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SPECTRAL ASYMPTOTICS FOR THE METROPOLIS ALGORITHM ON SINGULAR DOMAINS

BY LAURENT MICHEL

ABSTRACT. — We study the Metropolis algorithm on a bounded connected domain Ω of the Euclidean space with the proposal kernel localized at a small scale $h > 0$. We consider the case of a domain Ω that may have cusp singularities. For small values of the parameter h, we prove that the top of the spectrum of the Metropolis operator consists of eigenvalues of finite multiplicity, of which we compute an asymptotic as h goes to zero. As a consequence, we obtain an exponentially fast return to equilibrium in the total variation distance.

RÉSUMÉ (*Asymptotiques spectrales pour l'algorithme de Metropolis sur des domaines singuliers*). — On étudie l'algorithme de Metropolis sur un domaine borné connexe Ω de l'espace euclidien pour un noyau de proposition localisé à une petite échelle $h > 0$. Nous considérons le cas d'un domaine Ω qui peut avoir des singularités de type cusp. Pour des petites valeurs du paramètre h, nous prouvons que le haut du spectre de l'opérateur de Metropolis est constitué de valeurs propres de multiplicité finie, dont nous calculons une asymptotique lorsque h tend vers zéro. En conséquence, nous obtenons un retour à l'équilibre exponentiellement rapide en distance de variation totale.

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1. Introduction

Let Ω be a bounded connected open subset of $\mathbb{R}^d$ and let $\rho(x)$ be a positive measurable function on $\bar{\Omega}$ such that

$$\forall x \in \Omega,\ m \leq \rho(x) \leq M, \tag{1}$$

for some constants $m, M > 0$. We denote $\mu_\rho = \rho(x)dx$ the associated measure on Ω and we assume that $\mu_\rho(\Omega) = \int_\Omega \rho(x)dx = 1$. We consider the Metropolis algorithm associated to the density ρ defined as follows. For all $h \in]0,1]$, we define the distribution kernel

$$k_{h,\rho}(x,y) = h^{-d}\phi\left(\frac{x-y}{h}\right)\min\left(\frac{\rho(y)}{\rho(x)},1\right) \tag{2}$$

where $\phi(z) = \frac{1}{\mathscr{V}_d}\mathbb{1}_{B(0,1)}(z)$, $B(0,1)$ denotes the open unit ball in $\mathbb{R}^d$, and $\mathscr{V}_d$ is the volume of $B(0,1)$. The Metropolis kernel is then given by

$$t_{h,\rho}(x,dy) = m_{h,\rho}(x)\delta_{y=x} + k_{h,\rho}(x,y)dy, \tag{3}$$

where $m_{h,\rho}(x) = 1 - \int_\Omega k_{h,\rho}(x,y)dy$. The kernel $t_{h,\rho}(x,dy)$ is clearly a Markov kernel on the state space Ω, and the associated operator

$$T_{h,\rho}(u)(x) = m_{h,\rho}(x)u(x) + \int_\Omega k_{h,\rho}(x,y)u(y)dy \tag{4}$$

is a Markov operator. Throughout the paper, we sometimes omit the dependance of this operator with respect to ρ and write T_h instead of $T_{h,\rho}$ when there is no ambiguity. A straightforward computation shows that $T_{h,\rho}$ is self-adjoint on $L^2(\Omega,\rho(x)dx)$, which implies in particular that the measure μ_ρ is stationary for the kernel $t_{h,\rho}(x,dy)$. Since this kernel is also clearly aperiodically irreducible this implies that the iterated kernel $t^n_{h,\rho}(x,dy)$ converges to the measure μ_ρ as $n \to \infty$, which explains the use of this algorithm to sample the measure μ_ρ.

Introduced in [9] to compute thermodynamical functionals by the Monte-Carlo method, this algorithm has shown an impressive efficiency and is now used as a routine in many domains of science. From a theoretical point of view, the computation of the speed of convergence of the algorithm led to much work in the setting of discrete state spaces (see [2], [5] and references therein for an introduction to this topic). In [3], we obtained the first results on a continuous state space in the limit $h \to 0$. More precisely, given a bounded domain Ω of $\mathbb{R}^d$ with Lipschitz boundary, we proved that the operator T_h admits a spectral gap $g(h)$ of order h^2 and for smooth densities ρ, we computed the limit of $h^{-2}g(h)$. Eventually, we obtained some total variation estimates

$$\sup_{x\in\Omega} \|t^n_{h,\rho}(x,dy) - d\mu_\rho(y)\|_{TV} \leq Ce^{-ng(h)}, \tag{5}$$

for some constant $C > 0$ independent of h. In this approach, the fact that $\partial\Omega$ has Lipschitz regularity plays a fundamental role at several stages. In practice, there exists important examples where this assumption fails to be true. Consider, for example, the celebrated hard sphere model (N nonoverlapping spheres, of radius ϵ with centers in a fixed domain Ω of $\mathbb{R}^d$), for which the state space is

$$\mathcal{O}_{N,\epsilon} = \{X = (X_1, \dots, X_N) \in \Omega^N,\ \forall i \neq,\ |X_i - X_j|_{\mathbb{R}^d} > 2\epsilon\}.$$

When $N\epsilon$ is small, we proved in Prop 4.1 of [3] that $\mathcal{O}_{N,\epsilon}$ has a Lipschitz boundary. However, if $N\epsilon$ is not small, the physical model of low density of spheres $N\epsilon^d \ll 1$ is not Lipschitz, as observed in Remark 3 of [3]. A natural question is then to explore situations where the Lipschitz regularity assumption on $\partial\Omega$ fails to be true. In the present paper, we consider the case where $\partial\Omega$ may have cuspidal singularities. More precisely, we introduce the following assumption:

Assumption 1.1. — *There exist a finite collection of open subsets of* $\mathbb{R}^d$, $(\omega_i)_{i\in I_r\cup I_c}$ *such that* $\partial\Omega \subset (\bigcup_{i\in I_r\cup I_c} \omega_i)$ *and*

i) *for all* $i \in I_r$, $\partial\Omega \cap \omega_i$ *has Lipschitz regularity,*

ii) *for all* $i \in I_c$, *there exists a closed submanifold* S_i *of* $\mathbb{R}^d$ *with dimension* d_i'', *and there exist* $\alpha_i > 1, r_i > 0, \epsilon_i > 0$ *and a coordinate system* $(x_1, x', x'') \in \mathbb{R}^d = \mathbb{R} \times \mathbb{R}^{d_i'} \times \mathbb{R}^{d_i''}$, *such that*

$$\Omega \cap \omega_i = \{(x_1, x', x''), 0 < x_1 < \epsilon_i,\ |x'|_{d_i'} < x_1^{\alpha_i},\ |x''|_{d_i''} < r_i\}, \tag{6}$$

where $|\cdot|_k$ *stands for the Euclidean norm on* $\mathbb{R}^k$.

Throughout the paper we will denote

$$\gamma = \max_{i\in I_c} (\alpha_i - 1)d_i'. \tag{7}$$

In our main results, we need the cusp singularities to not be too sharp. We thus introduce the following

Assumption 1.2. — *The constant* γ *defined by* (7) *satisfies* $0 < \gamma < 2$.

Observe that as soon as I_c is nonempty (that is, there exists some cusps on the boundary), one has $\gamma > 0$. Under the above assumption, one has the following rough localization of the spectrum $\sigma(T_h)$ of T_h. The proof of this result will be given in the next section.

Proposition 1.3. — *Assume that Assumption 1.1 holds true. Then there exist* $\delta_1, \delta_2 > 0$ *and* $h_0 > 0$ *such that for all* $h \in]0, h_0]$, $\sigma(T_h) \subset [-1 + \delta_1 h^\gamma, 1]$, *and the essential spectrum satisfies* $\sigma_{ess}(T_h) \subset [-1 + \delta_1 h^\gamma, 1 - \delta_2 h^\gamma]$, *where* γ *is defined by* (7).

From the above result, it is clear that the spectrum of T_h in the interval $[1 - Ch^\gamma, 1]$ is made of eigenvalues of finite multiplicity. Our first main result will provide precise information on the spectrum of T_h in a box $[1 - Ch^2, 1]$