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OPTIMAL CONVERGENCE RATES OF MCMC INTEGRATION FOR FUNCTIONS WITH UNBOUNDED SECOND MOMENT

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Abstract

We study the Markov chain Monte Carlo estimator for numerical integration for functions that do not need to be square integrable with respect to the invariant distribution. For chains with a spectral gap we show that the absolute mean error for L^p functions, with $p \in (1, 2)$, decreases like $n^{(1/p)-1}$, which is known to be the optimal rate. This improves currently known results where an additional parameter $\delta > 0$ appears and the convergence is of order $n^{((1+\delta)/p)-1}$.

Keywords: Markov chain Monte Carlo; spectral gap; absolute mean error

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1. Introduction

Let $(\mathcal{X}, \mathcal{F}_{\mathcal{X}}, \pi)$ be a probability space and $f: \mathcal{X} \to \mathbb{R}$ be measurable as well as π-integrable. For a random variable $X \sim \pi$ we are interested in approximating the expectation

$$\mathbb{E}[f(X)] = \int_{\mathcal{X}} f(x)\, \pi(\mathrm{d}x) = \pi(f).$$

A common approach is to use a Markov chain Monte Carlo (MCMC) method. Requiring the density of π only in non-normalised form, many MCMC algorithms provide powerful tools for scientific and statistical applications. The main idea behind these approaches is to construct a Markov chain $(X_n)_{n\in\mathbb{N}}$, having π as the invariant distribution, and to estimate $\pi(f)$ via

$$S_n f = \frac{1}{n} \sum_{j=1}^{n} f(X_j).$$

Under fairly mild conditions we have $S_n f \to \pi(f)$ almost surely as $n \to \infty$; cf. [2] or [13, Chapter 17]. This ensures the strong consistency of the MCMC estimator, yet it is clearly of interest to have non-asymptotic error bounds. For instance, given some $p \in [1, \infty)$, we can consider the p-mean error,

$$\mathbb{E}[|S_n f - \pi(f)|^p]; \tag{1.1}$$

however, other criteria are also feasible – see, e.g., [9].

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Setting $p=2$ in (1.1), we speak of the *mean squared error*, and in different settings explicit bounds are known, e.g. under a Wasserstein contraction assumption [8], spectral gap conditions [17], or if we have geometric/polynomial ergodicity [10]. For the mean squared error to make sense we require a finite second moment of f, i.e. $\|f\|^2_{L^2(\pi)} = \pi(f^2) < \infty$. On the other hand, the *absolute mean error*, given by $\mathbb{E}|S_n f - \pi(f)|$, is well defined and finite as long as f is π-integrable. Bounds for the absolute mean error for functions with $\|f\|^p_{L^p(\pi)} = \pi(|f|^p) < \infty$, where $p < 2$, are still rare. In [18] it is shown that, under a spectral gap condition, for any $p \in (1, 2)$,

$$\sup_{\|f\|_{L^p(\pi)} \le 1} \mathbb{E}[|S_n f - \pi(f)|] \le \frac{C}{n^{1-((1+\delta)/p)}}, \tag{1.2}$$

with constants $\delta > 0$ and $C \in (0, \infty)$.

Setting $k=0$ in [15, Proposition 1, Section 2.2.9] (see also [7, Section 5]) shows that in general we have the lower bound

$$\sup_{\|f\|_{L^p(\pi)} \le 1} \mathbb{E}[|S_n f - \pi(f)|] \ge \frac{c}{n^{1-(1/p)}}, \tag{1.3}$$

where $c \in (0, \infty)$ is a constant independent of n.

Even though $\delta > 0$ in (1.2) may be chosen arbitrarily small, it is natural to ask whether it can be removed completely, such that we would have the same rate as in (1.3). Under the (strong) assumption of uniform ergodicity and reversibility we know that this is the case; cf. [18, Theorem 1]. To the best of the author's knowledge this is the only situation where optimal rates are known. The goal of this note is to extend this result to the spectral gap setting – see Theorem 2.1, where we show that

$$\sup_{\|f\|_{L^p(\pi)} \le 1} \mathbb{E}[|S_n f - \pi(f)|] \le \frac{\widetilde{C}_p}{n^{1-(1/p)}}$$

for $p \in (1, 2]$, with an explicit expression for the constant $\widetilde{C}_p$.

Let us sketch the proof. The main idea is to employ the Riesz–Thorin interpolation theorem, a technique which goes back at least to [7] in Monte Carlo theory, and was also used to derive (1.2) in [18]. To this end, we first derive a result for the case where $(X_n)_{n\in\mathbb{N}}$ is a stationary chain; see Proposition 3.1. Then we apply a change of measure argument to deduce Theorem 2.1. It is worth mentioning that, based on Proposition 3.1, it is also possible to generalise [17, Theorem 3.41]; see Corollary 3.1.

The rest of this note is organised as follows. In Section 2 we state and discuss our assumptions, as well as the main result. The proofs, together with some intermediate results, can be found in Section 3.

2. Error bounds for MCMC integration

This section contains our main result, Theorem 2.1, together with the required notation and assumptions. Let us start by specifying the general setting.

We assume that the state space $(\mathcal{X}, \mathcal{F}_\mathcal{X})$ is Polish with $\mathcal{F}_\mathcal{X}$ being countably generated. Let K be a Markov kernel and ν a probability measure, called the initial distribution, both defined on $(\mathcal{X}, \mathcal{F}_\mathcal{X})$. Then, the Markov chain corresponding to K and ν, say $(X_n)_{n\in\mathbb{N}}$, is defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P}_\nu)$. In particular, such a probability space exists. We assume that π is the unique invariant distribution of K and that $(X_n)_{n\in\mathbb{N}}$ is ψ-irreducible. For definitions and further details we refer to [4, 13].

Given $p \in [1, \infty)$, we define $L^p(\pi)$ as the set of all functions $f\colon \mathcal{X} \to \mathbb{R}$ such that $\|f\|^p_{L^p(\pi)} = \pi(|f|^p) < \infty$. Similarly, $L^\infty(\pi)$ denotes the set of functions with finite $\|f\|_{L^\infty(\pi)} = \operatorname{ess\,sup}_{x\in\mathcal{X}} |f(x)|$. We follow the usual convention that two functions in $L^p(\pi)$, with $p \in [1, \infty]$, are considered as equal if they are equal π-almost everywhere. Then, $(L^p(\pi), \|\cdot\|_{L^p(\pi)})$ is a normed space. Moreover, $L^2(\pi)$, equipped with $\langle f, g\rangle_{L^2(\pi)} = \int_{\mathcal{X}} f(x)g(x)\,\pi(\mathrm{d}x)$, is a Hilbert space with induced norm $\|\cdot\|_{L^2(\pi)}$, and so is the closed subspace $L_0^2(\pi) := \{f \in L^2(\pi)\colon \pi(f) = 0\}$.

Let $p \in [1, \infty]$; then the Markov kernel K induces a linear operator $K\colon L^p(\pi) \to L^p(\pi)$ via $f \mapsto Kf(\cdot) = \int_{\mathcal{X}} f(x')\,K(\cdot, \mathrm{d}x')$. Indeed, the operator K is well defined and we have $\|K\|_{L^p(\pi)\to L^p(\pi)} = 1$; we refer to [17, Section 3.1] for further details.

We denote by Id the identity on $L^2(\pi)$. The following condition about the operator $\mathrm{Id} - K$, restricted to $L_0^2(\pi)$, is our main assumption.

Assumption 2.1. *Assume that* $\mathrm{Id} - K$*, considered as an operator from* $L_0^2(\pi)$ *to* $L_0^2(\pi)$*, has a linear and bounded inverse with* $\|(\mathrm{Id} - K)^{-1}\|_{L_0^2(\pi)\to L_0^2(\pi)} \le s < \infty$.

Remark 2.1. The invertibility of $\mathrm{Id} - K$, restricted to a suitable subspace of $L^2(\pi)$, was also studied in [11] for uniformly ergodic chains and [12] for V-uniformly ergodic chains. In particular, the existence of $(\mathrm{Id} - K)^{-1}$ on an appropriate subspace was used there to characterise the convergence behaviour of the mean squared error. Moreover, non-reversible chains on finite state spaces were studied recently in [3]. There, bounds for the mean squared error are shown, where the second smallest singular value of $\mathrm{Id} - K$ plays an important role.

We note that Assumption 2.1 is closely related to a spectral gap; there are, however, different definitions for a spectral gap:

- Some authors (see, e.g., [1, 4]) say K admits a(n) (absolute L^2) spectral gap if $\sup_{\lambda\in\mathcal{S}_0} |\lambda| < 1$, where $\mathcal{S}_0$ is the spectrum of $K\colon L_0^2(\pi) \to L_0^2(\pi)$. This is equivalent to the existence of some $m \in \mathbb{N}$ such that $\|K^m\|_{L_0^2(\pi)\to L_0^2(\pi)} < 1$; cf. [4, Proposition 22.2.4].
- On the other hand, a different definition, for instance used in [6, 14, 17, 18], is to say that K admits a(n) (absolute L^2) spectral gap if $\|K\|_{L_0^2(\pi)\to L_0^2(\pi)} < 1$.

If K is reversible, which implies that the corresponding Markov operator is self-adjoint on $L^2(\pi)$, then both definitions are equivalent.

Let us emphasise that either of the above definitions of a spectral gap implies that Assumption 2.1 is true, including in the non-reversible case. Spectral gap results were established for a number of MCMC methods, see for instance [1, 6, 14]; see also [17, Section 3.4] and [16, Theorem 2.1]. Moreover, we note that under Assumption 2.1 we cover the setting of [18, Theorems 1 and 2].

If for the initial distribution we have $\nu \ll \pi$ with Radon–Nikodým derivative $\mathrm{d}\nu/\mathrm{d}\pi \in L^q(\pi)$ for some $q \in [1, \infty]$, then we set $M_q = \|\mathrm{d}\nu/\mathrm{d}\pi\|_{L^q(\pi)}$. In particular, for $q = \infty$ we have $\sup_{A\in\mathcal{F}_{\mathcal{X}}} [\nu(A)/\pi(A)] \le M_\infty$, in which case ν is called M_∞-warm.

The following theorem is our main result, which shows that under Assumption 2.1 we have the optimal rate of convergence for the absolute mean error.

Theorem 2.1. *Let Assumption 2.1 be true,* $p \in (1, 2]$*, and assume that* ν *is absolutely continuous with respect to* π *with Radon–Nikodým derivative* $\mathrm{d}\nu/\mathrm{d}\pi \in L^q(\pi)$*, where* $q > 0$ *satisfies*

$p^{-1}+q^{-1}=1$. *Then, for any* $f\in L^p(\pi)$ *and any* $n\in\mathbb{N}$,

$$\mathbb{E}_\nu[|S_nf-\pi(f)|]\le \frac{C_pM_q\|f\|_{L^p(\pi)}}{n^{1-1/p}},$$

where $C_p=2^{2/p-1}\cdot(4s)^{1-1/p}$ *and* $M_q=\|\mathrm{d}\nu/\mathrm{d}\pi\|_{L^q(\pi)}$.

Remark 2.2. We note that Theorem 2.1 is still true, with the same bound, if we replace S_nf by $S_{n,n_0}f=1/n\sum_{j=1}^n f(X_{j+n_0})$, which corresponds to using a *burn in* of length $n_0\in\mathbb{N}$.

Remark 2.3. Let $p\in(1,2]$, $q\in[1,\infty)$ with $p^{-1}+q^{-1}=1$, and C_p, M_q as specified in Theorem 2.1. Given $c\in\mathbb{R}$ and $f\in L^p(\pi)$, we set $f_c=f+c$, and note that $S_nf_c-\pi(f_c)=S_nf-\pi(f)$. Thus, for fixed $f\in L^p(\pi)$ and any $c\in\mathbb{R}$ we have

$$\mathbb{E}_\nu[|S_nf_c-\pi(f_c)|]=\mathbb{E}_\nu[|S_nf-\pi(f)|]\le \frac{C_pM_q\|f\|_{L^p(\pi)}}{n^{1-1/p}},$$

even though $\|\cdot\|_{L^p(\pi)}$ is not invariant with respect to linear shifts.

Remark 2.4. In Theorem 2.1 the quantity $\|\mathrm{d}\nu/\mathrm{d}\pi\|_{L^q(\pi)}$ appears. In some sense this penalises our choice of the initial distribution ν, which is allowed to differ from the target π. In the setting where a fixed computational budget is available it may be worth spending some effort to find a 'good' initial distribution ν. However, discussing optimal choices of ν with respect to different theoretical and/or practical aspects is beyond the scope of this note.

3. Proofs

In this section we prove our main results. Recall that the chain $(X_n)_{n\in\mathbb{N}}$ is defined on the probability space $(\Omega,\mathcal{F},\mathbb{P}_\nu)$. For $p\in[1,\infty]$ we define $L^p(\mathbb{P}_\nu)$ as the set of random variables Y on $(\Omega,\mathcal{F},\mathbb{P}_\nu)$ such that $\|Y\|^p_{L^p(\mathbb{P}_\nu)}=\mathbb{E}_\nu[|Y|^p]<\infty$. As for the $L^p(\pi)$ spaces, we consider two random variables $Y_1, Y_2\in L^p(\mathbb{P}_\nu)$ as equal if $Y_1=Y_2$ holds $\mathbb{P}_\nu$-almost surely. Then, $(L^p(\mathbb{P}_\nu), \|\cdot\|_{L^p(\mathbb{P}_\nu)})$ is a normed space.

The first result of this section provides a bound for the mean squared error of S_nh for the case where $(X_n)_{n\in\mathbb{N}}$ is stationary, i.e. where $X_1\sim\pi$, and h is a centred function.

Lemma 3.1. *Let Assumption 2.1 be true and assume that* $(X_n)_{n\in\mathbb{N}}$ *has initial distribution* π, *i.e.* $X_1\sim\pi$. *Then, for any* $h\in L_0^2(\pi)$ *and any* $n\in\mathbb{N}$, $\mathbb{E}_\pi[|S_nh|^2]\le(4s/n)\|h\|^2_{L^2(\pi)}$.

Proof. Expanding $\mathbb{E}_\pi[|S_nh|^2]$ and using [17, Lemma 3.25], we get

$$\mathbb{E}_\pi[|S_nh|^2]=\frac{1}{n^2}\sum_{j=1}^n\sum_{k=1}^n\mathbb{E}_\pi[h(X_j)h(X_k)]=\frac{1}{n^2}\sum_{j=1}^n\sum_{k=1}^n\langle h, K^{|j-k|}h\rangle_{L^2(\pi)}.$$

We have that $\sum_{j=1}^n\sum_{k=1}^n K^{|j-k|}=2\sum_{\ell=1}^{n-1}(n-\ell)K^\ell+n\mathrm{Id}=2\sum_{\ell=0}^{n-1}(n-\ell)K^\ell-n\mathrm{Id}$. Moreover, by induction it follows that $\sum_{\ell=0}^{n-1}(n-\ell)K^\ell=(\mathrm{Id}-K)^{-1}\sum_{m=1}^n(\mathrm{Id}-K^m)$, where all the operators are understood to act on $L_0^2(\pi)$.

Hence, again considering all operators to act on $L_0^2(\pi)$, the following identity holds:

$$\begin{aligned}\sum_{j=1}^{n}\sum_{k=1}^{n} K^{|j-k|} &= 2(\mathrm{Id}-K)^{-1}\sum_{m=1}^{n}(\mathrm{Id}-K^m) - n\mathrm{Id}\\ &= 2n(\mathrm{Id}-K)^{-1} - 2(\mathrm{Id}-K)^{-1}\sum_{m=1}^{n} K^m - n\mathrm{Id}\\ &= n(\mathrm{Id}-K)^{-1}(\mathrm{Id}+K) - 2(\mathrm{Id}-K)^{-1}\sum_{m=1}^{n} K^m. \end{aligned} \tag{3.1}$$

Set $R_n = n(\mathrm{Id}-K)^{-1}(\mathrm{Id}+K) - 2(\mathrm{Id}-K)^{-1}\sum_{m=1}^{n} K^m$. By the triangle inequality and the bounds $\|(\mathrm{Id}-K)^{-1}\|_{L_0^2(\pi)\to L_0^2(\pi)} \le s$ and $\|K^m\|_{L_0^2(\pi)\to L_0^2(\pi)} \le 1$, which are true for any $m \in \mathbb{N}$, we obtain $\|R_n\|_{L_0^2(\pi)\to L_0^2(\pi)} \le 2sn + 2sn = 4sn$. Since $\langle h, K^{|j-k|}h\rangle_{L^2(\pi)} = \langle h, K^{|j-k|}h\rangle_{L_0^2(\pi)}$ for any $j, k \in \{1, \dots, n\}$, it follows from (3.1) and the bound on $\|R_n\|_{L_0^2(\pi)\to L_0^2(\pi)}$ that

$$\mathbb{E}_\pi[|S_n h|^2] = \frac{1}{n^2}\langle h, R_n h\rangle_{L_0^2(\pi)} \le \frac{\|h\|_{L^2(\pi)}^2}{n^2}\|R_n\|_{L_0^2(\pi)\to L_0^2(\pi)} \le \frac{4s\|h\|_{L^2(\pi)}^2}{n},$$

which completes the proof. □

Proposition 3.1. *Let Assumption 2.1 be true, let $p \in [1, 2]$, and assume that $(X_n)_{n\in\mathbb{N}}$ has initial distribution π, i.e. $X_1 \sim \pi$. Then, for any $f \in L^p(\pi)$ and any $n \in \mathbb{N}$ we have*

$$\mathbb{E}_\pi[|S_n f - \pi(f)|^p] \le 2^{2-p}\left(\frac{4s}{n}\right)^{p-1}\|f\|_{L^p(\pi)}^p.$$

Proof. For any $g \in L^2(\pi)$ set $\bar{g} = g - \pi(g) \in L_0^2(\pi)$. Moreover, we set $T_n f = S_n f - \pi(f)$ for $f \in L^p(\pi)$ with $p \in [1, 2]$.

By Lemma 3.1 and the inequality $\|\bar{g}\|_{L^2(\pi)}^2 = \pi(g^2) - \pi(g)^2 \le \pi(g^2) = \|g\|_{L^2(\pi)}^2$, which is true for any $g \in L^2(\pi)$, we obtain

$$\mathbb{E}_\pi[|T_n g|^2] = \mathbb{E}_\pi[|S_n\bar{g}|^2] \le \frac{4s}{n}\|\bar{g}\|_{L^2(\pi)}^2 \le \frac{4s}{n}\|g\|_{L^2(\pi)}^2,$$

which implies that $\|T_n\|_{L^2(\pi)\to L^2(\mathbb{P}_\pi)} \le \sqrt{4s/n}$. Moreover, using the triangle inequality we see that $\|T_n\|_{L^1(\pi)\to L^1(\mathbb{P}_\pi)} \le 2$. Thus, by the Riesz–Thorin interpolation theorem, see [5, Theorem 1.3.4] in the setting $p_0 = q_0 = 1$, $p_1 = q_1 = 2$, and $\theta = 2 - 2/p$, we obtain that

$$\|T_n\|_{L^p(\pi)\to L^p(\mathbb{P}_\pi)} \le 2^{2/p-1}\left(\frac{4s}{n}\right)^{1-1/p},$$

which implies the result. □

Using a change of measure argument and Proposition 3.1 we are able to prove our main result. However, before we turn to the proof of Theorem 2.1 let us state another consequence of

Proposition 3.1. We note that the upcoming result generalises [17, Theorem 3.41] by providing a bound for the mean squared error of S_nf for $L^2(\pi)$ functions.

Corollary 3.1. *Let Assumption 2.1 be true, let $p \in [1, 2]$, and assume that $\nu \ll \pi$ with Radon–Nikodým derivative $\mathrm{d}\nu/\mathrm{d}\pi \in L^\infty(\pi)$. Then, for any $f \in L^p(\pi)$ and any $n \in \mathbb{N}$,*

$$\mathbb{E}_\nu[|S_nf - \pi(f)|^p] \le \frac{C_p M_\infty \|f\|^p_{L^p(\pi)}}{n^{p-1}},$$

where $C_p = 2^{2-p} \cdot (4s)^{p-1}$ and $M_\infty = \|\mathrm{d}\nu/\mathrm{d}\pi\|_{L^\infty(\pi)}$.

Proof. Since $\mathbb{P}_\nu$ and $\mathbb{P}_\pi$ only differ by the choice of the initial distribution of $(X_n)_{n\in\mathbb{N}}$, we have

$$\mathbb{E}_\nu[|S_nf - \pi(f)|^p] = \mathbb{E}_\pi\left[\frac{\mathrm{d}\nu}{\mathrm{d}\pi}(X_1)|S_nf - \pi(f)|^p\right] \le \left\|\frac{\mathrm{d}\nu}{\mathrm{d}\pi}\right\|_{L^\infty(\pi)} \mathbb{E}_\pi[|S_nf - \pi(f)|^p].$$

Hence, the result follows from Proposition 3.1. □

Finally, we turn to the proof of Theorem 2.1.

Proof of Theorem 2.1. By the same change of measure argument as before and Hoelder's inequality,

$$\mathbb{E}_\nu[|S_nf - \pi(f)|] = \mathbb{E}_\pi\left[\frac{\mathrm{d}\nu}{\mathrm{d}\pi}(X_1)|S_nf - \pi(f)|\right] \le \left\|\frac{\mathrm{d}\nu}{\mathrm{d}\pi}\right\|_{L^q(\pi)} \mathbb{E}_\pi[|S_nf - \pi(f)|^p]^{1/p}.$$

Now the desired result is a consequence of Proposition 3.1. □

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