QUANTITATIVE APPROXIMATIONS OF EVOLVING PROBABILITY MEASURES AND SEQUENTIAL MARKOV CHAIN MONTE CARLO METHODS

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Abstract. We study approximations of evolving probability measures by an interacting particle system. The particle system dynamics is a combination of independent Markov chain moves and importance sampling/resampling steps. Under global regularity conditions, we derive non-asymptotic error bounds for the particle system approximation. The main motivation are applications to sequential MCMC methods for Monte Carlo integral estimation.

1. Introduction

1.1. **Evolving probability measures.** Let $(\mu_t)_{t\geq 0}$ denote a family of mutually absolutely continuous probability measures on a set S. To keep the presentation as simple and non-technical as possible, we assume that S is finite. We will explain how to obtain Fokker-Planck type evolution equations on the space of probability measures on S that are satisfied by μ_t, and how to approximate these equations by interacting particle systems. The main purpose of this paper is to study the error of the particle system approximations in an L^p sense.

We assume that the measures are represented in the form

$$\mu_t(x) = \frac{1}{Z_t} \exp\left(-\mathcal{U}_t(x)\right) \mu_0(x), \qquad t \geq 0, \tag{1.1}$$

where Z_t is a normalization constant, and $(t,x) \mapsto \mathcal{U}_t(x)$ is a given function on $[0,\infty)\times S$ that is continuously differentiable in the first variable. If, for example, $\mathcal{U}_t(x) = t\,\mathcal{U}(x)$ for some function $\mathcal{U} : S \to \mathbb{R}$, then $(\mu_t)_{t\geq 0}$ is the exponential family corresponding to $\mathcal{U}$ and μ_0. Let

$$H_t(x) := -\frac{\partial}{\partial t}\log \mu_t(x) = -\frac{\partial}{\partial t}\log\frac{\mu_t(x)}{\mu_0(x)}$$

denote the negative logarithmic time derivative of the measures μ_t. Note that

$$\mu_t(x) = \exp\left(-\int_0^t H_s(x)\,ds\right)\,\mu_0(x)\,, \tag{1.2}$$

and

$$\langle H_t, \mu_t\rangle = -\frac{d}{dt}\mu_t(S) = 0 \qquad \text{for all } t \geq 0, \tag{1.3}$$

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where

$$\langle f,\nu\rangle := \int_S f\,d\nu \;= \sum_{x\in S} f(x)\,\nu(x)$$

denotes the integral of a function $f : S \to \mathbb{R}$ w.r.t. a measure ν on S. In particular,

$$H_t = \frac{\partial}{\partial t}\mathcal{U}_t - \langle \frac{\partial}{\partial t}\mathcal{U}_t, \mu_t\rangle.$$

In applications we have in mind, the functions $\mathcal{U}_t$ are given explicitly. Hence H_t is known explicitly up to an additive time-dependent constant. The evaluation of this constant, however, would require integration w.r.t. μ_t.

If all the functions H_t, $t \geq 0$, vanish then $\mu_t = \mu_0$ for all $t \geq 0$. In this case the measures are invariant for a Markov transition semigroup $(p_t)_{t\geq 0}$, i.e.,

$$\mu_s p_{t-s} = \mu_t \qquad \text{for all } t \geq s \geq 0,$$

provided the generator $\mathcal{L}$ of $(p_t)_{t\geq 0}$ satisfies $\mu_0\mathcal{L} = 0$, i.e.

$$\sum_{x\in S} \mu_0(x)\mathcal{L}(x,y) = 0 \qquad \text{for all } y \in S.$$

This fact is exploited in Markov Chain Monte Carlo (MCMC) methods for approximating expectation values w.r.t. the measure μ_0. The particle systems studied below can be applied for the same purpose when the measures μ_t are time-dependent.

1.2. **Fokker-Planck equation and particle system approximation.** To obtain approximations of the measures μ_t, we consider generators (Q-matrices) $\mathcal{L}_t$, $t \geq 0$, of a time-inhomogeneous Markov process on S satisfying the detailed balance conditions

$$\mu_t(x)\mathcal{L}_t(x,y) = \mu_t(y)\mathcal{L}_t(y,x) \quad \forall\, t \geq 0,\; x,y \in S. \tag{1.4}$$

For example, $\mathcal{L}_t$ could be the generator of a Metropolis dynamics w.r.t. μ_t, i.e.,

$$\mathcal{L}_t(x,y) \;=\; K_t(x,y)\cdot \min\left(\frac{\mu_t(y)}{\mu_t(x)}, 1\right) \text{ for } x \neq y,$$

$\mathcal{L}_t(x,x) = -\sum_{y\neq x}\mathcal{L}_t(x,y)$, where the proposal matrix K_t is a given symmetric transition matrix on S. In the sequel we will use the notation $\mathcal{L}_t^*\mu$ to denote the adjoint action of the generator on a probability measure μ, i.e.,

$$(\mathcal{L}_t^*\mu)(y) := (\mu\mathcal{L}_t)(y) = \sum_{x\in S}\mu(x)\mathcal{L}_t(x,y).$$

By (1.4), $\mathcal{L}_t^*\mu_t = 0$, i.e.,

$$\langle \mathcal{L}_t f, \mu_t\rangle = 0 \qquad \text{for all } f : S \to \mathbb{R} \text{ and } t \geq 0.$$

We fix non-negative constants λ_t, $t \geq 0$, such that $t \mapsto \lambda_t$ is continuous. Since the state space S is finite, the measures μ_t are the *unique* solution of the evolution equation for measures

$$\frac{\partial}{\partial t}\nu_t = \lambda_t\,\mathcal{L}_t^*\nu_t - H_t\nu_t \tag{1.5}$$

with initial condition $\nu_0 = \mu_0$. In general, solutions of (1.5) are not necessarily probability measures, even if ν_0 is a probability measure. Therefore, we consider the equation

$$\frac{\partial}{\partial t}\eta_t \;=\; \lambda_t\,\mathcal{L}_t^*\eta_t \;-\; H_t\eta_t \;+\; \langle H_t, \eta_t\rangle\,\eta_t \tag{1.6}$$

satisfied by the normalized measures $\eta_t = \frac{\nu_t}{\nu_t(S)}$. Note that, by (1.3), μ_t also solves (1.6). Moreover, if η_t is a solution of (1.6), then

$$\nu_t = \exp\left(-\int_0^t \langle H_s, \eta_s\rangle\right)\,\eta_t$$

is the unique solution of (1.5) with initial condition $\nu_0 = \eta_0$.

The Fokker-Planck equation (1.6) is an evolution equation for probability measures which, in contrast to the unnormalized equation, is not modified by adding constants to the functions H_t. We now introduce interacting particle systems that discretize the evolution equations (1.6) and (1.5). Consider right continuous time-inhomogeneous Markov processes $(X_t^N, \mathbb{P})$, $N \in \mathbb{N}$, with state space S^N and generators at time t given by

$$\begin{aligned} \mathcal{L}_t^N \varphi(x_1, \ldots, x_N) = \lambda_t \sum_{i=1}^N \mathcal{L}_t^{(i)} \varphi(x_1, \ldots, x_N) \\ + \frac{1}{N} \sum_{i,j=1}^N (H_t(x_i) - H_t(x_j))^+ (\varphi(x^{i\to j}) - \varphi(x)). \end{aligned} \tag{1.7}$$

Here $x = (x_1, \ldots, x_N) \in S^N$ and

$$(x^{i\to j})_k \;=\; \begin{cases} x_k & \text{if } k \neq i, \\ x_j & \text{if } k = i. \end{cases}$$

Moreover, $\mathcal{L}_t^{(i)}$ stands for the operator $\mathcal{L}_t$ applied to the i-th component of x. Thus the components $X_{t,i}^N$, $i = 1, \ldots, N$, of the process X_t^N move like independent Markov processes with generator $\lambda_t \mathcal{L}_t$ and are occasionally replaced by components with a lower value of H_t. Note that to compute the generator (and hence to simulate the Markov process) it is enough to know the functions H_t up to an additive constant.

One can show that if the initial distributions of the Markov processes are the N-fold products π^N of a probability measure π on S, then almost surely, the empirical distributions

$$\eta_t^N = \frac{1}{N} \sum_{i=1}^N \delta_{X_{t,i}^N} \tag{1.8}$$

and the reweighted empirical distributions

$$\nu_t^N = \exp\left(-\int_0^t \langle H_s, \eta_s^N\rangle\right)\,\eta_t^N \tag{1.9}$$

converge to the solutions of the equations (1.6) and (1.5) with initial conditions $\eta_0 = \nu_0 = \pi$ (see Corollary 2.7 below). As a consequence, simulating the Markov process X_t^N with initial distribution μ_0^N yields a Monte Carlo method for approximating sequentially the probability measures μ_t, $t \geq 0$. This Monte Carlo method can be viewed as a combination of Markov Chain Monte Carlo and Importance Sampling/Resampling. It is a continuous-time analogue of a particular type of Sequential Monte Carlo sampler. Sequential Monte Carlo samplers in discrete time have been introduced and systematically studied in [2]. They are closely related to particle filters (see e.g. [5]) and have been used in various applications to estimate expectation values w.r.t. multimodal distributions. The sequential Markov Chain Monte Carlo methods considered here are also related to several multi-level sampling methods including parallel tempering [9, 12, 16] and the equi-energy sampler [14].

1.3. **Quantitative convergence bounds.** Our main aim is to quantify the approximation properties of the particle systems when the initial distribution is μ_0^N. There is a substantial literature on asymptotic properties of corresponding particle system approximations, see e.g. [1, 4] and references therein. In particular, a law of large numbers type convergence theorem and a corresponding central limit theorem have been established in [3, 4] for a related particle system approximation, cf. also [18]. A crucial question for algorithmic applications, however, are quantitative bounds on the approximation error

$$\langle f, \eta_t^N \rangle - \langle f, \mu_t \rangle \tag{1.10}$$

for a given function $f : S \to \mathbb{R}$ and fixed N. The central limit theorem in [4] yields such bounds asymptotically as $N \to \infty$ (at least for a modified particle system). However, two important questions remain open:

- The expression for the asymptotic variance in the central limit theorem derived in [4] is not very explicit, as it involves L^2 norms of an associated Feynman-Kac semigroup. Methods that allow to bound this expression *efficiently* in a general setup and in concrete models have to be developed.
- For applications it is crucial to derive *non-asymptotic bounds* (i.e., bounds for fixed N), because the asymptotic estimates could be misleading when only a limited number of particles is available. The arguments in the proof of the CLT in [4] and the results in [18] in principle yield non-asymptotic bounds but the constants showing up are of order $\exp \int_0^t \mathrm{osc}(H_s)\, ds$, where $\mathrm{osc}(H_s) := \sup H_s - \inf H_s$ stands for the oscillation of H_s. Even in simple models with strong mixing properties, this quantity can be extremely large. Hence in spite of the LLN and CLT, even in "nice" cases it is not clear if the empirical distributions yield a reasonable approximation of μ_t for a realistic number N of particles/replicas (e.g. $N = 10,000$).

Dobrushin contraction coefficients do not seem to be an appropriate tool to answer these more delicate questions. In [8] (see also [6]) we propose an L^2 approach to quantify asymptotic stability properties of the Fokker-Planck equations for multimodal distributions where good global mixing properties fail. When studying the error of particle system approximations, we are forced to leave the L^2 framework and to work with various L^p norms. The purpose of the present article is hence to develop foundations of an L^p approach to non-asymptotic bounds for the particle system approximations. A key tool are L^p estimates for Feynman-Kac propagators that have been derived in [7].

1.4. **Outline.** The main results of our work are stated in Section 2. Here we also consider examples where the approximation errors can be quantified explicitly. In Section 3 we derive, by martingale arguments, an explicit formula for the variances of the estimators $\langle f, \nu_t^N \rangle$, see Proposition 2.1 below. In Section 4 we apply this formula to prove Theorem 2.4 below, which is a non-asymptotic bound for the variances. Finally, in Section 5 we combine this bound with the results from [7] to prove the bounds in Theorems 2.5 and 2.9 below.

2. Main results

To state our results in detail let us consider the Markov process $(X_t^N, \mathbb{P})$ with initial distribution μ_0^N. To derive error bounds for the particle system approximation it is convenient to consider at first the error for the Monte Carlo estimates based on the reweighted empirical distributions ν_t^N defined in (1.9). By a martingale argument it can be shown that $\langle f, \nu_t^N \rangle$ is an unbiased estimator of $\langle f, \mu_t \rangle$ for any function $f : S \to \mathbb{R}$ and $t \geq 0$, and an explicit formula for the variance can be given.

2.1. **An expression for the variance.** To state the formula for the variance, we introduce Feynman-Kac type transition operators $q_{s,t}$ related to the dynamics. For $0 \leq s \leq t < \infty$ and a function $f : S \to \mathbb{R}$, let $q_{s,t}f(x)$ denote the unique solution of the backward equation

$$-\frac{\partial}{\partial s} q_{s,t}f = \lambda_s \mathcal{L}_s q_{s,t} f - H_s q_{s,t} f, \qquad s \in [0,t], \tag{2.1}$$

with terminal condition $q_{t,t}f = f$. It can be shown that $q_{s,t}f$ is also the unique solution of the corresponding forward equation

$$\frac{\partial}{\partial t} q_{s,t} f = q_{s,t}(\lambda_t \mathcal{L}_t f - H_t f), \qquad t \in [s, \infty), \tag{2.2}$$

with initial condition $q_{s,s}f = f$. As a consequence, a probabilistic representation of $q_{s,t}$ is given by the Feynman-Kac formula

$$(q_{s,t}f)(x) = \mathbb{E}_{s,x}\left[e^{-\int_s^t H_r(X_r)\,dr} f(X_t)\right] \qquad \text{for all } x \in S, \tag{2.3}$$

where $(X_t)_{t \geq s}$ is a time-inhomogeneous Markov process w.r.t. $\mathbb{P}_{s,x}$ with generator $\mathcal{L}_t$ and initial condition $X_s = x$ $\mathbb{P}_{s,x}$-a.s., see e.g. [10], [11].

Proposition 2.1. *For all $f : S \to \mathbb{R}$,*

$$\begin{aligned} \mathbb{E}\left[\langle f, \nu_t^N \rangle\right] &= \langle f, \mu_t \rangle, \qquad \textit{and} \\ \mathbb{E}\left[\left|\langle f, \nu_t^N \rangle - \langle f, \mu_t \rangle\right|^2\right] &= \frac{1}{N}\operatorname{Var}_{\mu_t}(f) + \frac{1}{N}\int_0^t \mathbb{E}\left[V_{s,t}^N(f)\right] ds\,, \end{aligned}$$

where

$$\begin{aligned} V_{s,t}^N(f) = &- \langle H_s (q_{s,t}f)^2, \nu_s^N \rangle \langle 1, \nu_s^N \rangle - \langle H_s, \nu_s^N \rangle \langle q_{s,t} f^2 - (q_{s,t}f)^2, \nu_s^N \rangle \\ &+ \frac{1}{2} \iint |H_s(z) - H_s(y)| (q_{s,t}f(z) - q_{s,t}f(y))^2 \, \nu_s^N(dy)\, \nu_s^N(dz). \end{aligned} \tag{2.4}$$

Here and in the following $\operatorname{Var}_\mu(f) := \langle f^2, \mu \rangle - \langle f, \mu \rangle^2$ stands for the variance of f with respect to the measure μ. The proof of Proposition 2.1 relies on the identification of appropriate martingales, and is given in Section 3 below. A corresponding formula for the variance of a similar (but not identical) particle system has been derived in [4]. Elementary estimates now show that the approximation error (1.10) for estimates based on the empirical distributions η_t^N can be controlled by the variance of estimators based on ν_t^N:

Lemma 2.2. *For all functions $f : S \to \mathbb{R}$ and $t \geq 0$ we have*

$$\mathbb{E}\left[\left|\langle f, \eta_t^N \rangle - \langle f, \mu_t \rangle\right|^2\right] \leq 2 \operatorname{Var}\left(\langle f, \nu_t^N \rangle\right) + 2\|f - \langle f, \mu_t \rangle\|_{\sup}^2 \operatorname{Var}\left(\langle 1, \nu_t^N \rangle\right) \tag{2.5}$$

and

$$\begin{aligned} \mathbb{E}\left[\left|\langle f, \eta_t^N \rangle - \langle f, \mu_t \rangle\right|\right] \leq &\operatorname{Var}\left(\langle f, \nu_t^N \rangle\right)^{1/2} + \sqrt{2}\|f - \langle f, \mu_t \rangle\|_{\sup} \operatorname{Var}\left(\langle 1, \nu_t^N \rangle\right) \\ &+ \sqrt{2}\operatorname{Var}\left(\langle f, \nu_t^N \rangle\right)^{1/2} \operatorname{Var}\left(\langle 1, \nu_t^N \rangle\right)^{1/2}, \end{aligned} \tag{2.6}$$

where $\|g\|_{\sup} := \sup_{x \in S} |g(x)|$ for any $g : S \to \mathbb{R}$.

The proof is given in Section 5 below.

2.2. **A quantitative variance bound.** Let $p \in [2,\infty[$. Our goal is to prove quantitative bounds for the approximation errors that hold uniformly for all functions $f : S \to \mathbb{R}$ with L^p norm less than one. Because of Lemma 2.2, the errors can be quantified in terms of the variance bounds

$$\varepsilon_t^{N,p} := \sup\left\{ \mathbb{E}\left[\left|\langle f,\nu_s^N\rangle - \langle f,\mu_s\rangle\right|^2 \right] \,\middle|\, f : S \to \mathbb{R} \text{ s.t. } \|f\|_{L^p(\mu_s)} \le 1,\ s \in [0,t] \right\}, \quad (2.7)$$

with $p \in [2,\infty)$. To efficiently bound the quantities $\varepsilon_t^{N,p}$ we apply estimates of L^p-L^q operator norms for the operators $q_{s,t}$. Corresponding estimates are derived systematically in [7]. We first state a general result that bounds the error in terms of the expression (2.11) and appropriate operator norms, see Theorem 2.4 below.

For p, $q \in [2,\infty]$ with $p \le q$, let us consider the operator norms

$$\begin{aligned} C_{s,t}(p) &:= \sup_{f\neq 0} \frac{\|q_{s,t}f\|_{L^p(\mu_s)}}{\|f\|_{L^p(\mu_t)}}, \\ C_{s,t}(p,q) &:= \sup_{f\neq 0} \frac{\|q_{s,t}f\|_{L^{2r}(\mu_s)}}{\|f\|_{L^p(\mu_t)}} \vee \sup_{f\neq 0} \frac{\|q_{s,t}f\|_{L^p(\mu_s)}}{\|f\|_{L^{p/2}(\mu_t)}} \vee 1, \end{aligned}$$

where $r \in [p,\infty]$ is chosen such that $p^{-1} = q^{-1} + r^{-1}$. Moreover, for $\delta > 0$, we set

$$\bar{C}_t(p,q,\delta) := \sup_{\tau\in[0,t]} \int_0^{(\tau-\delta)^+} \|H_s\|_{L^q(\mu_s)} C_{s,\tau}(p,q)^2\, ds.$$

We fix a constant $t_0 > 0$, and set

$$\omega := \sup_{s\in[0,t_0]} \operatorname{osc}(H_s). \quad (2.8)$$

Since $H_s = -\frac{\partial}{\partial s}\log\mu_s$, the constant ω controls the logarithmic time change rate of the measures μ_t. Note that

$$\bar{C}_t(p,q,\delta) \le t\,\omega \sup\left\{ C_{s,\tau}(p,q)^2 \,\middle|\, s,\tau \in [0,t] \text{ s.t. } \tau \ge s+\delta \right\}.$$

Remark 2.3. Since we assume that the state space is finite, all the constants are finite, but their numerical values can be very large. It is a straightforward consequence of the forward equation (2.2) that

$$\mu_s q_{s,t} = \mu_t, \qquad 0 \le s \le t, \quad (2.9)$$

and hence $C_{s,t}(1) = 1$. On the other hand, in contrast to Markov transition operators which are contractions on L^∞, the constant $C_{s,t}(\infty)$ can be extremely large in typical applications. Therefore bounds on $C_{s,t}(p)$ are very sensitive to the choice of p, see [7] for details. The constants $C_{s,t}(p,q)$ and $\bar{C}_t(p,q,\delta)$ are related to hypercontractivity properties and can only be expected to be bounded in a feasible way if $t-s$ and δ, respectively, are not too small.

For a function $f : S \to \mathbb{R}$, set

$$V_{s,t}(f) := -\langle H_s(q_{s,t}f)^2,\mu_s\rangle + \iint |H_s(x)|(q_{s,t}f(y) - q_{s,t}f(x))^2\,\mu_s(dx)\,\mu_s(dy). \quad (2.10)$$

Our first main result shows that for $p > 4$ the asymptotic (as $N \to \infty$) variance of the estimator $\langle f,\nu_t^N\rangle$ is bounded from above by

$$N^{-1}\left(\operatorname{Var}_{\mu_t}(f) + \int_0^t V_{s,t}(f)\,ds + \|f\|^2_{L^p(\mu_t)} \right), \quad (2.11)$$

and, more importantly, it gives a non-asymptotic bound for the mean square error $\mathrm{Var}\left(\langle f, \nu_t^N\rangle\right)$ of the same order:

Theorem 2.4. *Fix $q \in]6,\infty]$ and $p \in]\frac{4q}{q-2}, q[$. Let $N \in \mathbb{N}$ be such that*

$$N \geq 25 \max\left(2, \bar{C}_{t_0}(p,q,\delta), \bar{C}_{t_0}(\tilde{p},q,\delta)\right),$$

where $\tilde{p}$ is defined by $\tilde{p}^{-1} = q^{-1} + (p/2)^{-1}$ and $\delta := (17\omega)^{-1}$. Then, for $t \in [0,t_0]$, we have

$$\begin{aligned} N\,\mathbb{E}\left[|\langle f,\nu_t^N\rangle - \langle f,\mu_t\rangle|^2\right] \;\leq\; & \mathrm{Var}_{\mu_t}(f) + \int_0^t V_{s,t}(f)\,ds \\ & + \left[1 + 7\bar{C}_t(p,q,\delta)\varepsilon_t^{N,p}\right] \|f\|^2_{L^p(\mu_t)}. \end{aligned} \tag{2.12}$$

In particular,

$$\varepsilon_t^{N,p} \leq (2 + v_t(p))N^{-1}\big(1 + 10\bar{C}_t(p,q,\delta)N^{-1}\big) \tag{2.13}$$

where

$$v_t(p) := \sup_{\tau\in[0,t]} \sup_{f\neq 0} \frac{\int_0^\tau V_{s,\tau}(f)\,ds}{\|f\|^2_{L^p(\mu_\tau)}}.$$

The proof is given in Section 4 below. To apply Theorem 2.4 we need bounds for the constants $v_t(p)$ and $\bar{C}_t(p,q,\delta)$. We will now discuss how to derive such bounds from Poincaré and logarithmic Sobolev inequalities in the following particular cases:

a) The Markov processes with generators $\mathcal{L}_t$, $t \geq 0$, have "good" global mixing properties.
b) The state space S can be decomposed into disjoint subsets S_i, $i \in I$, such that $\mathcal{L}_t(x,y) = 0$ for all $t \geq 0$, $x \in S_i$ and $y \in S_j$ with $i \neq j$, and "good" mixing properties hold on each of the subsets S_i.

2.3. **Non-asymptotic bounds from global Poincaré and log Sobolev inequalities.** For $t \geq 0$ and $q \in [1,\infty]$ let us define

$$K_t(q) = \int_0^t \|H_s\|_{L^q(\mu_s)}\,ds.$$

The quantities $K_t(q)$ are a way to control how much the measures μ_s change for $s \in [0,t]$. A rough estimate yields

$$v_t(p) \leq 5K_t(2)\sup\left\{C_{s,\tau}(4)^2 \,\middle|\, 0 \leq s \leq \tau \leq t\right\} \quad \text{for any } p \geq 4, \tag{2.14}$$

$$\bar{C}_t(p,q,\delta) \leq K_t(q)\sup\left\{C_{s,\tau}(p,q)^2 \,\middle|\, 0 \leq s \leq s+\delta \leq \tau \leq t\right\} \quad \text{for any } q \geq p \geq 1. \tag{2.15}$$

Hence estimates for $v_t(p)$ and $\bar{C}_t(p,q,\delta)$ follow from appropriate L^p-L^q bounds for the Feynman-Kac propagators $q_{s,t}$. In [7], we derive such bounds systematically from Poincaré and logarithmic Sobolev inequalities. To apply these results let us define the weighted Poincaré and log Sobolev constants

$$A_t := \sup_{f\in\mathcal{S}_0} \frac{-\int H_t f^2\,d\mu_t}{\mathcal{E}_t(f)},$$

$$B_t := \sup_{f\in\mathcal{S}_0} \frac{\left|\int H_t f\,d\mu_t\right|^2}{\mathcal{E}_t(f)},$$

$$\gamma_t := \sup_{f\in\mathcal{S}_1} \frac{\int f^2 \log|f|\,d\mu_t}{\mathcal{E}_t(f)},$$

where $\mathcal{S}_0 = \big\{f : S \to \mathbb{R} | \ \langle f, \mu_t\rangle = 0,\ f \not\equiv 0\big\}$, $\mathcal{S}_1 = \big\{f : S \to \mathbb{R} | \ \langle f^2, \mu_t\rangle = 1,\ f \not\equiv 1\big\}$, and

$$\mathcal{E}_t(f) \ = \ -\int f\mathcal{L}_t f \, d\mu_t \ = \ \frac{1}{2}\sum_{x,y\in S}(f(y)-f(x))^2\mathcal{L}_t(x,y)\mu_t(x)$$

denotes the Dirichlet form of the self-adjoint operator $\mathcal{L}_t$ on $L^2(S,\mu_t)$. We refer to [19] for background on Poincaré and logarithmic Sobolev inequalities and their applications to estimate L^p contractivity properties of transition semigroups and mixing times of reversible time-homogeneous Markov chains. In [7] we apply similar techniques to derive L^p-L^q bounds for Feynman-Kac propagators. We show that $C_{s,t}(p)$ and $C_{s,t}(p,q)$ are small (in particular less than 2) if the intensities λ_s, $0 \le s \le t$, of MCMC moves are sufficiently large in terms of the constants A_s, B_s and γ_s, respectively. By combining these results with Theorem 2.4 we obtain:

Theorem 2.5. *Fix $t_0 \ge 0$, $q \in]6,\infty[$ and $p \in]\frac{4q}{q-2}, q[$. Suppose that*

$$N \ge 40\ \max(K_{t_0}(q), 1), \qquad \textit{and} \tag{2.16}$$

$$\lambda_s \ge \max\left(\frac{pA_s}{4} + \frac{p(p+3)}{4}t_0 B_s\ ,\ \frac{17}{4}a(p,q)\,\omega\gamma_s\right) \qquad \textit{for all } s\in[0,t_0], \tag{2.17}$$

where ω is defined by (2.8) and

$$a(p,q) := \log\max\left(\frac{2r-1}{p-1}, \frac{2p-2}{p-2}, \frac{p-1}{\tilde p -1}, \frac{2\tilde p-2}{\tilde p-2}\right),$$

with $\tilde p$ and r determined by $\tilde p^{-1} = q^{-1} + 2p^{-1}$ and $p^{-1} = q^{-1} + r^{-1}$. Then, for $t \in [0,t_0]$,

$$\varepsilon_t^{N,p} \ \le \ (2 + 8\,K_t(2))\,N^{-1}\big(1 + 16K_t(q)N^{-1}\big). \tag{2.18}$$

The proof is given in Section 5 below.

Remark 2.6. (i) The assumptions on p and q guarantee that $\tilde p > 2$, so that $a(p,q)$ is finite.

(ii) If (2.17) holds, then, by (2.18), a number

$$N \ge \frac{3 + 10K_t(q)}{\alpha}$$

of particles/replicas guarantees $\varepsilon_t^{N,p} \le \alpha$ for a given $\alpha \in]0,1/8[$. In particular, as $\alpha \to 0$, a number of particles/replicas of order $O(K_t(q)/\alpha)$ is sufficient to bound the error by α.

(iii) Rough bounds for the constants $K_t(q)$, A_t and B_t for $t \in [0,t_0]$ are given by

$$K_t(q) \le \omega\, t, \qquad A_t \le C_t^{\mathrm{Poi}}, \qquad B_t \le \omega\, C_t^{\mathrm{Poi}},$$

where ω is defined by (2.8) and

$$C_t^{\mathrm{Poi}} := \sup_{f\in\mathcal{S}_0}\frac{\int f^2\,d\mu_t}{\mathcal{E}_t(f)}$$

denotes the Poincaré constant, i.e., the inverse spectral gap of the generator $\mathcal{L}_t$. Therefore, assumptions (2.16) and (2.17) in Theorem 2.5 are satisfied if

$$N \ge 40\max(\omega\, t_0, 1) \tag{2.19}$$

and

$$\lambda_s \ge \omega\max\Big(\frac{p}{4}\big(1 + t_0(p+3)/4\big)C_s^{\mathrm{Poi}}, \frac{17}{4}\gamma_s\log a(p,q)\Big). \tag{2.20}$$

Theorems 2.4 and 2.5 provide non-asymptotic bounds on the variances of the Monte Carlo estimators $\langle f, \nu_t^N \rangle$ that hold uniformly over all functions $f \in L^p(\mu_t)$. One can combine these bounds with (2.12) and (2.6) to obtain more precise non-asymptotic error bounds for the Monte Carlo estimators $\langle f, \nu_t^N \rangle$ and $\langle f, \eta_t^N \rangle$ for a fixed function f:

Corollary 2.7. *Suppose that the assumptions of Theorem 2.5 hold, and let $f \in L^p(\mu_t)$. Then*

$$N\,\mathbb{E}\left[\left|\langle f, \nu_t^N\rangle - \langle f, \mu_t\rangle\right|^2\right] \;\leq\; \mathrm{Var}_{\mu_t}(f) + \int_0^t V_{s,t}(f)\,ds + \|f\|^2_{L^p(\mu_t)} + R(t,N)\,\|f\|^2_{L^p(\mu_t)},$$

$$N^{1/2}\,\mathbb{E}\left[\left|\langle f, \eta_t^N\rangle - \langle f, \mu_t\rangle\right|\right] \;\leq\; \left(\mathrm{Var}_{\mu_t}(f) + \int_0^t V_{s,t}(f)\,ds + \|f - \langle f, \mu_t\rangle\|^2_{L^p(\mu_t)}\right)^{1/2} + \tilde{R}(t,N)\,\|f - \langle f, \mu_t\rangle\|_{\sup}$$

with explicit constants $R(t,N)$ of order $O(N^{-1})$ and $\tilde{R}(t,N)$ of order $O(N^{-1/2})$.

The proof is given in Section 5 below.

2.4. **Scope and Examples.** Summarizing our results, we make the following observations: the derived error bounds of a given size for the particle system approximation rely on the following quantities:

(i) A uniform upper bound on the oscillations of the logarithmic time derivatives $H_t = -\frac{\partial}{\partial t} \log \mu_t$.

(ii) A minimal intensity λ_t of MCMC moves. A lower bound for the required intensity can be given in terms of the constants A_t, B_t and γ_t, or alternatively in terms of ω, C_t^{Poi} and γ_t.

(iii) A minimal number N of particles. On a time interval of length t_0, a number of particles of order $O(\omega t_0 \alpha^{-1})$ is sufficient to bound the error $\varepsilon_{t_0}^{N,p}$ by α (provided λ_t is large enough).

We now illustrate range and limits of applicability of the results in two examples. The first is a simple one-dimensional example, while the second discusses the dimensional dependence of the estimates in the case of product measures.

Example 1. Moving Gaussians – one dimensional case. Suppose that $S = \{a, a+1, \ldots, a+\Delta-1\}$ for some $a \in \mathbb{Z}$ and $\Delta \in \mathbb{N}$, and $(\mu_t)_{t\geq 0}$ are probability measures on S such that

$$\mu_t(x) \propto \exp\Big(-\frac{(x-m_t)^2}{2\sigma_t^2}\Big), \qquad x \in S.$$

We assume that $t \mapsto m_t$ and $t \mapsto \sigma_t$ are continuously differentiable functions such that $\sigma_t \in]0,\infty[$ and $m_t \in [a, a+\Delta-1]$ for all $t \geq 0$. Moreover, we assume that the Markov chain moves are given by a Random Walk Metropolis dynamics (in continuous time), that is,

$$\mathcal{L}_t(x,y) = \begin{cases} \frac{1}{2}\min\big(\frac{\mu_t(y)}{\mu_t(x)}, 1\big), & \text{if } |y-x| = 1, \\ 0, & \text{if } |y-x| \geq 1. \end{cases}$$

In this case, the following upper bounds for C_t^{Poi} and γ_t hold (see the Appendix):

$$C_t^{\mathrm{Poi}} \leq 30\big((\sigma_t \wedge \Delta) \vee 2\big)^2 \tag{2.21}$$

$$\gamma_t \leq 300\frac{\Delta^2}{(\sigma_t \wedge 1)^2} + 300\big((\sigma_t \wedge \Delta) \vee 2\big)^2 \log \Delta \tag{2.22}$$

It can be shown that the upper bound for C_t^{Poi} is of the correct order in σ_t and Δ. The upper bound for γ_t could be improved, but γ_t is always bounded from below by a positive multiple of $(\Delta/\sigma_t)^2$. Our results can be applied in the following way. For $t \geq 0$ and $x, y \in S$ we have

$$\begin{aligned} H_t(x) - H_t(y) &= \frac{\partial}{\partial t}\Big(\frac{(x-m_t)^2}{\sigma_t^2} - \frac{(y-m_t)^2}{\sigma_t^2}\Big) \\ &= -\frac{\sigma_t'}{\sigma_t}\frac{(x-y)(x+y-2m_t)}{\sigma_t^2} - m_t'\frac{x-y}{\sigma_t^2} \\ &\leq \Big(2\frac{|\sigma_t'|}{\sigma_t} + \frac{|m_t'|}{\Delta}\Big)\frac{\Delta^2}{\sigma_t^2}. \end{aligned} \tag{2.23}$$

Therefore, if we choose the time scale in such a way that the condition

$$2\frac{|\sigma_t'|}{\sigma_t} + \frac{|m_t'|}{\Delta} \leq \frac{\sigma_t^2}{\Delta^2} \qquad \forall t \in [0, t_0] \tag{2.24}$$

is satisfied, then

$$\omega = \sup_{t\in[0,t_0]} \operatorname{osc}(H_t) \leq 1.$$

Condition (2.24) is an upper bound on the relative change rates of the parameters σ_t and m_t. Note that if Δ is large compared to σ_t, then only small change rates are possible. The reason is that in this case the Gaussian measure μ_t changes too rapidly in the tails, so that our arguments break down.

Assuming (2.24), Theorem 2.5 and Remark 2.6(iii) imply that

$$\varepsilon_t^{N,p} \leq (2+8t)N^{-1}(1+16N^{-1}),$$

provided $N \geq 40(t_0 \vee 1)$, and (2.20) holds with $\omega = 1$, and C_s^{Poi}, γ_s replaced by the upper bounds in (2.21), (2.22). If $(\sigma_t \wedge 1)/\Delta$ is not too small, this yields reasonably sized (although far from optimal) lower bounds on λ_t and N. On the other hand, if $\sigma_t/\Delta \to 0$, then the upper bounds in both (2.23) and (2.22) degenerate drastically.

Example 2. Product measures – dependence on the dimension. In our second example we study the dependence of (2.19), (2.20) and (2.18) on the dimension in the case when the evolving measures are all product measures. Suppose that

$$S = \prod_{i=1}^d S_i, \qquad \mu_t = \bigotimes_{i=1}^d \mu_t^{(i)},$$

with probability measures $\mu_t^{(i)}$, $t \geq 0$, $i = 1, \ldots, d$, on finite sets S_i such that $t \mapsto \mu_t^{(i)}(x)$ is continuously differentiable and strictly positive for all $1 \leq i \leq d$ and $x \in S_i$. In this case one has

$$H_t(x) = \sum_{i=1}^d H_t^{(i)}(x),$$

where H_t and $H_t^{(i)}$ denote the negative logarithmic time derivatives of the measures μ_t and $\mu_t^{(i)}$, respectively. If we assume

$$\operatorname{osc}(H_t^{(i)}) \leq 1 \qquad \forall t \in [0, t_0],\ i = 1, \ldots, d,$$

then

$$\omega = \sup_{t\in[0,t_0]} \operatorname{osc}(H_t) \leq d. \tag{2.25}$$

Moreover, suppose that

$$\mathcal{L}_t(x,y) = \sum_{i=1}^{d} \mathcal{L}_t^{(i)}(x_i,y_i)$$

for generators $\mathcal{L}_t^{(i)}$, $t \geq 0$, $i = 1,\dots,d$, of time-inhomogeneous Markov processes on S_i, i.e. $\mathcal{L}_t$ is the generator of the product dynamics on S with component generators $\mathcal{L}_t^{(i)}$. It is well known that $\mathcal{L}_t$ satisfies Poincaré and logarithmic Sobolev inequalities with constants

$$C_t^{\mathrm{Poi}} = \max_{i=1,\dots,d} C_t^{\mathrm{Poi},(i)}, \qquad \gamma_t = \max_{i=1,\dots,d} \gamma_t^{(i)},$$

respectively, where $C_t^{\mathrm{Poi},(i)}$ and $\gamma_t^{(i)}$ are the Poincaré and logarithmic Sobolev constants for the generators $\mathcal{L}_t^{(i)}$. In particular, if the component generators $\mathcal{L}_t^{(i)}$ satisfy Poincaré and logarithmic Sobolev inequalities with constants independent of i, then $\mathcal{L}_t$ satisfies the corresponding inequalities with the same constants – independently of the dimension d. Therefore, in this case, the values of N and λ_s required to satisfy conditions (2.19), (2.18) and (2.20) are of order $O(d)$. Hence both the number of particles/replicas and the intensity of MCMC moves required are of order $O(d)$. Since simulating from the product dynamics also requires $O(d)$ steps, the total effort to keep track of the evolving product measures up to a given precision is of order $O(d^3)$.

Remark 2.8 (Independent particles)**.** We compare briefly with the particle dynamics without importance sampling/resampling, i.e., when the second summand is omitted in the definition (1.7) of the generator $\mathcal{L}_t^N$. In this case, the particles/replicas move independently according to the time-inhomogeneous Markovian dynamics with generators $\mathcal{L}_t$, $t \geq 0$. Hence the positions of the particles at time t are independent random variables with distribution $\tilde{\mu}_t = \mu_0 p_{0,t}$, where $p_{s,t}$, $0 \leq s \leq t$, is the time-inhomogeneous transition function. A corresponding dynamics is used for example in the classical simulated annealing algorithm (see e.g. [15]). Since in general $\tilde{\mu}_t \neq \mu_t$, the empirical distribution of the independent particle system is an asymptotically biased estimator for μ_t. However, under strong mixing conditions as imposed above, the difference between $\tilde{\mu}_t$ and μ_t, and hence the asymptotic bias, will be small. Therefore it is possible that, for fixed N, the empirical distribution of the independent particles process is a better estimate for μ_t than η_t^N. On the other hand, if the mixing properties break down, the bias of the independent particles estimator will not be small, whereas the empirical measures ν_t^N and η_t^N may still be suitable estimators. This will be demonstrated now in a particular case.

2.5. **Non-asymptotic bounds from local estimates.** With suitable modifications the above analysis can also be applied to derive bounds when good mixing properties hold only locally. As an illustration, we consider another extreme case in which the state space is decomposed into several components that are not connected by the underlying Markovian dynamics. Suppose that

$$S = \bigcup_{i \in I} S_i,$$

is a decomposition of S into disjoint non-empty subsets S_i, $i \in I$, such that

$$\mathcal{L}_t(x,y) \;=\; 0 \qquad \text{for any } t \geq 0,\ x \in S_i \text{ and } y \in S_j \text{ with } i \neq j.$$

Let $\mu_t^i := \mu_t(\cdot|S_i)$ denote the measure μ_t conditioned by S_i. Then we can apply the arguments above with the L^p norm replaced by the stronger norm

$$\|f\|_{\widetilde{L^p(\mu_t)}} \;:=\; \max_{i\in I} \|f\|_{L^p(S_i,\mu_t^i)}.$$

Since Hölder's inequality and related estimates hold for these modified L^p norms as well, the assertion of Theorem 2.4 still remains true if $\varepsilon_t^{N,p}$ is replaced by

$$\tilde{\varepsilon}_t^{N,p} := \sup\left\{\mathbb{E}\left[\left|\langle f,\nu_s^N\rangle - \langle f,\mu_s\rangle\right|^2\right] \;\middle|\; f:S\to\mathbb{R} \text{ s.t. } \|f\|_{\widetilde{L^p(\mu_s)}}\le 1,\ s\in[0,t]\right\},$$

and the constants $C_{s,t}(p,q)$ and $\bar{C}_t(p,q,\delta)$ are defined w.r.t. the modified L^p and L^q norms as well. Moreover, the representations (1.2) and (1.3) hold for μ_t^i in place of μ_t if H_t is replaced by

$$H_t^i \;:=\; H_t - \langle H_t,\mu_t^i\rangle\,.$$

Let A_t^i, B_t^i and γ_t^i denote the Poincaré and logarithmic Sobolev constants defined as above but with S, μ_t and H_t replaced by S_i, μ_t^i and H_t^i, respectively. Let us also set

$$\tilde{A}_t := \max_{i\in I} A_t^i,\qquad \tilde{B}_t := \max_{i\in I} B_t^i,\qquad \tilde{\gamma}_t := \max_{i\in I}\gamma_t^i,$$

$$\tilde{K}_t(q) \;:=\; \int_0^t \|H_s\|_{\widetilde{L^q(\mu_s)}}\,ds,\qquad\text{and}$$

$$\tilde{M}_t \;:=\; \max_{i\in I}\sup_{0\le r\le s\le t}\frac{\mu_s(S_i)}{\mu_r(S_i)}\,.$$

Then, by estimating L^p norms separately on each component, we can prove the following extension of Theorem 2.5:

Theorem 2.9. *Fix $t_0\ge 0$, $q\in]6,\infty[$ and $p\in]\frac{4q}{q-2},q[$. Suppose that*

$$N\ge 40\max(\tilde{K}_{t_0}(q),1),\qquad \textit{and}$$

$$\lambda_s \ge \max\left(\frac{p\tilde{A}_s}{4}+\frac{p(p+3)}{4}t_0\tilde{B}_s,\ \frac{17}{4}a(p,q)\omega\tilde{\gamma}_s\right)\qquad \textit{for all } s\in[0,t_0]. \tag{2.26}$$

Then, for $t\in[0,t_0]$, one has

$$\tilde{\varepsilon}_t^{N,p} \;\le\; \left(2+8K_t(2)\tilde{M}_t^2\right)N^{-1}\left(1+16\tilde{K}_t(q)\tilde{M}_t^2\,N^{-1}\right).$$

Remark 2.10. (i) If there is only one component, the assertion of Theorem 2.9 reduces to that of Theorem 2.5.
(ii) Error bounds for the estimators $\langle f,\nu_t^N\rangle$ and $\langle f,\eta_t^N\rangle$ for a fixed function f hold analogously to Corollary 2.7.

2.6. **Open problems.** 1) The cases discussed in Sections 2.3 and 2.5 are extreme cases. In many typical applications, one would expect the state space to split up as time evolves into more and more components that get almost disconnected by the dynamics (local modes, metastable states). The study of such more complicated situations is an important topic for future research.

2) We have discussed here a setup with discrete state space and continuous time. Continuous state spaces can in principle be treated by similar techniques, although of course additional technical considerations are required. For algorithmic applications, the case of discrete time and a continuous state space is probably the most interesting one. This case will be studied in detail in the PhD thesis of N. Schweizer [20].

3. Variances of weighted empirical averages

In this section we will prove Proposition 2.1, which shows that $\langle f, \nu_t^N \rangle$ is an unbiased estimator for $\langle f, \mu_t \rangle$ and gives an explicit formula for the variance. The proof relies on the identification of appropriate martingales.

Recall that the carré du champ (square field) operator Γ_t^N associated to $\mathcal{L}_t^N$ is defined for functions $\varphi : S^N \to \mathbb{R}$ by

$$\Gamma_t^N(\varphi) \;=\; \mathcal{L}_t^N \varphi^2 - 2\varphi \mathcal{L}_t^N \varphi,$$

i.e.,

$$\Gamma_t^N(\varphi)(x) \;=\; \sum_{y \in S} \mathcal{L}_t^N(x,y)\,(\varphi(y) - \varphi(x))^2 \qquad \forall x \in S^N. \tag{3.1}$$

It is well-known that the processes

$$M_t^\varphi \;=\; \varphi(t, X_t^N) - \varphi(0, X_0^N) - \int_0^t \big(\frac{\partial}{\partial s} + \mathcal{L}_s^N\big)\varphi(s, X_s^N)\, ds, \qquad \text{and} \tag{3.2}$$

$$N_t^\varphi \;=\; (M_t^\varphi)^2 - \int_0^t \Gamma_s^N(\varphi(s,\,\cdot\,))(X_s^N)\, ds \tag{3.3}$$

are martingales w.r.t. the filtration induced by the process X_t^N for any function $\varphi : \mathbb{R}^+ \times S^N \to \mathbb{R}$ that is twice continuously differentiable in the first variable, cf. e.g. [13, Appendix 1, Lemma 5.1]. For $x \in S^N$ let

$$\eta(x) = \frac{1}{N} \sum_{i=1}^N \delta_{X_i}$$

denote the corresponding empirical average. In the next lemma we derive expressions for $\mathcal{L}_t^N$ and Γ_t^N acting on linear functions on S^N of the form

$$\varphi_f(x) \;=\; \langle f, \eta(x) \rangle \;=\; N^{-1} \sum_{i=1}^N f(x_i).$$

Lemma 3.1. *For any function $f : S \to \mathbb{R}$ and $t \geq 0$, one has*

$$\mathcal{L}_t^N \langle f, \eta \rangle \;=\; \lambda_t \langle \mathcal{L}_t f, \eta \rangle + \langle H_t, \eta \rangle \langle f, \eta \rangle - \langle H_t f, \eta \rangle$$

and

$$\Gamma_t^N(\langle f, \eta \rangle) \;=\; \frac{\lambda_t}{N} \langle \Gamma_t(f), \eta \rangle + \frac{1}{N} \iint \big(H_t(y) - H_t(z)\big)^+ \big(f(z) - f(y)\big)^2\, \eta(dy)\, \eta(dz),$$

where Γ_t denotes the carré du champ operator w.r.t. $\mathcal{L}_t$.

Proof. The definition of $\mathcal{L}_t^N$ immediately yields

$$\mathcal{L}_t^N \langle f, \eta \rangle(x) \;=\; \frac{\lambda_t}{N} \sum_{i=1}^N \mathcal{L}_t f(x_i) + \frac{1}{N^2} \sum_{i,j=1}^N (H_t(x_i) - H_t(x_j))^+ (f(x_j) - f(x_i)). \tag{3.4}$$

Moreover,

$$\begin{aligned}\sum_{i,j=1}^{N}&(H_t(x_i)-H_t(x_j))^+(f(x_j)-f(x_i))\\ &=\sum_{i,j:H_t(x_i)>H_t(x_j)}(H_t(x_i)-H_t(x_j))(f(x_j)-f(x_i))\\ &=\sum_{i,j:H_t(x_j)>H_t(x_i)}(H_t(x_j)-H_t(x_i))(f(x_i)-f(x_j))\\ &=\sum_{i,j:H_t(x_j)>H_t(x_i)}(H_t(x_i)-H_t(x_j))(f(x_j)-f(x_i))\\ &=-\sum_{i,j=1}^{N}(H_t(x_i)-H_t(x_j))^-(f(x_j)-f(x_i)),\end{aligned}$$

and hence

$$\sum_{i,j=1}^{N}(H_t(x_i)-H_t(x_j))(f(x_j)-f(x_i))=2\sum_{i,j=1}^{N}(H_t(x_i)-H_t(x_j))^+(f(x_j)-f(x_i)).$$

Therefore the second term on the right hand side of (3.4) is equal to

$$\begin{aligned}\frac{1}{2N^2}&\sum_{i,j=1}^{N}(H_t(x_i)-H_t(x_j))(f(x_j)-f(x_i))\\ &=\Big(\frac{1}{N}\sum_{i=1}^{N}H_t(x_i)\Big)\Big(\frac{1}{N}\sum_{j=1}^{N}f(x_j)\Big)-\frac{1}{N}\sum_{i=1}^{N}H_t(x_i)f(x_i)\\ &=\langle H_t,\eta(x)\rangle\langle f,\eta(x)\rangle-\langle H_tf,\eta(x)\rangle,\end{aligned}$$

from which the first claim follows.

Furthermore, since

$$\langle f,\eta(x^{i\to j})\rangle-\langle f,\eta(x)\rangle \;=\; N^{-1}\,(f(x_j)-f(x_i))\,,$$

(3.1) and (1.7) imply

$$\begin{aligned}\Gamma_t^N\langle f,\eta\rangle(x)\;&=\frac{\lambda_t}{N^2}\sum_{i=1}^{N}\sum_{y\in S}\mathcal{L}_t(x_i,y)(f(y)-f(x_i))^2\\ &+\frac{1}{N^3}\sum_{i,j=1}^{N}\big(H_t(x_i)-H_t(x_j)\big)^+\big(f(x_j)-f(x_i)\big)^2,\end{aligned}$$

from which the second claim follows noting that the first term on the right hand side of the previous expression is equal to

$$\frac{\lambda_t}{N^2}\sum_{i=1}^{N}\Gamma_t(f)(x_i)\;=\;\frac{\lambda_t}{N}\langle\Gamma_t(f),\eta(x)\rangle. \qquad\square$$

Now let us define

$$\bar{A}^f_{s,t}\;=\;\langle q_{s,t}f,\eta^N_s\rangle\;=\;\frac{1}{N}\sum_{i=1}^{N}(q_{st}f)(X^N_{s,i})\,.$$

As a consequence of Lemma 3.1 we obtain:

Proposition 3.2. *The processes $\bar{M}_u^f$ and $\bar{N}_u^f$, $u \in [0,t]$, defined by*

$$\begin{aligned}
\bar{M}_u^f &= \bar{A}_{u,t}^f - \bar{A}_{0,t}^f - \int_0^u \langle H_s, \eta_s^N \rangle \langle q_{s,t} f, \eta_s^N \rangle \, ds, \\
\bar{N}_u^f &= (\bar{M}_u^f)^2 - \frac{1}{N} \int_0^u \lambda_s \, \langle \Gamma_s(q_{s,t} f), \eta_s^N \rangle \, ds \\
& \quad - \frac{1}{N} \int_0^u \iint \big(H_s(y) - H_s(z) \big)^+ \big(q_{s,t} f(z) - q_{s,t} f(y) \big)^2 \, \eta_s^N(dy) \, \eta_s^N(dz) \, ds
\end{aligned}$$

are martingales w.r.t. the filtration $\mathcal{F}_t = \sigma(X_s^N \mid s \in [0,t])$.

Proof. Note that $\bar{A}_s^f = \varphi(s, X_s^N)$, where

$$\varphi(s,x) = N^{-1} \sum_{i=1}^N q_{st} f(x_i).$$

By the backward equation (2.1),

$$\begin{aligned}
\frac{\partial}{\partial s} \varphi(s,x) &= -\frac{\lambda_s}{N} \sum_{i=1}^N \mathcal{L}_s q_{st} f(x_i) + \frac{1}{N} \sum_{i=1}^N H_s q_{st} f(x_i) \\
&= -\lambda_s \langle \mathcal{L}_s q_{st} f, \eta(x) \rangle + \langle H_s q_{st} f, \eta(x) \rangle,
\end{aligned}$$

and by lemma 3.1,

$$\left(\mathcal{L}_s^N \varphi \right)(s,x) = \lambda_s \langle \mathcal{L}_s q_{s,t} f, \eta(x) \rangle + \langle H_s, \eta(x) \rangle \langle q_{s,t} f, \eta(x) \rangle - \langle H_s q_{s,t} f, \eta(x) \rangle$$

Hence

$$\left(\frac{\partial}{\partial s} + \mathcal{L}_s^N \right) \varphi(s,x) = \langle H_s, \eta(x) \rangle \langle q_{s,t} f, \eta(x) \rangle,$$

which proves that $\bar{M}^f = M^\varphi$ is a martingale, cf. (3.2). Similarly, by Lemma 3.1,

$$\begin{aligned}
\Gamma_s^N(\varphi)(s,x) &= \frac{\lambda_s}{N} \langle \Gamma_s(q_{s,t} f), \eta(x) \rangle \\
& \quad + \frac{1}{N} \iint \big(H_s(y) - H_s(z) \big)^+ \big(q_{s,t} f(z) - q_{s,t} f(y) \big)^2 \, \eta_s^N(dy) \, \eta_s^N(dz),
\end{aligned}$$

which proves that $\bar{N}^f = N^\varphi$ is a martingale, cf. (3.3). □

Since in general, $\bar{A}_{s,t}^f$ is not a martingale, $\langle f, \eta_t^N \rangle$ is not an unbiased estimator for $\langle f, \mu_t \rangle$. This motivates considering $\langle f, \nu_t^N \rangle$ instead. Let

$$A_{s,t}^f = \langle q_{s,t} f, \nu_s^N \rangle = e^{-\int_0^s \langle H_r, \eta_r^N \rangle \, dr} \bar{A}_{s,t}^f. \tag{3.5}$$

Proposition 3.3. *The process $A_{u,t}^f$, $u \in [0,t]$, is a martingale with increasing process given by*

$$\begin{aligned}
\langle A_{\bullet,t}^f \rangle_u &= \frac{1}{N} \int_0^u \lambda_s \, \langle 1, \nu_s^N \rangle \langle \Gamma_s(q_{s,t} f), \nu_s^N \rangle \, ds \\
& \quad + \frac{1}{N} \int_0^u \iint \big(H_s(x) - H_s(y) \big)^+ \big(q_{s,t} f(y) - q_{s,t} f(x) \big)^2 \, \nu_s^N(dx) \, \nu_s^N(dy) \, ds.
\end{aligned}$$

Proof. By the integration by parts formula for Stieltjes integrals and Proposition 3.2, we get

$$\begin{aligned} A^f_{u,t} - A^f_{0,t} &= \int_0^u e^{-\int_0^s \langle H_r,\eta^N_r\rangle\,dr} d\bar{A}^f_{s,t} - \int_0^u \langle H_s,\eta^N_s\rangle e^{-\int_0^s \langle H_r,\eta^N_r\rangle\,dr} \bar{A}^f_{s,t}\,ds \\ &= \int_0^u e^{-\int_0^s \langle H_r,\eta^N_r\rangle\,dr} d\bar{M}^f_s + \langle H_s,\eta^N_s\rangle A^f_s\,ds - \langle H_s,\eta^N_s\rangle A^f_s\,ds. \end{aligned}$$

Hence $[0,t] \ni s \mapsto A^f_{s,t}$ is a martingale whose increasing process can be written as

$$\langle A^f_{\bullet,t}\rangle_u = \int_0^u e^{-2\int_0^s \langle H_r,\eta^N_r\rangle\,dr}\, d\langle \bar{M}^f\rangle_s.$$

The result now follows by Proposition 3.2 and Equation (1.9). □

The purpose of the next lemma is to obtain an alternative representation (modulo martingale terms) of the term involving the carré du champ operator in the expression for $\langle A^f_{\bullet,t}\rangle$.

Lemma 3.4. *The following decomposition holds:*

$$\begin{aligned} &\int_0^u \lambda_s\langle 1,\nu^N_s\rangle\langle\Gamma_s(q_{st}f),\nu^N_s\rangle\,ds \\ &= \tilde{M}_u + \langle 1,\nu^N_u\rangle\left\langle (q_{ut}f)^2,\nu^N_u\right\rangle + \int_0^u \langle H_s,\nu^N_s\rangle\langle (q_{st}f)^2,\nu^N_s\rangle\,ds \\ &\quad - \int_0^u \langle 1,\nu^N_s\rangle\langle H_s(q_{st}f)^2,\nu^N_s\rangle\,ds, \end{aligned}$$

where $\tilde{M}$ is a martingale.

Proof. Let

$$Y_u := \langle 1,\nu^N_u\rangle\langle (q_{ut}f)^2,\nu^N_u\rangle = e^{-2\int_0^u \langle H_r,\eta^N_r\rangle\,dr}\left\langle (q_{ut}f)^2,\eta^N_u\right\rangle.$$

By applying the martingale problem to the functions $\varphi(s,x) = \left\langle (q_{st}f)^2,\eta(x)\right\rangle$, we obtain

$$\begin{aligned} Y_u = e^{-2\int_0^u \langle H_r,\eta^N_r\rangle\,dr}\left\langle (q_{ut}f)^2,\eta^N_u\right\rangle \;\sim\; &-2\int_0^u e^{-2\int_0^s \langle H_r,\eta^N_r\rangle\,dr}\langle H_s,\eta^N_s\rangle\left\langle (q_{st}f)^2,\eta^N_s\right\rangle\,ds \\ &+ \int_0^u e^{-2\int_0^s \langle H_r,\eta^N_r\rangle\,dr}\left(\frac{\partial}{\partial s} + \mathcal{L}^N_s\right)\varphi(s,X^N_s)\,ds. \end{aligned}$$

Here and in the following we write $Y_u \sim Z_u$ if the processes Y_u and Z_u differ only by a martingale term. Proceeding as in the proof of proposition 3.2, we get that

$$\frac{\partial}{\partial s}\varphi(s,X^N_s) = 2\langle q_{st}f\frac{\partial}{\partial s}q_{st}f,\eta^N_s\rangle = -2\lambda_s\langle q_{st}f\mathcal{L}_s q_{st}f,\eta^N_s\rangle + 2\langle H_s(q_{st}f)^2,\eta^N_s\rangle,$$

and

$$\mathcal{L}^N_s\varphi(s,X^N_s) = \lambda_s\langle\mathcal{L}_s(q_{st}f)^2,\eta^N_s\rangle + \langle H_s,\eta^N_s\rangle\langle (q_{st}f)^2,\eta^N_s\rangle - \langle H_s(q_{st}f)^2,\eta^N_s\rangle.$$

Recalling that $\mathcal{L}_s(q_{st}f)^2 - 2q_{st}f\mathcal{L}_s q_{st}f = \Gamma_s(q_{s,t}f)$ and $\nu^N_s = \exp(-\int_0^s\langle H_r,\nu^N_r\rangle dr)\,\eta^N_s$, we conclude

$$\begin{aligned} \langle 1,\nu^N_u\rangle\langle (q_{ut}f)^2,\nu^N_u\rangle \;\sim\; &-\int_0^u \langle H_s,\nu^N_s\rangle\langle (q_{st}f)^2,\nu^N_s\rangle\,ds \\ &+ \int_0^u \langle 1,\nu^N_s\rangle\langle H_s(q_{st}f)^2,\nu^N_s\rangle\,ds + \int_0^u \lambda_s\,\langle 1,\nu^N_s\rangle\langle\Gamma_s(q_{st}f),\nu^N_s\rangle\,ds, \end{aligned}$$

which proves the assertion. □

Lemma 3.5. *For all* $t \geq 0$,

$$\mathbb{E}\Big[\langle 1, \nu_t^N\rangle\langle f^2, \nu_t^N\rangle\Big] \;=\; \langle f^2, \mu_t\rangle - \mathbb{E}\left[\int_0^t \langle H_s, \nu_s^N\rangle\langle q_{st} f^2, \nu_s^N\rangle\, ds\right].$$

Proof. By the product rule for Stieltjes integrals,

$$\begin{aligned}\langle 1, \nu_s^N\rangle\langle q_{st} f^2, \nu_s^N\rangle &= e^{-\int_0^s \langle H_r, \eta_r^N\rangle\, dr} A_{s,t}^{f^2} \\ &= \int_0^s e^{-\int_0^u \langle H_r, \eta_r^N\rangle\, dr} dA_{u,t}^{f^2} \;-\; \int_0^s \langle H_u, \nu_u^N\rangle A_{u,t}^{f^2}\, du.\end{aligned}$$

Since $s \mapsto A_{s,t}^{f^2}$ is a martingale,

$$\mathbb{E}\left[\langle 1, \nu_t^N\rangle\langle f^2, \nu_t^N\rangle\right] \;=\; \langle q_{0,t} f^2, \mu_0\rangle - \mathbb{E}\left[\int_0^t \langle H_u, \nu_u^N\rangle A_{u,t}^{f^2}\, du\right].$$

The proof is completed by noting that $\langle q_{0,t} f^2, \mu_0\rangle = \langle f^2, \mu_t\rangle$. □

Proof of Proposition 2.1. Fix a function $f : S \to \mathbb{R}$ and $t \geq 0$. Recalling that, by (2.9), $\langle f, \mu_t\rangle = \langle q_{0,t} f, \mu_0\rangle$, we have

$$\begin{aligned}\langle f, \nu_t^N\rangle - \langle f, \mu_t\rangle &= \langle q_{t,t} f, \nu_t^N\rangle - \langle q_{0,t} f, \nu_0^N\rangle + \langle q_{0,t} f, \nu_0^N\rangle - \langle q_{0,t} f, \mu_0\rangle \\ &= A_{t,t}^f - A_{0,t}^f + \langle q_{0,t} f, \nu_0^N\rangle - \langle q_{0,t} f, \mu_0\rangle.\end{aligned}$$

Taking expectations on both sides, we immediately obtain

$$\mathbb{E}\left[\langle f, \nu_t^N\rangle\right] \;=\; \langle f, \mu_t\rangle,$$

because $s \mapsto A_{s,t} f$ is a martingale by Proposition 3.3, and ν_0^N is the empirical distribution of N i.i.d. random variables with distribution μ_0. Moreover, by Proposition 3.3 and Lemma 3.4,

$$\begin{aligned} N\,\mathbb{E}\left[\left|\langle f, \nu_t^N\rangle - \langle f, \mu_t\rangle\right|^2\right] &= N\,\mathbb{E}\left[(A_{t,t}^f - A_{0,t}^f)^2\right] + N\,\mathbb{E}\left[\big(\langle q_{0,t} f, \nu_0^N\rangle - \langle q_{0,t} f, \mu_0\rangle\big)^2\right] \\ &= N\,\mathbb{E}\left[\langle A_{\bullet,t}^f\rangle_t\right] + \mathrm{Var}_{\mu_0}(q_{0,t} f) \\ &= \mathbb{E}\Big[\langle 1, \nu_t^N\rangle\langle f^2, \nu_t^N\rangle - \langle (q_{0,t} f)^2, \nu_0^N\rangle\Big] + \mathrm{Var}_{\mu_0}(q_{0,t} f) \\ &\quad + \mathbb{E}\int_0^t \langle H_s, \nu_s^N\rangle\langle (q_{st} f)^2, \nu_s^N\rangle\, ds \;-\; \mathbb{E}\int_0^t \langle 1, \nu_s^N\rangle\langle H_s (q_{st} f)^2, \nu_s^N\rangle\, ds \\ &\quad + \mathbb{E}\int_0^t \iint \big(H(x) - H(y)\big)^+ \big(q_{s,t} f(y) - q_{s,t} f(x)\big)^2\, \nu_s^N(dx)\, \nu_s^N(dy)\, ds.\end{aligned}$$

The assertion now follows from Lemma 3.5 observing that

$$\begin{aligned} -\mathbb{E}\Big[\langle (q_{0,t} f)^2, \nu_0^N\rangle\Big] + \mathrm{Var}_{\mu_0}(q_{0,t} f) &= -\langle (q_{0,t} f)^2, \mu_0\rangle + \mathrm{Var}_{\mu_0}(q_{0,t} f) \\ &= -\langle q_{0,t} f, \mu_0\rangle^2 = -\langle f, \mu_t\rangle^2.\end{aligned}$$

□

4. Proof of Theorem 2.4

Proposition 4.1. *Let* p, q, $r \in [1, \infty]$ *be such that* $p^{-1} = q^{-1} + r^{-1}$. *Then, for* $0 \leq s \leq t$,

$$\begin{aligned}\mathbb{E}\left[V_{s,t}^N(f)\right] \leq & V_{s,t}(f) \\ & + \big(6\|H_s\|_{L^q(\mu_s)} \|q_{s,t} f\|_{L^{2r}(\mu_s)}^2 + \|H_s\|_{L^p(\mu_s)} \|q_{s,t} f^2\|_{L^p(\mu_s)}\big)\varepsilon_s^{N,p}.\end{aligned}$$

Proof. Since $\langle f,\nu_s^N\rangle$ and $\langle g,\nu_s^N\rangle$ are unbiased estimators of $\langle f,\mu_s\rangle$ and $\langle g,\mu_s\rangle$, respectively, we have, by the Cauchy-Schwarz inequality,

$$\begin{aligned}
&\big|\mathbb{E}[\langle f,\nu_s^N\rangle\langle g,\nu_s^N\rangle] - \langle f,\mu_s\rangle\langle g,\mu_s\rangle\big| \\
&\qquad = \big|\mathbb{E}\big[(\langle f,\nu_s^N\rangle - \langle f,\mu_s\rangle)(\langle g,\nu_s^N\rangle - \langle g,\mu_s\rangle)\big]\big| \\
&\qquad \le \big(\mathbb{E}\big|\langle f,\nu_s^N\rangle - \langle f,\mu_s\rangle\big|^2\big)^{1/2}\big(\mathbb{E}\big|\langle g,\nu_s^N\rangle - \langle g,\mu_s\rangle\big|^2\big)^{1/2} \\
&\qquad \le \varepsilon_s^{N,p}\, \|f\|_{L^p(\mu_s)}\, \|g\|_{L^p(\mu_s)}
\end{aligned} \tag{4.1}$$

for all $0 \le s \le t$ and all functions $f,\, g : S \to \mathbb{R}$. Since the last term on the right-hand side of (2.4) can be bounded by

$$\iint |H_s(y)|(q_{s,t}f(z) - q_{s,t}f(y))^2\, \nu_s^N(dz)\, \nu_s^N(dy),$$

an application of (4.1) yields, by (1.3) and (2.10),

$$\begin{aligned}
\mathbb{E}\big[V_{s,t}^N(f)\big] &\le -\langle H_s(q_{s,t}f)^2,\mu_s\rangle\langle 1,\mu_s\rangle - \langle H_s,\mu_s\rangle\langle q_{s,t}f^2 - (q_{s,t}f)^2,\mu_s\rangle \\
&\quad + \iint |H_s(y)|(q_{s,t}f(z) - q_{s,t}f(y))^2\, \mu_s(dz)\, \mu_s(dy)\, + \varepsilon_s^{N,p} R_{s,t}(f) \\
&= V_{s,t}(f) + \varepsilon_s^{N,p} R_{s,t}(f),
\end{aligned}$$

where

$$\begin{aligned}
R_{s,t}(f) &= \|H_s(q_{s,t}f)^2\|_{L^p(\mu_s)} + \|H_s\|_{L^p(\mu_s)}\big\|q_{s,t}f^2 - (q_{s,t}f)^2\big\|_{L^p(\mu_s)} \\
&\quad + \|H_s\|_{L^p(\mu_s)}\big\|(q_{s,t}f)^2\big\|_{L^p(\mu_s)} + 2\|H_s q_{s,t}f\|_{L^p(\mu_s)}\|q_{s,t}f\|_{L^p(\mu_s)} \\
&\quad + \big\|H_s(q_{s,t}f)^2\big\|_{L^p(\mu_s)} \\
&\le \|H_s\|_{L^p(\mu_s)}\|q_{s,t}f^2\|_{L^p(\mu_s)} + 6\|H_s\|_{L^q(\mu_s)}\|q_{s,t}f\|_{L^{2r}(\mu_s)}^2.
\end{aligned}$$

□

In order to bound $V_{s,t}^N(f)$ uniformly over $f \in L^p(\mu_t)$ with $\|f\|_{L^p(\mu_t)} \le 1$, one needs to be able to control $\|q_{s,t}f\|_{L^{2r}(\mu_t)}$ in terms of $\|f\|_{L^p(\mu_t)}$. This is possible if hypercontractivity holds and $t-s$ is sufficiently large. Over short time intervals $[s,t]$ we apply in a first step another rough estimate instead:

Lemma 4.2. *Let $p \ge 2$ and $N \in \mathbb{N}$. Then for $0 \le s \le t$,*

$$\frac{1}{N}\,\mathbb{E}\big[V_{s,t}^N(f)\big] \le 4\,\mathrm{osc}(H_s)\Big(1 + \varepsilon_s^{N,p} \exp\Big(2\int_s^t \mathrm{osc}(H_r)\, dr\Big)\Big)\|f\|_{L^p(\mu_t)}^2.$$

Proof. Setting

$$A_t^f \;:=\; \langle f,\nu_t^N\rangle \;=\; \langle f,\eta_t^N\rangle\, \exp\Big(-\int_0^t \langle H_s,\eta_s^N\rangle\, ds\Big),$$

we have $A_t^f = \langle f,\eta_t^N\rangle\, A_t^1$ for all $f : S \to \mathbb{R}$. Since

$$\langle f^2,\eta_t^N\rangle = \frac{1}{N}\sum_{i=1}^N f(X_{t,i})^2 \le \frac{1}{N}\Big(\sum_{i=1}^N |f(X_{t,i})|\Big)^2 = N\langle |f|,\eta_t^N\rangle^2,$$

we obtain, recalling that η_t^N is a probability measure,

$$\begin{aligned} V_{s,t}^N(f) &\leq N\,(A_s^1)^2\Big((\max H_s^- + \max H_s^+)\langle |q_{s,t}f|, \eta_s^N\rangle^2 + \max H_s^- \langle (q_{s,t}f^2)^{1/2}, \eta_s^N\rangle^2 \\ &\qquad + 2\,\mathrm{osc}(H_s)\langle |q_{s,t}f|, \eta_s^N\rangle^2\Big) \\ &\leq N\,\mathrm{osc}(H_s)\Big(3\langle q_{s,t}|f|, \nu_s^N\rangle^2 + \langle (q_{s,t}f^2)^{1/2}, \nu_s^N\rangle^2\Big). \end{aligned} \tag{4.2}$$

Moreover, by inequality (4.1),

$$\mathbb{E}\left[\langle f, \nu_t^N\rangle^2\right] \leq \langle f, \mu_t\rangle^2 + \varepsilon_t^{N,p}\|f\|_{L^p(\mu_t)}^2,$$

hence, taking expectations on both sides of (4.2), we obtain

$$\begin{aligned} \frac{1}{N}\,\mathbb{E}\big[V_{s,t}^N(f)\big] &\leq 3\,\mathrm{osc}(H_s)\big[\langle q_{s,t}|f|, \mu_s\rangle^2 + \varepsilon_s^{N,p}\big\|q_{s,t}|f|\big\|_{L^p(\mu_s)}^2\big] \\ &\quad + \mathrm{osc}(H_s)\big[\langle q_{s,t}f^2, \mu_s\rangle + \varepsilon_s^{N,p}\big\|q_{s,t}f^2\big\|_{L^{p/2}(\mu_t)}^2\big] \\ &\leq 4\,\mathrm{osc}(H_s)\,\left[\langle f^2, \mu_t\rangle + \varepsilon_s^{N,p}\exp\left(2\int_s^t \mathrm{osc}(H_r)\,dr\right)\|f\|_{L^p(\mu_t)}^2\right], \end{aligned}$$

where we have used the fact that $\langle q_{s,t}f, \mu_s\rangle = \langle f, \mu_t\rangle$, and the estimate

$$\big\|q_{s,t}f\big\|_{L^p(\mu_t)} \;\leq\; \exp\left(\int_s^t \mathrm{osc}(H_r)\,dr\right)\|f\|_{L^p(\mu_s)}. \tag{4.3}$$

The proof of (4.3) is elementary and can be found in [7]. □

Combining Proposition 4.1 and Lemma 4.2 we obtain the following (rough) a priori estimate:

Lemma 4.3. *Let p, q, $r \in [2,\infty]$ be such that $p^{-1} = q^{-1} + r^{-1}$, and choose δ as in Theorem 2.4. If*

$$N \geq 25\,\max\big(1, \bar{C}_t(p,q,\delta)\big)$$

then

$$\varepsilon_t^{N,p} < 1.$$

Proof. Note that, by (2.10),

$$V_{s,t}(f) \leq 5\,\|H_s\|_{L^q(\mu_s)}\,\|q_{s,t}f\|_{L^{2r}(\mu_s)}$$

for any $f : S \to \mathbb{R}$ and $0 \leq s \leq t$. Hence Proposition 4.1 implies

$$\mathbb{E}\big[V_{s,t}^N(f)\big] \leq \|H_s\|_{L^q(\mu_s)}C_{s,t}(p,q)^2\|f\|_{L^p(\mu_t)}^2\big(5 + 7\varepsilon_s^{N,p}\big).$$

Choosing N as stated we get

$$\frac{1}{N}\int_0^{(t-\delta)^+}\mathbb{E}\big[V_{s,t}^N(f)\big]\,ds \leq \frac{12}{25}\|f\|_{L^p(\mu_t)}^2\max\big(\varepsilon_t^{N,p}, 1\big).$$

On the other hand, by Lemma 4.2 and since $17\,\delta\;\mathrm{osc}(H_s) \leq 1$ for any $s \leq t$, we obtain

$$\begin{aligned} \frac{1}{N}\int_{(t-\delta)^+}^t \mathbb{E}\big[V_{s,t}^N(f)\big]\,ds &\leq \frac{4}{17}\big(1 + \varepsilon_t^{N,p}e^{2/17}\big)\|f\|_{L^p(\mu_t)}^2 \\ &< \frac{1}{2}\|f\|_{L^p(\mu_t)}^2\max\big(\varepsilon_t^{N,p}, 1\big). \end{aligned}$$

Hence by Proposition 2.1, since $N \geq 50$, we get

$$\varepsilon_t^{N,p} = \sup\left\{ \frac{1}{N}\,\mathrm{Var}_{\mu_t}(f) + \frac{1}{N}\int_0^t \mathbb{E}\big[V_{s,t}^N(f)\big]\,ds \,\Big|\, f:S\to\mathbb{R} \text{ with } \|f\|_{L^p(\mu_r)} \leq 1,\ r\in[0,t]\right\}$$
$$< \left(\frac{1}{50}+\frac{12}{25}+\frac{1}{2}\right)\max\big(\varepsilon_t^{N,p},1\big). \qquad \square$$

The a priori estimate just obtained can be used instead of Lemma 4.2 to estimate $\mathbb{E}\left[V_{s,t}^N(f)\right]$ when $t-s$ is small:

Lemma 4.4. *Let $q\in]6,\infty]$ and $p\in]4q/(q-2),\infty[$. Suppose that*

$$N \geq 25\max\big(1,\bar{C}_t(\tilde{p},q,\delta)\big),$$

where $\tilde{p}$ is defined by $\tilde{p}^{-1}=q^{-1}+(p/2)^{-1}$. Then for $0\leq s\leq t\leq t_0$,

$$\mathbb{E}\left[V_{s,t}^N(f)\right] \;\leq\; V_{s,t}(f) + 7\,\exp\left(2\int_s^t \mathrm{osc}(H_r)\,dr\right)\|H_s\|_{L^q(\mu_s)}\|f\|_{L^p(\mu_t)}^2.$$

Proof. Note that $\tilde{p}^{-1}=q^{-1}+(p/2)^{-1}<1/2$ by the assumptions on p and q. Applying Proposition 4.1 with p, q, r replaced by $\tilde{p}$, $\tilde{q}:=q$, and $\tilde{r}:=p/2$, respectively, yields

$$\mathbb{E}\big[V_{s,t}^N(f)\big] \leq V_{s,t}(f) + \big(\|H_s\|_{L^{\tilde{p}}(\mu_s)}\|q_{s,t}f^2\|_{L^{\tilde{p}}(\mu_s)} + 6\|H_s\|_{L^q(\mu_t)}\|q_{s,t}f\|_{L^p(\mu_s)}^2\big)\,\varepsilon_s^{N,\tilde{p}}$$

Since $\tilde{p}<\min(q,p/2)$, the claim follows by Lemma 4.3 and the estimate (4.3). $\square$

We are now ready to prove the theorem:

Proof of Theorem 2.4. By Proposition 4.1 we have

$$\mathbb{E}\big[V_{s,t}^N(f)\big] \leq V_{s,t}(f) + 7\|H_s\|_{L^q(\mu_s)}C_{s,t}(p,q)^2\|f\|_{L^p(\mu_t)}^2\varepsilon_t^{N,p}$$

for any $f:S\to\mathbb{R}$ and $0\leq s\leq t$. Therefore by Proposition 2.1, Lemma 4.4, and the choice of δ,

$$N\,\mathbb{E}\big|\langle f,\nu_t^N\rangle - \langle f,\mu_t\rangle\big|^2 = \mathrm{Var}_{\mu_t}(f) + \int_0^{(t-\delta)^+}\mathbb{E}\big[V_{s,t}^N(f)\big]\,ds + \int_{(t-\delta)^+}^t \mathbb{E}\big[V_{s,t}^N(f)\big]\,ds$$
$$\leq \mathrm{Var}_{\mu_t}(f) + \int_0^t V_{s,t}(f)\,ds$$
$$+\Big[7\bar{C}_t(p,q,\delta)\varepsilon_t^{N,p} + 7e^{2/17}\int_{(t-\delta)^+}^t \|H_s\|_{L^q(\mu_s)}\,ds\Big]\,\|f\|_{L^p(\mu_t)}^2.$$

Observing that $\|H_s\|_{L^q(\mu_s)}\leq \mathrm{osc}(H_s)$ and that $7\,e^{2/17}/17<1$, we obtain (2.12).

Furthermore, by maximizing (2.12) over all $f:S\to\mathbb{R}$ such that $\|f\|_{L^p(\mu_t)}\leq 1$ and over t, we get

$$N\varepsilon_t^{N,p} \leq 2+v_t^p+7\bar{C}_t(p,q,\delta)\varepsilon_t^{N,p}$$

for all $t\in[0,t_0]$. Recalling that $N>25\bar{C}_t(p,q,\delta)$ by assumption, we obtain

$$\varepsilon_t^{N,p} \leq \frac{2+v_t^p}{N-7\bar{C}_t(p,q,\delta)} = (2+v_t^p)\left(\frac{1}{N}+\frac{7\bar{C}_t(p,q,\delta)}{N(N-7\bar{C}_t(p,q,\delta))}\right)$$
$$\leq (2+v_t^p)\,N^{-1}\left(1+\frac{7\cdot 25}{18}\bar{C}_t(p,q,\delta)N^{-1}\right),$$

which implies (2.13). $\square$

5. Proofs of Theorems 2.5 and 2.9

Proof of Theorem 2.5. By the estimates in [7] we have, for $0 \le s \le t \le t_0$,

$$\|q_{s,t}f\|_{L^p(\mu_s)} \le 2^{1/4}\|f\|_{L^p(\mu_s)}$$

for all $f : S \to \mathbb{R}$, provided

$$\lambda_s \;\ge\; \frac{p}{4}\,A_s + \frac{p(p+3)}{4}\,t_0\,B_s \qquad \text{for all } s \in [0,t_0]. \tag{5.1}$$

Hence, under this condition, we get $C_{s,t}(p) \le 2^{1/4}$. Moreover, by [7],

$$\|q_{t-\delta,t}f\|_{L^q(\mu_{t-\delta})} \;\le\; \exp\Big(\int_{t-\delta}^{t} \max H_r^-\,dr\Big)\,\|f\|_{L^p(\mu_t)}$$

for all $f : S \to \mathbb{R}$ and $0 \le \delta \le t \le t_0$, provided

$$\lambda_s \ge \frac{\gamma_s}{4\delta}\log\frac{q-1}{p-1} \qquad \text{for all } s \in [0,t_0]. \tag{5.2}$$

Choosing $\delta = (17\omega)^{-1}$, we obtain that, for $s \le t-\delta$,

$$\|q_{s,t}f\|_{L^p(\mu_s)} \;=\; \|q_{s,t-\delta}q_{t-\delta,t}f\|_{L^p(\mu_s)} \;\le\; 2^{1/4}e^{1/17}\|f\|_{L^q(\mu_t)},$$

if both (5.1) and (5.2) hold. Hence

$$C_{s,t}(p,q) \le 2^{1/4}e^{1/17}$$

provided (5.1) holds and

$$\lambda_s \ge \frac{\gamma_s}{4\delta}\log\max\Big(\frac{2r-1}{p-1},\frac{2p-2}{p-2}\Big) \qquad \text{for all } s \in [0,t_0].$$

Since $2 < \tilde{p} < p$ and $\tilde{p}^{-1} = q^{-1} + (p/2)^{-1}$, we obtain similarly that $C_{s,t}(\tilde{p},q) \le 2^{1/4}e^{1/17}$ provided (5.1) holds and

$$\lambda_s \ge \frac{\gamma_s}{4\delta}\log\max\Big(\frac{p-1}{\tilde{p}-1},\frac{2\tilde{p}-2}{\tilde{p}-2}\Big) \qquad \text{for all } s \in [0,t_0].$$

Hence by (2.14) and (2.15) we obtain

$$v_t(p) \le 5\cdot 2^{1/2}\,K_t(2), \qquad \bar{C}_t(p,q,\delta) \le 2^{1/2}\,e^{2/17}\,K_t(q), \qquad \bar{C}_t(\tilde{p},q,\delta) \le 2^{1/2}\,e^{2/17}\,K_t(q)$$

for any $t \le t_0$. The assertion now follows from Theorem 2.4. □

Proof of Lemma 2.2. For a function $f : S \to \mathbb{R}$ and $t \ge 0$ let $f_t := f - \langle f,\mu_t\rangle$. Then

$$\langle f_t,\eta_t^N\rangle = \langle f,\eta_t^N\rangle - \langle f,\mu_t\rangle$$

and, by (1.9),

$$\langle f_t,\nu_t^N\rangle = \langle 1,\nu_t^N\rangle\langle f_t,\eta_t^N\rangle. \tag{5.3}$$

Hence

$$\begin{aligned}
\mathbb{E}\big[\langle f_t,\eta_t^N\rangle^2\big] &\le 2\,\mathbb{E}\Big[\big(\langle f_t,\eta_t^N\rangle - \langle f_t,\nu_t^N\rangle\big)^2\Big] + 2\,\mathbb{E}\big[\langle f_t,\nu_t^N\rangle^2\big] \\
&= 2\,\mathbb{E}\Big[\big(\langle 1,\nu_t^N\rangle - 1\big)^2\langle f_t,\eta_t^N\rangle^2\Big] + 2\,\mathbb{E}\big[\langle f_t,\nu_t^N\rangle^2\big] \\
&\le 2\,\|f_t\|_{\sup}^2\,\mathbb{E}\Big[\big(\langle 1,\nu_t^N\rangle - 1\big)^2\Big] + 2\,\mathbb{E}\big[\langle f_t,\nu_t^N\rangle^2\big]\,.
\end{aligned}$$

Applying this bound and (5.3), we obtain the L^1 estimate:

$$\begin{aligned}\mathbb{E}\big[|\langle f_t,\eta_t^N\rangle|\big] &= \mathbb{E}\big[|\langle f_t,\eta_t^N\rangle\big(1-\langle 1,\nu_t^N\rangle\big)|\big] + \mathbb{E}\big[|\langle f_t,\nu_t^N\rangle|\big] \\ &\le \mathbb{E}\left[\langle f_t,\eta_t^N\rangle^2\right]^{1/2}\mathbb{E}\big[\big(\langle 1,\nu_t^N\rangle-1\big)^2\big]^{1/2} + \mathbb{E}\left[\langle f_t,\nu_t^N\rangle^2\right]^{1/2} \\ &\le \mathbb{E}\left[\langle f_t,\nu_t^N\rangle^2\right]^{1/2} + \sqrt{2}\,\|f_t\|_{\sup}\mathbb{E}\left[\big(\langle 1,\nu_t^N\rangle-1\big)^2\right] \\ &\quad + \sqrt{2}\,\mathbb{E}\left[\langle f_t,\nu_t^N\rangle^2\right]^{1/2}\mathbb{E}\left[\big(\langle 1,\nu_t^N\rangle-1\big)^2\right]^{1/2}.\end{aligned}$$

This proves Lemma 2.2. □

Proof of Corollary 2.7. The first assertion is an immediate consequence of (2.12) and (2.18). The second assertion follows by the first one and (2.6). □

Proof of Theorem 2.9. Fix $i \in I$ and define

$$h_t(i) := \langle H_t, \mu_t^i\rangle = \int_{S_i} H_t\, d\mu_t/\mu_t(S_i).$$

Note that

$$h_t(i) = -\frac{d}{dt}\log \mu_t(S_i).$$

Since (1.2) and (1.3) hold, $H_t^i = H_t - h_t(i)$ is the negative logarithmic time derivative of μ_t^i. If we define $q_{s,t}^i f$ for functions $f : S_i \to \mathbb{R}$ in the same way as $q_{s,t}f$ with H_t replaced by H_t^i, then

$$q_{s,t}f(x) \;=\; \exp\big(-\int_s^t h_r(i)\,dr\big)\, q_{s,t}^i f(x) \;=\; \frac{\mu_t(S_i)}{\mu_s(S_i)}\, q_{s,t}^i f(x).$$

In particular, for $p \in [1,\infty]$, we have

$$\|q_{s,t}f\|_{\widetilde{L^p}(\mu_s)} \;=\; \max_{i\in I}\|q_{s,t}f\|_{L^p(\mu_s^i)} \;\le\; \max_{i\in I}\frac{\mu_t(S_i)}{\mu_s(S_i)}\,\|q_{s,t}^i f\|_{L^p(\mu_s^i)}. \tag{5.4}$$

Assuming Poincaré and log Sobolev inequalities with respect to the measures μ_t^i and the functions H_t^i, we obtain the same type of L^p-L^q bounds for the operators $q_{s,t}^i$ as we did for the operators $q_{s,t}$ in the proof of Theorem 2.5. Because of (5.4) the assertion then follows similarly as above. □

Appendix A. Spectral gap and LSI for 1D Metropolis

In this appendix we prove upper bounds for the Poincaré and logarithmic Sobolev constants for Random Walk Metropolis algorithms on a finite subset S of $\mathbb{Z}$. Let $S := \{a, a+1, \ldots, -1, 0, 1, \ldots, a+\Delta-1\}$ with $a \in \mathbb{Z}$ and $\Delta \in \mathbb{N}$ such that $0 \in S$. We assume that μ is a probability measure on S satisfying

(i) $\mu(x) \le \rho\mu(y)$ for any x, $y \in [-s, s]$;
(ii) $\mu(x+1) \le \alpha\mu(x)$ for any $x \ge s$, and $\mu(x-1) \le \alpha\mu(x)$ for any $x \le -s$,

for appropriate constants $s \in \mathbb{Z}_+$, $\rho \in [1, +\infty[$, and $\alpha \in]0, 1[$. For notational convenience, we set

$$b := a+\Delta-1, \qquad r := \frac{1}{1-\alpha}\wedge\Delta, \qquad u := s\wedge\Delta.$$

The Random Walk Metropolis chain for sampling from μ is the Markov chain on S with generator $\mathcal{L}$ satisfying

$$\mathcal{L}(x,y) = \begin{cases} \frac{1}{2}\min\left(\frac{\mu(y)}{\mu(x)}, 1\right), & \text{if } |y-x| = 1, \\ 0, & \text{if } |y-x| > 1. \end{cases}$$

To estimate the Poincaré constant for this dynamics, we can apply a general upper bound for one-dimensional Markov chains due to Miclo [17], which implies in our case

$$C^{\text{Poi}} \le 4\,\max(B^+, B^-), \tag{A.1}$$

where

$$B^+ := \max_{1\le k\le b} B_k^+, \qquad B_k^+ := \sum_{x=1}^{k} \frac{1}{\mu(x-1)\wedge\mu(x)} \sum_{x=k}^{b} \mu(x),$$

$$B^- := \max_{a\le k\le -1} B_k^-, \qquad B_k^- := \sum_{x=k}^{-1} \frac{1}{\mu(x+1)\wedge\mu(x)} \sum_{x=a}^{k} \mu(x).$$

The bound is sharp up to a factor 4, see [17]. We are going to estimate B_k^+ in the cases $k > s$ and $k \le s$ separately. Corresponding bounds hold for B_k^-. Let us assume first that $k > s$. Then we have, by (ii),

$$\sum_{x=s+1}^{k} \frac{1}{\mu(x-1)\wedge\mu(x)} = \sum_{x=s+1}^{k} \frac{1}{\mu(x)} \le \frac{1}{\mu(k)} \sum_{i=0}^{k-s-1} \alpha^i \le \frac{r}{\mu(k)}.$$

and, by (i) and (ii),

$$\sum_{x=1}^{s} \frac{1}{\mu(x-1)\wedge\mu(x)} \le \frac{\rho u}{\mu(s)} \le \frac{\alpha^{k-s}\rho u}{\mu(k)}.$$

Hence

$$\sum_{x=1}^{k} \frac{1}{\mu(x-1)\wedge\mu(x)} \le (r + \alpha^{k-s}\rho u)\frac{1}{\mu(k)}. \tag{A.2}$$

Similarly, by (ii),

$$\sum_{x=k}^{b} \mu(x) \le \mu(k) \sum_{i=0}^{b-k} \alpha^i \le r\mu(k). \tag{A.3}$$

Therefore (A.2) and (A.3) yield

$$B_k^+ \le r\big(r + \alpha^{k-s}\rho u\big) \le r^2 + \rho\, u\, r \qquad \text{for any } k > s. \tag{A.4}$$

Let us now consider the case $k \le s$: by (i) and since $s \wedge b \le u$, we have

$$\sum_{x=1}^{k} \frac{1}{\mu(x-1)\wedge\mu(x)} \sum_{x=k}^{s\wedge b-1} \mu(x) = \sum_{x=1}^{k} \sum_{y=k}^{s\wedge b-1} \frac{\mu(y)}{\mu(x-1)\wedge\mu(x)} \le \rho k(u-k) \le \rho u^2/4.$$

Moreover, similarly to (A.3), we have

$$\sum_{x=s\wedge b}^{b} \mu(x) \le r\mu(s\wedge b),$$

hence, by (i) and since $k \le s$ and $k \le \Delta$,

$$\sum_{x=1}^{k} \frac{1}{\mu(x-1)\wedge\mu(x)} \sum_{x=s\wedge b}^{b} \mu(x) \le r \sum_{x=1}^{k} \frac{\mu(s\wedge b)}{\mu(x-1)\wedge\mu(x)} \le \rho\, k\, r \le \rho\, u\, r.$$

Combining these estimates, we obtain

$$B_k^+ \le \frac{1}{4}\rho u^2 + \rho u r, \qquad \text{for any } k \le s. \tag{A.5}$$

By (A.4) and (A.5), we finally obtain

$$B^+ := \max_{k=1,\dots,b} B_k^+ \le \rho u r + \max(r^2, \rho u^2/4).$$

Observing that the same estimate holds for B^-, we have shown:

Theorem A.1. *The Poincaré constant C^{Poi} for the Random Walk Metropolis chain with stationary distribution μ satisfies*

$$C^{\mathrm{Poi}} \le 4\rho u r + \max(4r^2, \rho u^2)$$

Proof. The result holds by the upper bound (A.1). □

For the corresponding logarithmic Sobolev constant the following upper bound follows from the results in [17]:

$$\gamma \le 20 \max(\beta^+, \beta^-),$$

where

$$\beta^+ := \max_{1\le k\le b} \beta_k^+, \qquad \beta_k^+ := \sum_{x=1}^{k} \frac{2}{\mu(x-1)\wedge\mu(x)} \sum_{x=k}^{b} \mu(x) \Big| \log \sum_{x=k}^{b} \mu(x) \Big|,$$

$$\beta^- := \max_{a\le k\le -1} \beta_k^-, \qquad \beta_k^- := \sum_{x=k}^{-1} \frac{2}{\mu(x+1)\wedge\mu(x)} \sum_{x=a}^{k} \mu(x) \Big| \log \sum_{x=a}^{k} \mu(x) \Big|.$$

Again, the bound is sharp up to an explicit numerical constant. A rough estimate for β_k^+ can easily be obtained observing that

$$\Big| \log \sum_{x=k}^{b} \mu(x) \Big| = \log \Big(\sum_{x=k}^{b} \mu(x) \Big)^{-1} \le \log \frac{1}{\mu(k)} \le \log \frac{1}{\mu_*},$$

where $\mu_* = \min_x \mu(x)$. In fact, this implies

$$\beta_k^+ \le 2B_k^+ \log \frac{1}{\mu_*},$$

hence upper bounds for β^+ and β^- can be obtained from the corresponding bounds for B^+ and B^- simply by multiplying by a factor $2\log \mu_*^{-1}$. In particular, the upper bound for C^{Poi} derived above yields an upper bound for γ:

Theorem A.2. *One has*

$$\gamma \le 10\big(4\rho u r + \max(\rho u^2, 4r^2)\big) \log \frac{1}{\mu_*}.$$

Example: A discrete Gauss model. Assume that

$$\mu(x) \propto \exp\Big(-\frac{x^2}{2\sigma^2}\Big)$$

for some finist constant $\sigma > 0$. Then one can check that (i) and (ii) above are satisfied with

$$s = \lfloor \sigma \rfloor, \qquad \rho = e^{1/2}, \qquad \alpha = \frac{\mu(s+1)}{\mu(s)} = \exp\Big(-\frac{\lfloor \sigma \rfloor + 1/2}{\sigma^2}\Big).$$

Note that $\alpha \le e^{-1/2}$ for $\sigma < 1$ and $\alpha \le e^{-3/4\sigma}$ for $\sigma \ge 1$. Applying the elementary inequality $1 - e^{-x} \ge \min(2x/3, 1/2)$, we obtain $1-\alpha \ge 1/(2\sigma)$ if $\sigma > 1$ and $1 - \alpha \ge 1/3$ if $\sigma \le 1$. Hence

$$r = \frac{1}{1-\alpha} \wedge \Delta \le (2\sigma \vee 3) \wedge \Delta \le 2\big((\sigma \wedge \Delta) \vee 2\big).$$

By Theorem A.1, we then obtain

$$C^{\mathrm{Poi}} \le 30\,\big((\sigma \wedge \Delta) \vee 2\big)^2.$$

Moreover, since $-\Delta \le a \le b \le \Delta$, one has

$$\frac{\mu(k)}{\mu(0)} = \exp\Big(-\frac{k^2}{2\sigma^2}\Big) \ge \exp\Big(-\frac{1}{2}\frac{\Delta^2}{\sigma^2}\Big) \qquad \text{for any } k \in S,$$

and thus

$$\log\frac{1}{\mu_*} \le \frac{1}{2}\big(\Delta/\sigma\big)^2 + \log\frac{1}{\mu(0)} \le \frac{1}{2}\big(\Delta/\sigma\big)^2 + \log\Delta.$$

Therefore we obtain, by Theorem A.2,

$$\begin{aligned}\gamma &\le 150\big((\sigma\wedge\Delta)\vee 2\big)^2\big(\Delta/\sigma\big)^2 + 300\big((\sigma\wedge\Delta)\vee 2\big)^2\log\Delta \\ &\le 300\Big(\frac{\Delta}{\sigma\wedge 1}\Big)^2 + 300\big((\sigma\wedge\Delta)\vee 2\big)^2\log\Delta.\end{aligned}$$

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