Convergence of the Wang-Landau algorithm

G. Fort[1], B. Jourdain[2], E. Kuhn[3], T Lelièvre[2,4] and G. Stoltz[2,4]

1: LTCI, CNRS & Telecom ParisTech, 46 rue Barrault, 75634 Paris Cedex 13, France

2: Université Paris Est, CERMICS, Ecole des Ponts ParisTech, 6 & 8 Av. Pascal, 77455 Marne-la-Vallée Cedex 2, France

3: INRA Unité MIA, Domaine de Vilvert, 78352 Jouy-en-Josas Cedex, France

4: Project-team MICMAC, INRIA Rocquencourt, Domaine de Voluceau, B.P. 105, 78153 Le Chesnay Cedex, France

September 27, 2013

Abstract

We analyze the convergence properties of the Wang-Landau algorithm. This sampling method belongs to the general class of adaptive importance sampling strategies which use the free energy along a chosen reaction coordinate as a bias. Such algorithms are very helpful to enhance the sampling properties of Markov Chain Monte Carlo algorithms, when the dynamics is metastable. We prove the convergence of the Wang-Landau algorithm and an associated central limit theorem.

1 Introduction

The Wang-Landau algorithm was originally proposed in the physics literature to efficiently sample the density of states of Ising-type systems [31, 32]. From a computational statistical point of view, it can be seen as some adaptive importance sampling strategy combined with a Metropolis algorithm: the instrumental distribution is updated at each iteration of the algorithm in order to have a sampling of the configuration space as uniform as possible along a given direction. There are numerous physical and biochemical works using this technique to overcome sampling problems such as the ones encountered in the computation of macroscopic properties around critical points and phase transitions. The original paper [32] is cited more than one thousand times, according to Web of Knowledge. The success of the technique motivated its use and study in the statistics literature, see [24, 25, 2, 16, 5] for instance for previous mathematical and numerical studies.

1.1 Free energy biasing techniques

The Wang-Landau algorithm belongs to the class of *free energy biasing techniques* [20] which have been introduced in computational statistical physics to efficiently sample thermodynamic ensembles and to compute free energy differences. These algorithms can be seen as *adaptive importance sampling techniques*, the biasing factor being adapted on-the-fly in order to flatten the target probability measure along a given direction. Let us explain this with more details.

Let π be a multimodal probability measure over a high-dimensional space $\mathsf{X} \subseteq \mathbb{R}^D$. Classical algorithms to sample π (such as a Metropolis-Hastings procedure with local proposal moves) typically converge very slowly to equilibrium since high probability regions are separated by low probability regions. Averages have to be taken over very long trajectories in order to visit all the modes of the target probability measure π. The idea of free energy biasing techniques is to *flatten the target probability along a well-chosen direction* through an importance sampling procedure in order to more easily sample π. More precisely, assume that we are given a measurable function $\mathcal{O}$ defined on X and with values in a low dimensional compact space, or in a discrete space. This function is sometimes called a reaction coordinate or an order parameter in the physics literature. Let us introduce $\mathcal{O} * \pi$ the image of the measure π by $\mathcal{O}$: for any test function φ on the image $\mathcal{O}(\mathsf{X})$ of X by $\mathcal{O}$, $\int_{\mathcal{O}(\mathsf{X})} \varphi(y) \mathcal{O} * \pi(dy) = \int_{\mathsf{X}} \varphi(\mathcal{O}(x)) \pi(dx)$. The free energy biased probability measure $\pi^\star$ is defined by the two following properties: *(i)* the image $\mathcal{O} * \pi^\star$ of $\pi^\star$ by $\mathcal{O}$ is the uniform measure on $\mathcal{O}(\mathsf{X})$ and *(ii)* for each $y \in \mathcal{O}(\mathsf{X})$, the conditional distributions of x given $\mathcal{O}(x) = y$ under $\pi(dx)$ and $\pi^\star(dx)$ coincide i.e. there exists a measurable function $h : \mathcal{O}(\mathsf{X}) \to \mathbb{R}_+$ such that $\pi^\star(dx) = h(\mathcal{O}(x))\pi(dx)$.

Let us give two prototypical examples. When $\mathcal{O} = \xi$ is a smooth function with values in a continuous space, for example $\xi : \mathsf{X} \to \mathbb{T}$ (where $\mathbb{T} = \mathbb{R}/\mathbb{Z}$ is the one-dimensional torus), we have

$$\pi^\star(dx) = (1/\rho) \circ \xi(x) \pi(dx) \;, \tag{1.1}$$

where the measure $\xi * \pi$ is assumed to admit the density $\rho : \mathbb{T} \to \mathbb{R}_+$ with respect to the Lebesgue measure on $\mathbb{T}$. In this case, $A(z) = -\ln \rho(z)$ can be interpreted as a free energy [22]. This explains the name "free energy biasing techniques". When $\mathcal{O} = I$ is a function with values in a discrete finite set (this will be the case considered in this paper), $I : \mathsf{X} \to \{1, \ldots, d\}$, we have

$$\pi^\star(dx) = \frac{1}{d} \sum_{i=1}^{d} \frac{\mathbb{1}_{I(x)=i}}{\theta_\star(i)} \pi(dx) \;, \tag{1.2}$$

where $\theta_\star(i) = \pi\left(\{x \in \mathsf{X}, \, I(x) = i\}\right) = I * \pi(i)$ for $i \in \{1, \ldots, d\}$.

The bottom line of free energy biasing techniques is that it should be easier to sample $\pi^\star$ than to sample π since, by construction, $\mathcal{O} * \pi^\star$ is the uniform probability measure. Then, sampling from π could be obtained by importance sampling from $\pi^\star$. The fact that $\pi^\star$ is indeed much easier to sample than π actually depends on the choice of $\mathcal{O}$. It is not an easy task to define and to design in practice a good choice for $\mathcal{O}$ and we do not discuss further these aspects here. This is related to the choice of a "good" reaction coordinate in the physics literature, which is a very debatable subject. We refer for example to [7] for such an analysis in the context of free energy biasing techniques used to sample posterior distributions in Bayesian statistics.

Of course, the difficulty is that in general, $\mathcal{O} * \pi$ is unknown (equivalently ρ in (1.1), or $\theta_\star$ in (1.2), are unknown) so that it is not possible to sample from $\pi^\star$. The idea is then *to approximate* $\mathcal{O} * \pi$ *on the fly* in order to, in the longtime limit, sample from $\pi^\star$. This is the adaptive feature of these algorithms: the importance sampling factor is computed as time goes, in order to penalize states (namely level sets of $\mathcal{O}$) which have already been visited. To approximate $\pi^\star$ at a given time, one could either use the occupation measure of the Markov chain up to the current time (this is typically what is done in practice in the molecular dynamics community) or one could use an approximation over many Markov chains running in parallel [20, 29]. Moreover, one could either think of approximating $\mathcal{O} * \pi$ (these are the so-called Adaptive Biasing Potential (ABP) techniques) or, in the case $\mathcal{O}$ is a continuous order parameter, approximating $A'(z)$ (these are the so-called Adaptive Biasing Force (ABF) techniques [8, 15]). This gives rise to many algorithms in the literature (see for instance the classification and references in [20]), which are more or less efficient and more or less difficult to analyze mathematically. We refer for example to [8, 15] for ABF techniques using the occupation measure, to [29, 17] for ABF techniques using many replicas in parallel, to [31] for ABP approaches using the occupation measure and to [3, 5] for ABP approaches using many replicas in parallel. Before discussing the efficiency and the mathematical analysis of these algorithms, let us emphasize that in many applications, computing the measure $\mathcal{O} * \pi$ (or equivalently the free energy) is actually the main goal [22].

Roughly speaking, from a practical point of view, most ABP approaches (like the Wang-Landau algorithm) are more involved to use since they typically require to introduce a vanishing adaption mechanism. Indeed, even if one starts with a very good approximation of $\mathcal{O} * \pi$, and thus with a probability measure very close to $\pi^\star$, the adaptive mechanism will introduce a non-zero biasing factor to penalize visited level sets of $\mathcal{O}$, as time goes. One crucial feature of ABP approaches is thus to penalize less and less (as time goes) the visited states, so that in the longtime limit, no adaption is performed anymore. The way this adaption mechanism is performed is made precise below in the Wang-Landau case. We would also like to mention that some ABP techniques without externally imposed vanishing adaption have been proposed, like the self-healing umbrella sampling [26, 9], but we do not discuss them here. ABF approaches do not require such a vanishing adaption mechanism since the approximation of $A'(z)$ is based on conditional measures given the value of $\mathcal{O}$, which are not affected by the biasing factor (since it only depends on $\mathcal{O}$). However, ABF techniques cannot be used for discrete order parameters.

In terms of mathematical analysis, approximations based on many replicas in parallel are typically easier to analyze, since they can be related (in the limit of infinitely many replicas) to mean field models for which powerful longtime convergence analysis techniques can be used. We refer for example to [21, 19] for such an analysis for an ABF technique. In [21] for example, it is shown that the method is efficient if for each $y \in \mathcal{O}(\mathsf{X})$, the conditional distribution of x given $\mathcal{O}(x) = y$ under $\pi(dx)$ has good mixing properties (namely large Logarithmic Sobolev Inequality constants). The convergence analysis and, more importantly, the study of the efficiency of free energy biased techniques for approximations based on the occupation measure are much more involved since correlations in time of the Markov process play a crucial role. The aim of this paper is to propose a convergence analysis for the Wang-Landau algorithm, which is an ABP approach.

We would like to stress that the convergence results are a necessary first step in the study of the Wang-Landau algorithm, but are by no means the end of the story. Indeed, the real practical interest of adaptive techniques are their improved convergence properties. Although this improvement is obvious to practitioners, it is mathematically more difficult to formalize. We refer to the companion paper [11] for a study of the efficiency of the algorithm on a very simple toy model. Further works to mathematically formalize the efficiency of the Wang-Landau algorithm are required.

1.2 Objectives and main results

In this paper, we consider the Wang-Landau algorithm applied to the case $\mathcal{O} = I$ with $I : \mathsf{X} \to \{1, \ldots, d\}$. It both computes a (penalty) sequence $\{\theta_n, n \geqslant 0\}$ approximating (in the longtime limit) the probability measure $I * \pi$ and samples draws $\{X_n, n \geqslant 0\}$ distributed (in the longtime limit) according to $\pi^\star$. The update of the penalty sequence follows a Stochastic

Approximation algorithm [30, 4] and is of the form

$$\theta_{n+1} = \theta_n + \gamma_{n+1} \mathcal{H}_n(X_{n+1}, \theta_n) \; .$$

Different strategies about the field $\mathcal{H}_n$ and the adaption schedule $\{\gamma_n, n \geqslant 1\}$ have been proposed in the literature. In the original paper [31], the authors came up with a stochastic adaption schedule hereafter called *flat histogram Wang-Landau*. In this procedure, the updating parameter γ_n remains constant up to the (random) time when the sampling along the chosen order parameter $\mathcal{O}$ is approximately uniform, the "amount of uniformity" being measured according to the current value of γ_n. Then γ_n is lowered and a new updating procedure of the weights starts with a constant stepsize. Another strategy consists in a deterministic update of the adaption sequence $\{\gamma_n, n \geqslant 1\}$.

Despite the Wang-Landau algorithm has been successfully applied for many problems of practical interest, there are many open questions about its longtime behavior and its efficiency. Such a longtime behavior study relies on the convergence of stochastic approximation algorithms with Markovian inputs [4, 1] combined with the convergence of adaptive Markov chain Monte Carlo samplers [12]; for both parts, the stability of the sequence $\{\theta_n, n \geqslant 0\}$ is a fundamental property. Stability here means that the sequence $\{\theta_n, n \geqslant 0\}$ remains in a compact subset of the probability measures on $\{1, \ldots, d\}$ with support equal to the support of $I * \pi$ (as explained in Section 3, this is related to a recurrence property).

The asymptotic behavior of the flat histogram Wang-Landau algorithm, when $\mathcal{H}_n$ is such that in some sense, θ_n counts the number of visits to the level sets of $\mathcal{O}$, has been considered in [2, 16]. One crucial step is to show that the time τ to reach the flat histogram criterium is finite with probability one. In [2], it is proved for a specific field $\mathcal{H}_n$, that τ is finite almost-surely, the sequence $\{\theta_n, n \geqslant 0\}$ is stable and converges almost-surely. A strong law of large numbers for the draws $\{X_n, n \geqslant 0\}$ is also established for a wide family of unbounded functions. In [16], the authors show that the precise form of $\mathcal{H}_n$ plays a role on the convergence of the flat histogram Wang-Landau algorithm (see Section 2.2 for more details).

In this paper, we consider the Wang-Landau algorithm with a deterministic adaption sequence $\{\gamma_n, n \geqslant 1\}$ (see again Section 2.2 for a precise definition of the algorithm). The aim of this article is to address both the convergence of $\{\theta_n, n \geqslant 0\}$ to $I * \pi$ and the convergence of $\{X_n, n \geqslant 0\}$ to $\pi^\star$. More precisely, we prove first that the sequence $\{\theta_n, n \geqslant 0\}$ is stable, which is a crucial point for applications: no *ad hoc* stabilization techniques (such as truncation at randomly varying bounds [6]) is required. We also prove the almost-sure convergence of $\{\theta_n, n \geqslant 0\}$ as well as a Central Limit Theorem. We then prove the ergodicity and a strong law of large numbers for the draws $\{X_n, n \geqslant 0\}$.

Concerning the convergence result, we would like to mention the previous work [25] where some results about the longtime analysis for Wang-Landau with deterministic adaption can be found. In this paper, the authors combine the Wang-Landau algorithm with a reprojection technique on a fixed compact subset of probability measures on $\{1, \ldots, d\}$ with support equal to the support of $I * \pi$ so that the sequence $\{\theta_n, n \geqslant 0\}$ is stable by definition; then, they prove the convergence of the sequence whenever the limiting point is in the interior of the reprojection subset. Therefore, our results extend the work in [25] by precisely analyzing the stability of the algorithm, by addressing the convergence of $\{\theta_n, n \geqslant 0\}$ under weaker assumptions and by proving additional asymptotic analysis.

The paper is organized as follows. We describe in Section 2 the algorithm we consider and compare it to previously proposed Wang-Landau type algorithms. We then study its asymptotic behavior in Section 3. We first prove in Section 3.2 a fundamental stability result. Then we deduce convergence properties relying on previous results on stochastic approximation with Markovian inputs and on the theory of adaptive Markov chain Monte Carlo samplers. The proofs of the results presented in Sections 3 are gathered in Section 4.

2 Description of the Wang-Landau algorithm

2.1 Notation and preliminaries

The system that we consider is described by a normalized target probability density π defined on a Polish space X, endowed with a reference measure λ defined on the Borel σ-algebra $\mathcal{X}$. Notice that, as for classical Metropolis-Hastings procedure, the practical implementation of the algorithm only requires to specify π up to a multiplicative constant. In statistical physics, X typically is the set of all admissible configurations of the system while π is a Gibbs measure with density $\pi(x) = Z_\beta^{-1} \exp(-\beta U(x))$, U being the potential energy function and β the inverse temperature. In condensed matter physics for instance, actual simulations are performed on systems composed of N particles in dimension 2 or 3, living in a cubic box with periodic boundary conditions. In this case, $\mathsf{X} = (L\mathbb{T})^{2N}$ or $\mathsf{X} = (L\mathbb{T})^{3N}$, where L is the length of the sides of the box and $\mathbb{T} = \mathbb{R}/\mathbb{Z}$ is the one-dimensional torus.

Consider now a partition $\mathsf{X}_1, \ldots, \mathsf{X}_d$ of X in $d \geqslant 2$ elements, and define, for any $i \in \{1, \ldots, d\}$,

$$\theta_\star(i) \stackrel{\text{def}}{=} \int_{\mathsf{X}_i} \pi(x)\lambda(dx) \; . \tag{2.1}$$

In the following, X_i will be called the i-th *stratum*. Each weight $\theta_\star(i)$, which is assumed to be positive, gives the relative likelihood of the stratum $\mathsf{X}_i \subset \mathsf{X}$. In practice, the partitioning could be obtained by considering some smooth function $\xi : \mathsf{X} \to [a, b]$ (called a reaction coordinate in the physics literature) and defining, for $i = 1, \ldots, d-1$,

$$\mathsf{X}_i = \xi^{-1}\Big([\alpha_{i-1}, \alpha_i)\Big) \; , \tag{2.2}$$

and $\mathsf{X}_d = \xi^{-1}([\alpha_{d-1}, \alpha_d])$, with $a = \alpha_0 < \alpha_1 < \ldots \alpha_d = b$ (possibly, $a = -\infty$ and/or $b = +\infty$). In the notation of the introduction, the order parameter is thus the discrete function $I : \mathsf{X} \to \{1, \ldots, d\}$ defined by

$$\forall x \in \mathsf{X}, \; I(x) = i \text{ if and only if } x \in \mathsf{X}_i \; . \tag{2.3}$$

As mentioned above, the choice of an appropriate function I is a difficult issue, and is mostly based on intuition at the time being: practitioners identify some slowly evolving degree of freedom responsible for the metastable behavior of the system (the fact that trajectories generated by the numerical method remain trapped for a long time in some region of the phase space, and only occasionally hop to another region, where they also remain trapped). There are however ways to quantify the relevance of the choice of the reaction coordinate, see for instance the discussion in [7].

The above discussion motivates the fact that the weights $\theta_\star(i)$ typically span several orders of magnitude, some sets X_i having very large weights, and other ones being very unlikely under π. Besides, trajectories bridging two very likely states may need to go through unlikely regions. To efficiently explore the configuration space, and sample numerous configurations in all the strata X_i, it is therefore a natural idea to resort to importance sampling strategies and reweight appropriately each subset X_i. A possible way to do so is the following. Let Θ be the subset of (non-degenerate) probability measures on $\{1, \dots, d\}$ given by

$$\Theta = \left\{ \theta = (\theta(1), \dots, \theta(d)) \;\middle|\; 0 < \theta(i) < 1 \text{ for all } i \in \{1, \dots, d\} \text{ and } \sum_{i=1}^d \theta(i) = 1 \right\} .$$

For any $\theta \in \Theta$, we define the probability density π_θ on $(\mathsf{X}, \mathcal{X})$ (endowed with the reference measure λ) as

$$\pi_\theta(x) = \left(\sum_{i=1}^d \frac{\theta_\star(i)}{\theta(i)} \right)^{-1} \sum_{i=1}^d \frac{\pi(x)}{\theta(i)} \mathbb{1}_{\mathsf{X}_i}(x) . \tag{2.4}$$

This measure is such that the weight of the set X_i under π_θ is proportional to $\theta_\star(i)/\theta(i)$. In particular, all the strata X_i have the same weight under $\pi_{\theta_\star}$. Unfortunately, $\theta_\star$ is unknown and sampling under $\pi_{\theta_\star}$ is typically unfeasible.

The Wang-Landau algorithm precisely is a way to overcome these difficulties: at each iteration of the algorithm, a weight vector $\theta_n = (\theta_n(1), \dots, \theta_n(d))$ is updated based on the past behavior of the algorithm and a point is drawn from a Markov kernel P_{θ_n} with invariant density π_{θ_n}. The intuition for the convergence of this algorithm is that if $\{\theta_n, n \geqslant 0\}$ converges to $\theta_\star$ then the draws are asymptotically distributed according to the density $\pi_{\theta_\star}$. Conversely, if the draws are under $\pi_{\theta_\star}$, then the update of $\{\theta_n, n \geqslant 0\}$ is chosen such that it converges to $\theta_\star$. We will derive below sufficient conditions on the sequence $\{\gamma_n, n \geqslant 1\}$ of step-sizes used to update $\{\theta_n, n \geqslant 0\}$ and on the Markov kernels $\{P_\theta, \theta \in \Theta\}$ in order to prove the convergence of a version of the Wang-Landau algorithm, namely a linearized Wang-Landau algorithm with a deterministic adaption where the step-size γ_n is used at the n-th iteration of the Markov chain.

2.2 The linearized Wang-Landau algorithm with deterministic adaption

We now describe the algorithm we study in this article. Let $\{\gamma_n, n \geqslant 1\}$ be a $[0, 1)$-valued deterministic sequence. For any $\theta \in \Theta$, denote by P_θ a Markov transition kernel onto $(\mathsf{X}, \mathcal{X})$ with unique stationary distribution $\pi_\theta(x)\lambda(dx)$; for example, P_θ is one step of a Metropolis-Hastings algorithm [27, 14] with target probability measure $\pi_\theta(x)\lambda(dx)$.

Consider an initial value $X_0 \in \mathsf{X}$ and an initial set of weights $\theta_0 \in \Theta$ (typically, in absence of any prior information, $\theta_0(i) = 1/d$). Define the process $\{(X_n, \theta_n), n \geqslant 0\}$ as follows: given the current value (X_n, θ_n),

(1) Draw X_{n+1} under the conditional distribution $P_{\theta_n}(X_n, \cdot)$;

(2) Set $i = I(X_{n+1})$ where I is given by (2.3). The weights are then updated as

$$\begin{cases} \theta_{n+1}(i) = \theta_n(i) + \gamma_{n+1}\, \theta_n(i)\, (1 - \theta_n(i)) \,, & \\ \theta_{n+1}(k) = \theta_n(k) - \gamma_{n+1}\, \theta_n(k)\, \theta_n(i) & \text{for } k \neq i. \end{cases} \tag{2.5}$$

Note that since $\gamma_n \in [0, 1)$, $\theta_n \in \Theta$ for any $n \geqslant 0$. As explained in the introduction, the idea of the updating strategy (2.5) is that the weights of the visited stratas are increased, in order to penalize already visited states. The update of the probability vector θ_n can be recast equivalently into the stochastic approximation framework upon writing

$$\theta_{n+1} = \theta_n + \gamma_{n+1} H(X_{n+1}, \theta_n) \,, \tag{2.6}$$

where $H : \mathsf{X} \times \Theta \to [-1,1]^d$ is defined componentwise by

$$H_i(x,\theta) = \theta(i) \left(\mathbb{1}_{\mathsf{X}_i}(x) - \theta(I(x)) \right) , \tag{2.7}$$

with the function I given by (2.3).

The updating strategy (2.5) (or equivalently (2.6)) is a modification of the original Wang-Landau algorithm obtained by (i) using a deterministic schedule for the evolution of the step-sizes used to modify the values of the weights (instead of reducing the value of these step-sizes at random times when the empirical frequencies of the strata are sufficiently uniform: this is the flat histogram version of the Wang-Landau algorithm mentioned in the introduction) and (ii) linearizing at first order in γ_n the update of the weight θ_n.

Concerning this second point, the standard Wang-Landau update is

$$\theta_{n+1}(i) = \theta_n(i) \frac{1 + \gamma_{n+1} \mathbb{1}_{\mathsf{X}_i}(X_{n+1})}{1 + \gamma_{n+1}\theta_n(I(X_{n+1}))} . \tag{2.8}$$

The update (2.5) is obtained from (2.8) in the limit of small γ_n. For the stability and the convergence analysis in Section 3, we adopt this linear update. The main advantage is that it makes the proof of convergence simpler: with the standard Wang-Landau update, an additional remainder term would have to be considered in Proposition 4.10. Nevertheless, since γ_n converges to zero, the stability and convergence results stated in Section 3 could be proved using similar arguments for the standard Wang-Landau update (see Section 4.2.4 below concerning the stability).

By contrast, we would like to emphasize here that this distinction between the two updating strategies (2.5) and (2.8) *does matter* when considering the flat histogram criterium for the vanishing adaption procedure, as proved in [16]. Indeed it is shown in [16] that the linearized version of the update (2.5) allows to satisfy in finite time the uniformity criterion required in the original Wang-Landau algorithm, whereas this is not guaranteed for the nonlinear update (2.8).

3 Convergence of the Wang-Landau algorithm

The proof of the convergence of the Wang-Landau algorithm described in Section 2.2 relies on its reformulation (2.6) as a stochastic approximation procedure. Since the draws $\{X_n, n \geqslant 1\}$ satisfy for any measurable non-negative function f:

$$\mathbb{E}\left[f(X_{n+1}) | \mathcal{F}_n\right] = P_{\theta_n} f(X_n) , \tag{3.1}$$

where $\mathcal{F}_n$ denotes the σ-field $\sigma(\theta_0, X_0, X_1, \ldots, X_n)$, it is a so-called "stochastic approximation procedure with Markovian dynamics" (see *e.g.* [4]).

The main difficulty, when proving the almost-sure convergence of such algorithms, is the stability, namely how to ensure that the sequence $\{\theta_n, n \geqslant 0\}$ remains in a compact subset of Θ. We use a traditional approach to answer this question: we first prove that our algorithm satisfies a recurrence property *i.e.* the sequence $\{\theta_n, n \geqslant 0\}$ visits infinitely often a compact subset of Θ; we then show that there exists a Lyapunov function with respect to the *mean-field* function $h : \Theta \to [-1,1]^d$

$$h(\theta) = \int_{\mathsf{X}} H(x,\theta)\, \pi_\theta(x)\, \lambda(dx) = \left(\sum_{j=1}^{d} \frac{\theta_\star(j)}{\theta(j)} \right)^{-1} (\theta_\star - \theta) , \tag{3.2}$$

with strong enough properties so that the recurrence property implies stability. Different strategies based on truncations are proposed in the literature to circumvent the stability problem (see *e.g.* [18]). The most popular technique is the truncation to a fixed compact set but this is not a satisfactory solution since the choice of this compact is delicate: a necessary condition for convergence is that the compact contains the unknown desired limit. An adaptive truncation has been proposed by [6] (and analyzed for example in [1, 23]) which avoids the main drawbacks of the deterministic truncation approach. We prove in Section 3.2 that, under conditions on the target density π and the step-size sequence $\{\gamma_n, n \geqslant 1\}$, the algorithm (2.6) is recurrent, so that such truncation techniques are not required.

In Section 3.3, we address the almost-sure convergence of the weight sequence $\{\theta_n, n \geqslant 0\}$. We then obtain in Section 3.4 the convergence in distribution and a strong Law of large numbers for the samples $\{X_n, n \geqslant 0\}$. Finally, we obtain a central limit theorem in Section 3.5 for the weight sequence $\{\theta_n, n \geqslant 0\}$.

3.1 Assumptions on the Metropolis dynamics and on the adaption rate

Our conditions fall into three categories: conditions on the equilibrium measure (see A1), on the transition kernels $\{P_\theta, \theta \in \Theta\}$ (see A2) and conditions on the step-size sequence $\{\gamma_n, n \geqslant 1\}$ (see A3). It is assumed that

A1 The probability density π with respect to the measure λ is such that $0 < \inf_{\mathsf{X}} \pi \leqslant \sup_{\mathsf{X}} \pi < \infty$. In addition, $\inf_{1 \leqslant i \leqslant d} \theta_\star(i) > 0$ where $\theta_\star$ is given by (2.1).

The first part of Assumption A1 is satisfied, for example, for smooth positive densities on a compact state space $\mathsf{X} \subset \mathbb{R}^D$ with the Lebesgue measure as the reference measure λ, or for a positive probability measure on a discrete finite state space $\mathsf{X} = \{1, \dots, K\}$ with the uniform measure as the reference measure. Since $\inf_{\mathsf{X}} \pi$ is assumed to be positive, the second part of the assumption is satisfied as soon as $\inf_{1 \leqslant i \leqslant d} \lambda(\mathsf{X}_i) > 0$. The minorization condition on π certainly is the most restrictive assumption: it is introduced in order to prove the recurrence of the algorithm (2.6). This condition can be removed by adding a stabilization step to (2.6) (such as a truncation technique at random varying bounds [6, 18]) in order to ensure the recurrence.

The second assumption is:

A2 For any $\theta \in \Theta$, P_θ is a Metropolis-Hastings transition kernel with invariant distribution $\pi_\theta \; d\lambda$, where π_θ is given by (2.4), and with symmetric proposal kernel $q(x, y)\lambda(dy)$ satisfying $\inf_{\mathsf{X}^2} q > 0$.

The transition probability for a symmetric Metropolis-Hastings dynamics reads

$$P_\theta(x, dy) = q(x, y)\alpha_\theta(x, y)\, \lambda(dy) + \delta_x(dy) \left(1 - \int_{\mathsf{X}} q(x, z)\alpha_\theta(x, z)\, \lambda(dz)\right) ,$$

with

$$\alpha_\theta(x, y) = 1 \wedge \frac{\pi_\theta(y)q(y, x)}{\pi_\theta(x)q(x, y)} = 1 \wedge \frac{\pi_\theta(y)}{\pi_\theta(x)} ,$$

the last equality being a consequence of the symmetry of q. Assumption A2 is satisfied for instance when $\mathsf{X} = \mathbb{T}^n$ (a cubic simulation cell endowed with periodic boundary conditions), and $q(x, y) = \widetilde{q}(y - x)$ for a positive and even density $\widetilde{q}$ such that $\inf_{\mathsf{X}} \widetilde{q} > 0$.

The minorization condition on q implies that the transition kernels $\{P_\theta, \theta \in \Theta\}$ are uniformly (geometrically) ergodic, as stated in Proposition 3.1 below. This property allows a simple presentation of the main ingredients for the limiting behavior analysis of the algorithm. Extensions to a more general case could be done by using the same tools as in [12] (see also [1, Section 3]) and controlling the dependence upon θ of the ergodic behavior. These technical steps are out of the scope of this paper.

We prove in Section 4.1 the following result:

Proposition 3.1. *Under A1 and A2, there exists $\rho \in (0,1)$ such that for all $\theta \in \Theta$, for all $x \in \mathsf{X}$ and for all $A \in \mathcal{X}$, it holds:*

$$P_\theta(x, A) \geqslant \rho \int_A \pi_\theta(x)\, \lambda(dx) \ , \tag{3.3}$$

$$\sup_{\theta \in \Theta} \sup_{x \in \mathsf{X}} \| P_\theta^n(x, \cdot) - \pi_\theta \, d\lambda \|_{\mathrm{TV}} \leqslant 2(1-\rho)^n, \tag{3.4}$$

where for a signed measure μ, the total variation norm is defined as

$$\|\mu\|_{\mathrm{TV}} = \sup_{\{f \,:\, \sup_{\mathsf{X}} |f| \leqslant 1\}} |\mu(f)| \ .$$

We finally introduce conditions on the magnitude of the step-size sequence.

A3 The sequence $\{\gamma_n, n \geqslant 1\}$ is a $[0,1)$-valued deterministic sequence such that

a) $\{\gamma_n, n \geqslant 1\}$ is a non-increasing sequence and $\lim_n \gamma_n = 0$;

b) $\sum_n \gamma_n = \infty$;

c) $\sum_n \gamma_n^2 < \infty$.

For ease of exposition, it is assumed in A3 that the sequence is non-increasing and with values strictly smaller than 1. These hypotheses can be weakened by assuming that they are only satisfied ultimately: for some constant n_0, the sequence $\{\gamma_n,\, n \geq n_0\}$ is non-increasing and with values strictly smaller than 1, and $\gamma_n \leq 1$ for $n < n_0$. Examples of step-size sequence satisfying assumption A3 are the polynomial schedules $\gamma_n = \gamma_\star / n^\alpha$ with $1/2 < \alpha \leqslant 1$. As already observed in Section 2.2, the condition $\gamma_n \in [0,1)$ implies that if $\theta_0 \in \Theta$, then for any $n \geqslant 1$, $\theta_n \in \Theta$. Assumption A3a is introduced for the proof of the recurrence property. Assumptions A3b-c are standard conditions for the stability and the convergence of a stochastic approximation scheme since the pioneering work [30].

3.2 Recurrence property of the weight sequence $\{\theta_n, n \geqslant 0\}$

We state in this section that, almost surely, there exists a compact subset of Θ such that θ_n belongs to this compact subset for infinitely many n. For any $n \geq 0$, set

$$\underline{\theta}_n = \min_{1 \leqslant j \leqslant d} \theta_n(j) \ . \tag{3.5}$$

We prove in Section 4.2 the following theorem:

Theorem 3.2. *Assume A1, A2 and A3a. Then,* $\mathbb{P}\left(\limsup_{n \to \infty} \underline{\theta}_n > 0 \right) = 1.$

The proof is based on the following consideration. The value of the smallest weight increases when the chain goes into the corresponding stratum (see the updating formula (2.5)). Under the stated assumptions, we prove that the chain $\{X_n, n \geqslant 0\}$ returns in the strata of smallest weights often enough for the smallest weight to remain isolated from 0.

3.3 Convergence of the weight sequence $\{\theta_n, n \geqslant 0\}$

In this subsection, the almost-sure convergence of the sequence $\{\theta_n, n \geqslant 0\}$ to $\theta_\star$ is addressed. We prove in Section 4.3 the following convergence result:

Theorem 3.3. *Assume A1, A2 and A3. Then,* $\mathbb{P}\left(\lim_{n\to\infty} \theta_n = \theta_\star\right) = 1$.

The proof relies on [1] which provides sufficient conditions for convergence of stochastic approximation techniques. The first step consists in rewriting the weight update (2.6) as

$$\theta_{n+1} = \theta_n + \gamma_{n+1} h(\theta_n) + \gamma_{n+1}\Big(H(X_{n+1}, \theta_n) - h(\theta_n)\Big) , \tag{3.6}$$

where h is given by (3.2). The heuristic idea is that, if the step-size quickly is sufficiently small, and the Metropolis dynamics converges sufficiently fast to equilibrium for θ fixed (a result given by Proposition 3.1), the update of θ_n is indeed close to an update with the averaged drift $h(\theta_n)$. However, in order for the updates of the weights to be non-negligible, the step-sizes should not be too small. The balance between these two opposite effects is encoded in the conditions A3b-c.

From a technical viewpoint, the proof of the theorem relies on two main tools. The first one (see Proposition 4.5) is to show that the function $V : \Theta \to \mathbb{R}_+$ given by

$$V(\theta) \stackrel{\text{def}}{=} \sum_{i=1}^{d} \theta_\star(i) \log\left(\frac{\theta_\star(i)}{\theta(i)}\right) \tag{3.7}$$

is a Lyapunov function with respect to the mean-field h, namely $\langle \nabla V(\theta), h(\theta)\rangle < 0$ for $\theta \neq \theta_\star$ and $\langle \nabla V(\theta_\star), h(\theta_\star)\rangle = 0$ (here, $\langle \cdot, \cdot \rangle$ denotes the scalar product in $\mathbb{R}^d$). This motivates the fact that $\{\theta_n, n \geqslant 0\}$ may converge to $\theta_\star$. The second important result establishes that the remainder term $\gamma_{n+1}\left(H(X_{n+1}, \theta_n) - h(\theta_n)\right)$ in (3.6) vanishes in some sense (see Proposition 4.10). This step is quite technical and requires regularity-in-θ of the transition kernels P_θ and the invariant distributions π_θ (see Lemmas 4.6 and 4.7). The conclusion then follows from [1, Theorem 2.3] and Theorem 3.2.

3.4 Ergodicity and Law of large numbers for the samples $\{X_k, k \geqslant 0\}$

In this subsection, we discuss the asymptotic behavior of the chain $\{X_k, k \geqslant 0\}$. The main result is the following (see Section 4.4 for the proof).

Theorem 3.4. *Assume A1, A2 and A3. Then, for any bounded measurable function f,*

$$\lim_{n\to\infty} \mathbb{E}\left[f(X_n)\right] = \int_{\mathsf{X}} f(x)\, \pi_{\theta_\star}(x)\, \lambda(dx) , \tag{3.8}$$

$$\frac{1}{n}\sum_{k=1}^{n} f(X_k) \xrightarrow{\text{a.s.}} \int_{\mathsf{X}} f(x)\, \pi_{\theta_\star}(x)\, \lambda(dx) . \tag{3.9}$$

This theorem shows that the distribution of the sample X_n converges to $\pi_{\theta_\star}(x)\lambda(dx)$, where, we recall

$$\pi_{\theta_\star}(x) = \frac{1}{d}\sum_{i=1}^{d} \frac{\pi(x)}{\theta_\star(i)} \mathbb{1}_{\mathsf{X}_i}(x) .$$

Moreover, the empirical mean of the samples $\{f(X_k), k \geqslant 0\}$ converges to $\int f \, \pi_{\theta_\star} \, d\lambda$. Hence, although the weights θ_n evolve in the adaptive algorithm, ergodic averages can be thought of as averages with fixed weights $\theta_\star$.

In many practical cases, averages with respect to π are of interest. In this case, the Wang-Landau procedure is used as some adaptive importance sampling strategy. In order to obtain averages according to π along a trajectory of the algorithm, some reweighting has to be considered. A natural strategy is to use some stratified-type weighted sum of the samples $\{X_k, \, k \geqslant 1\}$:

$$\mathcal{I}_n(f) \stackrel{\text{def}}{=} d \sum_{i=1}^{d} \theta_n(i) \left(\frac{1}{n} \sum_{k=1}^{n} f(X_k) \mathbb{1}_{\mathsf{X}_i}(X_k) \right) .$$

We prove in Section 4.5 the following result:

Theorem 3.5. *Assume A1, A2 and A3. Then for any bounded measurable function f,*

$$\lim_{n \to \infty} d \, \mathbb{E} \left[\sum_{i=1}^{d} \theta_n(i) \, f(X_n) \, \mathbb{1}_{\mathsf{X}_i}(X_n) \right] = \int_{\mathsf{X}} f(x) \, \pi(x) \, \lambda(dx) \, , \tag{3.10}$$

$$\mathcal{I}_n(f) \xrightarrow{\text{a.s.}} \int_{\mathsf{X}} f(x) \, \pi(x) \, \lambda(dx) \, . \tag{3.11}$$

There are of course many other reweighting strategies. We have discussed one possible choice, but we do not claim that the above estimator is the best one.

3.5 Central limit theorem for the weight sequence

In this section, we state a Central Limit Theorem on the error $\theta_n - \theta_\star$. We show that the rate of convergence depends upon the step-size sequence $\{\gamma_n, n \geqslant 1\}$ and discuss an averaging strategy in order to reach the optimal rate of convergence. An additional assumption is required on the sequence $\{\gamma_n, n \geqslant 1\}$:

A4 $\lim_n \gamma_n \sqrt{n} = 0$, and one of the following condition holds:

- (i) $\log(\gamma_n / \gamma_{n+1}) = \mathrm{o}(\gamma_n)$;
- (ii) $\log(\gamma_n / \gamma_{n+1}) \sim \gamma_n / \gamma_\star$ with $\gamma_\star > d/2$.

The latter conditions are satisfied for sequences $\gamma_n = \gamma_\star / n^\alpha$, when $\alpha \in (1/2, 1)$ for (i), or when $\alpha = 1$ and $\gamma_\star > d/2$ for (ii). Under this additional assumption, the following result holds (see Section 4.6 for the proof).

Theorem 3.6. *Assume that A1, A2, A3 and A4 hold. Then $\{\gamma_n^{-1/2} \left(\theta_n - \theta_\star\right), n \geqslant 1\}$ converges in distribution to a centered Gaussian distribution with variance-covariance matrix $\sigma^2 U_\star$ where $\sigma^2 = d/2$ in case A4*(i) *and $\sigma^2 = \gamma_\star d / (2\gamma_\star - d)$ in case A4*(ii)*,*

$$U_\star \stackrel{\text{def}}{=} \int_{\mathsf{X}} \left\{ \widehat{H}_{\theta_\star}(x) \widehat{H}_{\theta_\star}^T(x) - P_{\theta_\star} \widehat{H}_{\theta_\star}(x) \; P_{\theta_\star} \widehat{H}_{\theta_\star}^T(x) \right\} \pi_{\theta_\star}(x) \, \lambda(dx) \, , \tag{3.12}$$

and

$$\widehat{H}_{\theta_\star} \stackrel{\text{def}}{=} \sum_{n \geqslant 0} P_{\theta_\star}^n \left(I - \pi_{\theta_\star}\right) H(\cdot, \theta_\star) = \sum_{n \geqslant 0} P_{\theta_\star}^n \left(H(\cdot, \theta_\star) - h(\theta_\star)\right) \, .$$

Notice that $\widehat{H}_{\theta_\star}$ is the Poisson solution associated to the pair $(P_{\theta_\star}, H(\cdot, \theta_\star))$, namely $\widehat{H}_{\theta_\star}$ is a solution to: find $g : \mathsf{X} \to \mathbb{R}$ such that

$$g - P_{\theta_\star} g = H(\cdot, \theta_\star) - \int_{\mathsf{X}} H(x, \theta_\star)\, \pi_{\theta_\star}(x)\, \lambda(dx) \; .$$

By Proposition 3.1 and the results of [28, Chapter 17], such a function exists and is unique up to an additive constant.

Theorem 3.6 shows that the rate of convergence depends upon the step-size sequence $\{\gamma_n, n \geqslant 1\}$: when $\gamma_n = \gamma_\star/n^\alpha$ for $\alpha \in (1/2, 1]$, the maximal rate of convergence is reached with $\alpha = 1$ and the rate is $\mathrm{O}(n^{-1/2})$.

When $\gamma_n = \gamma_\star/n$, Theorem 3.6 states that $\{\sqrt{n}\,(\theta_n - \theta_\star)\,,\, n \geqslant 1\}$ converges in distribution to a centered Gaussian distribution with variance-covariance matrix $dU_\star \gamma_\star^2/(2\gamma_\star - d)$, which is minimum for $\gamma_\star = d$ (in which case the variance-covariance matrix is $d^2 U_\star$). It is actually not possible to further reduce the asymptotic variance by introducing a gain matrix Γ in the algorithm (2.6) which yields the update

$$\check{\theta}_{n+1} = \check{\theta}_n + \gamma_{n+1} \Gamma \; H(X_{n+1}, \check{\theta}_n) \; .$$

It is proved in [4, Proposition 4 p.112] that for a large family of gain matrices (so-called "admissible gains") a Central Limit Theorem still holds for the sequence of random variables $\{\sqrt{n}(\theta_n - \theta_\star), n \geqslant 0\}$ and the minimal variance-covariance matrix $d^2 U_\star$ is indeed reached for $\Gamma = d\gamma_\star^{-1}\mathrm{Id}$.

From a practical point of view, it is known that stochastic approximation algorithms are more efficient when the step-size sequence decreases at a slow rate: in the polynomial schedule, this means that $\gamma_n = \gamma_\star/n^\alpha$ with α close to $1/2$. As shown by Theorem 3.6, this yields a slower rate of convergence. Nevertheless, combining Wang-Landau update with an *averaging technique* allows to reach the optimal rate of convergence and the optimal variance-covariance matrix: by applying [10, Theorem 1.4], it can be proved that $\{\sqrt{n}\left(\frac{1}{n}\sum_{k=1}^n \theta_k - \theta_\star\right), n \geqslant 1\}$ converges in distribution to a centered Gaussian distribution with variance-covariance matrix $d^2 U_\star$. The proof of this claim is along the same lines as the proof of Theorem 3.6 and details are therefore omitted.

4 Proofs

In the following, we denote by $\lfloor x \rfloor$ the integer part of $x \in \mathbb{R}$ namely the integer such that $\lfloor x \rfloor \leq x < \lfloor x \rfloor + 1$. We will also use the notation $\lceil x \rceil$ for the integer such that $\lceil x \rceil - 1 < x \leq \lceil x \rceil$.

4.1 Proof of Proposition 3.1

We prove (3.3); the second assertion follows by [28, Theorem 16.2.4]. Since q is symmetric, it holds by definition of the Metropolis kernel that

$$P_\theta(x, A) \geqslant \int_A q(x,y) \left(1 \wedge \frac{\pi_\theta(y)}{\pi_\theta(x)}\right) \lambda(dy) \geqslant \frac{\inf_{\mathsf{X}^2} q}{\sup_{\mathsf{X}} \pi_\theta} \int_A \pi_\theta(y)\, \lambda(dy) \; .$$

Under A2, $\inf_{\mathsf{X}} q > 0$. Furthermore, since $\theta(i) > 0$ and $\theta_\star(i) > 0$ for any $i \in \{1, \dots, d\}$,

$$\sup_{\mathsf{X}} \pi_\theta = \left(\sum_{k=1}^d \frac{\theta_\star(k)}{\theta(k)}\right)^{-1} \sup_{\mathsf{X}} \left(\sum_{i=1}^d \frac{\pi}{\theta(i)} \mathbb{1}_{\mathsf{X}_i}\right) \leqslant \sup_{\mathsf{X}} \sum_{i=1}^d \frac{\frac{\pi}{\theta(i)} \mathbb{1}_{\mathsf{X}_i}}{\frac{\theta_\star(i)}{\theta(i)}} \leqslant \frac{\sup_{\mathsf{X}} \pi}{\min_{i \in \{1,\dots,d\}} \theta_\star(i)} \; .$$

The right-hand side is finite by A1 and does not depend upon θ. Therefore, (3.3) holds with $\rho \stackrel{\text{def}}{=} (\inf_{\mathsf{X}^2} q)\,(\sup_{\mathsf{X}} \pi)^{-1} \min_{1\leqslant i\leqslant d} \theta_\star(i)$.

4.2 Proof of Theorem 3.2

Define the smallest index of stratum with smallest weight according to θ_n *i.e.*

$$I_n \stackrel{\text{def}}{=} \min\{i \,:\, \theta_n(i) = \underline{\theta}_n\}\;, \tag{4.1}$$

where $\underline{\theta}_n$ is given by (3.5). We also introduce the stopping times T_k as the times of return in the stratum of smallest weight: $T_0 = 0$ and, for $k \geqslant 1$,

$$T_k = \inf\{n > T_{k-1} \,:\, X_n \in \mathsf{X}_{I_n}\}\;,$$

with the convention that $\inf \emptyset = \infty$. With these notations, Theorem 3.2 is implied by the following proposition, the proof of which is the goal of this section.

Proposition 4.1. *Under A1, A2 and A3a, it holds*

$$\mathbb{P}\Big(\forall k \in \mathbb{N},\ T_k < \infty\Big) = 1\;, \tag{4.2}$$

$$\mathbb{P}\left(\limsup_{k\to\infty} \underline{\theta}_{T_k-1} > 0\right) = 1\;, \tag{4.3}$$

where $\underline{\theta}_n$ is given by (3.5).

When finite, the stopping times T_k are such that $\underline{\theta}_{T_k} - \underline{\theta}_{T_k-1}$ admits a known increase. Indeed, by the update rule (2.5),

$$\begin{aligned}\theta_{T_k-1}(I_{T_k}) &= \frac{\theta_{T_k}(I_{T_k})}{1+\gamma_{T_k}(1-\theta_{T_k-1}(I_{T_k}))} < \theta_{T_k}(I_{T_k}) \\ &\leqslant \min_{j\neq I_{T_k}} \theta_{T_k}(j) < \min_{j\neq I_{T_k}} \frac{\theta_{T_k}(j)}{1-\gamma_{T_k}\theta_{T_k-1}(I_{T_k})} = \min_{j\neq I_{T_k}} \theta_{T_k-1}(j)\;,\end{aligned}$$

so that

$$I_{T_k-1} = I_{T_k} \text{ and } \underline{\theta}_{T_k} = \underline{\theta}_{T_k-1}(1+\gamma_{T_k}(1-\underline{\theta}_{T_k-1}))\;. \tag{4.4}$$

In the evolution from $\underline{\theta}_{T_k-1}$ to $\underline{\theta}_{T_{k+1}-1}$, the increase provided by the return to the stratum $\mathsf{X}_{I_{T_k}}$ at time T_k compensates the decrease of $\underline{\theta}_n$ generated by the subsequent visits to the other strata for $n \in \{T_k+1, \dots, T_{k+1}-1\}$, provided that $T_{k+1} - T_k$ is small enough. This is indeed possible since the decrease arises from multiplicative factors $1 - \gamma_n\theta(I(X_n))$, where $\gamma_n\theta(I(X_n))$ is typically much smaller than the term $\gamma_{T_k}(1-\underline{\theta}_{T_k-1})$ appearing in (4.4).

4.2.1 Proof of (4.2)

To prove the first assertion, we proceed by induction on k and suppose that $\mathbb{P}(T_k < \infty) = 1$. This assertion is true for $k = 0$. To check the condition $\mathbb{P}(T_{k+1} < \infty) = 1$, we are going to construct a specific sequence ensuring that X_n returns in the stratum of smallest weight at some point (see (4.6) below), and show that this sequence has a positive probability of occurrence (see Lemma 4.2 below).

For $m \in \mathbb{N}$, let $\theta_{T_k+md}((1)_m) \leqslant \theta_{T_k+md}((2)_m) \leqslant \ldots \leqslant \theta_{T_k+md}((d)_m)$ denote the increasing reordering of $(\theta_{T_k+md}(i))_{1 \leqslant i \leqslant d}$ (notice that $\theta_{T_k+md}((1)_m) = \underline{\theta}_{T_k+md}$), and define

$$i_m = \max\{i \leqslant d : \theta_{T_k+md}((i)_m) < \underline{\theta}_{T_k+md}(1+\gamma_1)/(1-\gamma_1)\}. \tag{4.5}$$

The indices $(1)_m, \ldots, (i_m)_m$ are all the indices of the strata with weights close enough to the minimal weight. We then consider the sequence obtained by visiting successively the strata with indices $(i)_m$ for $i \leqslant i_m$, in decreasing order. This corresponds to the event

$$A_m = \left\{ X_{T_k+md+1} \in \mathsf{X}_{(i_m)_m}, X_{T_k+md+2} \in \mathsf{X}_{(i_m-1)_m}, \ldots, X_{T_k+md+i_m} \in \mathsf{X}_{(1)_m} \right\}. \tag{4.6}$$

On A_m, the weights are not updated for $j \geqslant i_m + 1$, so that

$$\frac{\theta_{T_k+md+i_m-1}((j)_m)}{\theta_{T_k+md+i_m-1}((1)_m)} = \frac{\theta_{T_k+md}((j)_m)}{\theta_{T_k+md}((1)_m)} \geqslant \frac{1+\gamma_1}{1-\gamma_1} > \frac{1+\gamma_{T_k+md+i_m}(1-\theta_{T_k+md+i_m-1}((1)_m))}{1-\gamma_{T_k+md+i_m}\theta_{T_k+md+i_m-1}((1)_m)} ,$$

where we have used successively the definition of i_m and A3a. The inequality between the left-most and right-most terms rewrites $\theta_{T_k+md+i_m}((j)_m) > \theta_{T_k+md+i_m}((1)_m)$. Now, for $j \in \{2, \ldots, i_m\}$, it holds on A_m

$$\frac{\theta_{T_k+md+i_m}((j)_m)}{\theta_{T_k+md+i_m}((1)_m)} = \frac{\theta_{T_k+md}((j)_m)}{\theta_{T_k+md}((1)_m)} \times \frac{1 + \dfrac{\gamma_{T_k+md+i_m+1-j}}{1-\gamma_{T_k+md+i_m+1-j}\theta_{T_k+md+i_m-j}((j)_m)}}{1 + \dfrac{\gamma_{T_k+md+i_m}}{1-\gamma_{T_k+md+i_m}\theta_{T_k+md+i_m-1}((1)_m)}} .$$

The second factor on the right-hand side is larger than 1 on A_m since $\gamma_{T_k+md+i_m} \leqslant \gamma_{T_k+md+i_m+1-j}$ by A3a and, using the fact that the stratum $\mathsf{X}_{(1)_m}$ is not visited until the last step,

$$\begin{aligned}\theta_{T_k+md+i_m-1}((1)_m) < \theta_{T_k+md+i_m-j}((1)_m) &= \theta_{T_k+md+i_m-j}((j)_m) \times \frac{\theta_{T_k+md}((1)_m)}{\theta_{T_k+md}((j)_m)} \\ &\leqslant \theta_{T_k+md+i_m-j}((j)_m) .\end{aligned}$$

Therefore, the stratum with smallest weight at iteration $T_k + md + i_m$ is still $(1)_m$, which means that $I_{T_k+md+i_m} = (1)_m$ on A_m and

$$\text{on } A_m, \qquad T_{k+1} \leqslant T_k + md + i_m \leqslant T_k + (m+1)d . \tag{4.7}$$

To deduce that $\mathbb{P}(T_{k+1} < \infty) = 1$, we use the following lemma (whose proof is postponed to Section 4.2.3).

Lemma 4.2. *Under A1 and A2, there exists a constant $p \in (0,1]$ not depending on k such that almost-surely*

$$\forall m \in \mathbb{N}, \qquad \mathbb{P}(A_m | \mathcal{F}_{T_k+md}) \geqslant p .$$

Lemma 4.2 implies that, for $m \in \mathbb{N}$,

$$\begin{aligned}\mathbb{P}\big(T_{k+1} > T_k + (m+1)d\big) &\leqslant \mathbb{P}(A_0^c \cap A_1^c \cap \ldots \cap A_m^c) \\ &= \mathbb{E}\left(\mathbb{1}_{\{A_0^c \cap A_1^c \cap \ldots \cap A_{m-1}^c\}}\big(1 - \mathbb{P}(A_m|\mathcal{F}_{T_k+md})\big)\right) \\ &\leqslant (1-p)\mathbb{P}(A_0^c \cap A_1^c \cap \ldots \cap A_{m-1}^c) ,\end{aligned}$$

which inductively leads to $\mathbb{P}(T_{k+1} > T_k + (m+1)d) \leqslant (1-p)^{m+1}$. The conclusion follows by taking the limit $m \to \infty$ in the latter inequality.

4.2.2 Proof of (4.3)

The proof of the second assertion relies on the following lemma (proved in Section 4.2.3). For $k \geqslant 1$, set

$$\mathcal{G}_k \stackrel{\text{def}}{=} \mathcal{F}_{T_k} , \qquad Y_k \stackrel{\text{def}}{=} \underline{\theta}_{T_k - 1} , \tag{4.8}$$

where $\underline{\theta}_\ell$ is defined by (3.5).

Lemma 4.3. *Let $v : (0, 1] \ni t \mapsto -\ln(t) \in \mathbb{R}_+$. Assume that A1, A2 and A3a hold. Then, there exist $\underline{k} \in \mathbb{N}$ and $\bar{y} \in (0, 1)$ such that almost-surely,*

$$\forall k \geqslant \underline{k}, \qquad Y_k \leqslant \bar{y} \Rightarrow \mathbb{E}(v(Y_{k+1})|\mathcal{G}_k) \leqslant v(Y_k) .$$

We then define by induction stopping times σ_m and τ_m as follows: $\sigma_0 = 0$, and for $m \geqslant 1$ (with the convention $\inf \emptyset = \infty$),

$$\tau_m = \inf\{k > \sigma_{m-1} \, : \, Y_k \leqslant \bar{y}\}, \qquad \sigma_m = \inf\{k > \tau_m \, : \, Y_k > \bar{y}\} .$$

All possible events can then be classified using the following partition of the underlying probability space:

$$\{\exists m \geqslant 0 : \sigma_m < \infty = \tau_{m+1}\} \cup \{\forall m \geqslant 1, \sigma_m < \infty\} \cup \{\exists m \geqslant 1 : \tau_m < \infty = \sigma_m\} .$$

On the first two sets, $Y_k > \bar{y}$ infinitely often so that $\limsup_{k\to\infty} Y_k \geqslant \bar{y}$. To deal with the last set, one remarks that for each $m \geqslant 1$, the process $(v(Y_{k\wedge\sigma_m}) - v(Y_{k\wedge\tau_m}))_{k\geqslant\underline{k}}$ is a $\mathcal{G}_k$-supermartingale by Lemma 4.3 and is not smaller than $-v(Y_{\tau_m}) \geqslant -v(\bar{y}(1-\gamma_1))$ by positivity and monotonicity of v and definition of τ_m. So this process converges almost surely to a finite limit V_m as $k \to \infty$. As a consequence, on $\{\exists m \geqslant 1 : \tau_m < \infty = \sigma_m\}$, $(Y_k)_k$ converges a.s. to $\sum_{m\geqslant 1} \mathbb{1}_{\{\tau_m<\infty=\sigma_m\}} Y_{\tau_m} e^{-V_m}$. In conclusion, $\mathbb{P}(\limsup_{k\to\infty} Y_k > 0) = 1$.

4.2.3 Proofs of some technical results

We now provide the proofs of the previously quoted lemmas.

Proof of Lemma 4.2. By A1 and A2, the constant $c \stackrel{\text{def}}{=} \frac{\inf_{\mathsf{X}^2} q}{\sup_{\mathsf{X}} \pi}$ is positive. The main ingredient of the proof is the following lower-bound: for all $i \in \{1, \ldots, d\}$ and $x \in \mathsf{X}$,

$$P_\theta(x, \mathsf{X}_i) \geqslant \int_{\mathsf{X}_i} q(x, y) \left(1 \wedge \frac{\theta(I(x))\pi(y)}{\theta(i)\pi(x)}\right) \lambda(dy) \geqslant c\, \theta_\star(i) \left(\frac{\theta(I(x))}{\theta(i)} \wedge 1\right). \tag{4.9}$$

For $j \in \{1, \ldots, i_m - 1\}$, it holds on $\{X_{T_k+md+1} \in \mathsf{X}_{(i_m)_m}, \ldots, X_{T_k+md+j} \in \mathsf{X}_{(i_m+1-j)_m}\}$,

$$\begin{aligned} &\frac{\theta_{T_k+md+j}((i_m + 1 - j)_m)}{\theta_{T_k+md+j}((i_m - j)_m)} \\ &= \frac{\theta_{T_k+md}((i_m + 1 - j)_m)}{\theta_{T_k+md}((i_m - j)_m)} \times \frac{1 + \gamma_{T_k+md+j}(1 - \theta_{T_k+md+j-1}((i_m + 1 - j)_m)}{1 - \gamma_{T_k+md+j}\theta_{T_k+md+j-1}((i_m + 1 - j)_m)} . \end{aligned}$$

Both factors on the right-hand side are larger than 1 (the first one by definition of the ordered indices $(i)_m$), so that, by (4.9),

$$P_{\theta_{T_k+md+j}}\left(X_{T_k+md+j}, \mathsf{X}_{(i_m-j)_m}\right) \geqslant c\, \theta_\star((i_m - j)_m) \geqslant c\, \underline{\theta}_\star ,$$

where $\underline{\theta}$ is defined by (3.5). Using successively the strong Markov property of the chain $(X_n, \theta_n)_n$, a backward induction on n, the definition of i_m, together with (4.9),

$$
\begin{aligned}
&\mathbb{P}(A_m | \mathcal{F}_{T_k+md}) \\
&= \mathbb{E}\left(\mathbb{1}_{\{X_{T_k+md+1} \in \mathsf{X}_{(i_m)_m}, \dots, X_{T_k+md+i_m-1} \in \mathsf{X}_{(2)_m}\}} P_{\theta_{T_k+md+i_m-1}}(X_{T_k+md+i_m-1}, \mathsf{X}_{(1)_m}) | \mathcal{F}_{T_k+md}\right) \\
&\geqslant c\,\underline{\theta}_\star \mathbb{E}\left(\mathbb{1}_{\{X_{T_k+md+1} \in \mathsf{X}_{(i_m)_m}, \dots, X_{T_k+md+i_m-2} \in \mathsf{X}_{(3)_m}\}} P_{\theta_{T_k+md+i_m-2}}(X_{T_k+md+i_m-2}, \mathsf{X}_{(2)_m}) \Big| \mathcal{F}_{T_k+md}\right) \\
&\geqslant (c\,\underline{\theta}_\star)^{i_m-1} P_{\theta_{T_k+md}}(X_{T_k+md}, \mathsf{X}_{(i_m)_m}) \\
&\geqslant (c\,\underline{\theta}_\star)^{i_m-1} c \frac{1-\gamma_1}{1+\gamma_1} \underline{\theta}_\star \geqslant \frac{1-\gamma_1}{1+\gamma_1} (c\,\underline{\theta}_\star)^d \ .
\end{aligned}
$$

It then suffices to define

$$
p = \frac{1-\gamma_1}{1+\gamma_1} (c\,\underline{\theta}_\star)^d \tag{4.10}
$$

in order to conclude the proof. □

Proof of Lemma 4.3. Note first that, apart from the case when $X_n \in \mathsf{X}_{I_n}$, the other situation ensuring that $\underline{\theta}_{n+1} > \underline{\theta}_n$ is the case when the chain visits the stratum of smallest weight, but the weight of this stratum is then increased while the weights of the other ones are decreased, in such a manner that this stratum no longer remains the one with smallest weight. In mathematical terms, $X_{n+1} \in \mathsf{X}_{I_n}$ and

$$
\frac{\underline{\theta}_n}{1-\gamma_{n+1}\underline{\theta}_n} < \min_{j \neq I_n} \theta_n(j) \leqslant \frac{\underline{\theta}_n(1+\gamma_{n+1}(1-\underline{\theta}_n))}{1-\gamma_{n+1}\underline{\theta}_n},
$$

where the first inequality actually implies that $\underline{\theta}_{n+1} > \underline{\theta}_n$ and the second one that $X_{n+1} \notin \mathsf{X}_{I_{n+1}}$.

Define $\mu(\omega) = \inf\{m \geqslant 1 : \omega \in A_{m-1}\}$. Then, recalling that $Y_k \stackrel{\text{def}}{=} \underline{\theta}_{T_k-1}$,

$$
\begin{aligned}
Y_{k+1} &\geqslant Y_k(1+\gamma_{T_k}(1-Y_k)) \prod_{n=T_k}^{T_{k+1}-2} (1-\gamma_{n+1}\theta_n(I(X_{n+1}))) \\
&\geqslant Y_k(1+\gamma_{T_k}(1-Y_k)) \prod_{n=T_k}^{T_k+\mu d-2} (1-\gamma_{T_k}\theta_n(I(X_{n+1}))),
\end{aligned} \tag{4.11}
$$

where the first factor comes from the definition of T_k (see (4.4)); the first inequality from the possibility that for some $n \in \{T_k, \dots, T_{k+1}-2\}$, $X_{n+1} \in \mathsf{X}_{I_n}$ and $I_{n+1} \neq I_n$; and the second inequality from A3a and the fact that $T_{k+1} \leqslant T_k + \mu d$ by (4.7). By Lemma 4.2 μ is smaller than some geometric random variable with parameter bounded from below by the positive constant p. Therefore, the number of terms smaller than 1 in the product on the right-hand side of (4.11) is small. If Y_k is chosen small enough, then $\gamma_{T_k}(1-Y_k)$ is much larger than $\gamma_{T_k} Y_k$ and if $\theta_n(I(X_{n+1}))$ remains of the same order as $\theta_{T_k-1}(I(X_{T_k})) = Y_k$ for $n \in \{T_k, \dots, T_k+\mu d-2\}$, then, in average, Y_{k+1} will be larger than Y_k. Unfortunately, since for $\theta \in \Theta$, $\max_{1 \leqslant i \leqslant d} \theta(i) \geqslant \frac{1}{d}$, $\theta_{T_k}(i)$ is large for i in some subset of $\{1, \dots, d\}$ and we need to control the probability for $(X_n)_{T_k+1 \leqslant n \leqslant T_k+\mu d-1}$ to visit the corresponding strata. Under A1, $C \stackrel{\text{def}}{=} \frac{\sup_{\mathsf{X}} \pi}{\inf_{\mathsf{X}} \pi} < \infty$ and, for all $i \neq j \in \{1, \dots, d\}$ and $x \in \mathsf{X}_i$,

$$
P_\theta(x, \mathsf{X}_j) = \int_{\mathsf{X}_j} q(x,y) \left(1 \wedge \frac{\theta(i)\pi(y)}{\theta(j)\pi(x)}\right) \lambda(dy) \leqslant C \left(\frac{\theta(i)}{\theta(j)} \wedge 1\right) . \tag{4.12}
$$

This ensures that the conditional probability to choose $X_{n+1} \in \mathsf{X}_j$ with large weight $\theta_n(j)$, given $X_n \in \mathsf{X}_i$ with low weight $\theta_n(i)$, is small.

To quantify this intuition, define $i_{T_k} \in \operatorname{argmax}_{1 \leqslant i \leqslant d-1} \dfrac{\theta_{T_k}((i+1)_0)}{\theta_{T_k}((i)_0)}$. Since

$$\prod_{i=1}^{d-1} \frac{\theta_{T_k}((i+1)_0)}{\theta_{T_k}((i)_0)} = \frac{\max_i \theta_{T_k}(i)}{Y_k(1+\gamma_{T_k}(1-Y_k))} \geqslant \frac{1}{2dY_k} , \tag{4.13}$$

it holds

$$\frac{\theta_{T_k}((i_{T_k}+1)_0)}{\theta_{T_k}((i_{T_k})_0)} \geqslant (2dY_k)^{-1/(d-1)} ,$$

so that, for all $i \in \{1, \ldots, i_{T_k}\}$,

$$\theta_{T_k}((i)_0) \leqslant \theta_{T_k}((i_{T_k})_0) = \frac{\theta_{T_k}((i_{T_k})_0)}{\theta_{T_k}((i_{T_k}+1)_0)} \times \theta_{T_k}((i_{T_k}+1)_0) \leqslant (2dY_k)^{1/(d-1)} .$$

Hereafter, the set

$$\mathsf{X}(k) \stackrel{\text{def}}{=} \cup_{i \geqslant i_{T_k}+1} \mathsf{X}_{(i)_0} , \tag{4.14}$$

plays the role of the union of strata with large weight according to θ_{T_k}. Define, for $m \in \mathbb{N}$,

$$\rho_m \stackrel{\text{def}}{=} 1 \wedge \left((2dY_k)^{1/(d-1)} \left(\frac{1+\gamma_{T_k}}{1-\gamma_{T_k}} \right)^{(m+1)d} \right), \qquad B_m \stackrel{\text{def}}{=} \bigcup_{n \in \{1,\ldots,d\}} \left\{ X_{T_k+md+n} \in \mathsf{X}(k) \right\} . \tag{4.15}$$

Then,

$$\forall m \in \mathbb{N},\ \forall n \leqslant (m+1)d, \qquad \frac{\max_{j \leqslant i_{T_k}} \theta_{T_k+n}((j)_0)}{\min_{i \geqslant i_{T_k}+1} \theta_{T_k+n}((i)_0)} \wedge 1 \leqslant \rho_m , \tag{4.16}$$

which implies

$$\forall j \in \{1, \ldots, i_{T_k}\}, n \leqslant (m+1)d, \qquad \theta_{T_k+n}((j)_0) \leqslant \rho_m . \tag{4.17}$$

Using (4.11), the definition of μ, then the inequality $-\ln(x) \leqslant \frac{1}{x} - 1$, it follows

$$\begin{aligned}
&\mathbb{E}(v(Y_{k+1})|\mathcal{G}_k) - v(Y_k) + \ln(1+\gamma_{T_k}(1-Y_k)) \\
&\leqslant -\sum_{m \in \mathbb{N}} \mathbb{E}\left(\ln\left(\prod_{n=T_k}^{T_k+(m+1)d-1} (1-\gamma_{T_k}\theta_n(I(X_{n+1}))) \right) \mathbb{1}_{\{A_0^c \cap \ldots \cap A_{m-1}^c \cap A_m\}} | \mathcal{G}_k \right) \\
&\leqslant -\sum_{m \in \mathbb{N}} \mathbb{E}\left(\ln\left(\prod_{n=T_k}^{T_k+(m+1)d-1} (1-\gamma_{T_k}\theta_n(I(X_{n+1}))) \right) \mathbb{1}_{\{A_0^c \cap \ldots \cap A_{m-1}^c\}} | \mathcal{G}_k \right) \\
&\leqslant \sum_{m \in \mathbb{N}} \sum_{l=0}^{m} E_{ml} ,
\end{aligned} \tag{4.18}$$

where the numbers E_{ml} are defined by decomposing the possible events using the partition

$B_0, B_0^c \cap B_1, \ldots, B_0^c \cap \cdots \cap B_{m-2}^c \cap B_{m-1}, B_0^c \cap \cdots \cap B_{m-1}^c$:

$$E_{ml} = \begin{cases} \mathbb{E}\left(\left((1-\gamma_{T_k})^{-(m+1)d} - 1\right)\mathbb{1}_{\{A_0^c\cap\ldots\cap A_{m-1}^c\cap B_0\}}|\mathcal{G}_k\right) & \text{for } l = 0, \\ \mathbb{E}\left(\left((1-\gamma_{T_k})^{-(m+1)d} - 1\right)\mathbb{1}_{\{A_0^c\cap\ldots\cap A_{m-1}^c\cap B_0^c\cap\ldots\cap B_{l-1}^c\cap B_l\}}|\mathcal{G}_k\right) & \text{for } 0 < l < m, \\ \mathbb{E}\left(\left((1-\gamma_{T_k}\rho_m)^{-(m+1)d} - 1\right)\mathbb{1}_{\{A_0^c\cap\ldots\cap A_{m-1}^c\cap B_0^c\cap\ldots\cap B_{m-1}^c\}}|\mathcal{G}_k\right) & \text{for } l = m. \end{cases}$$

The inequality (4.17) was used for the case $l = m$.

Let

$$\overline{m} \stackrel{\text{def}}{=} \left(-\frac{\ln(4d^2 Y_k)}{2d(d-1)\ln\left(\frac{1+\gamma_{T_k}}{1-\gamma_{T_k}}\right)}\right)^+ - 1.$$

Note that $\overline{m}$ is chosen so that $\rho_m \leqslant Y_k^{1/2(d-1)}$ for $0 \leqslant m \leqslant \overline{m}$. Besides, we may assume that k is large enough so that $1-p < (1-\gamma_{T_k})^d$, p being defined in Lemma 4.2 (indeed, $T_k \geqslant k$, and $\lim_{n\to\infty}\gamma_n = 0$ by A3a). Therefore, using Lemma 4.2 for the second inequality,

$$\begin{aligned} \sum_{m\in\mathbb{N}} E_{mm} \leqslant & \sum_{m\leqslant\overline{m}} \left((1-\gamma_{T_k}Y_k^{1/2(d-1)})^{-(m+1)d} - 1\right)\mathbb{P}(A_0^c\cap\ldots\cap A_{m-1}^c|\mathcal{G}_k) \\ & + \sum_{m>\overline{m}} (1-\gamma_{T_k})^{-(m+1)d}\mathbb{P}(A_0^c\cap\ldots\cap A_{m-1}^c|\mathcal{G}_k) \\ \leqslant & \sum_{m\in\mathbb{N}} ((1-\gamma_{T_k}Y_k^{1/2(d-1)})^{-(m+1)d} - 1)(1-p)^m + \sum_{m>\overline{m}} (1-\gamma_{T_k})^{-(m+1)d}(1-p)^m \\ = & \frac{1-(1-\gamma_{T_k}Y_k^{1/2(d-1)})^d}{p(p+(1-\gamma_{T_k}Y_k^{1/2(d-1)})^d - 1)} + \frac{1}{p+(1-\gamma_{T_k})^d-1}\left(\frac{1-p}{(1-\gamma_{T_k})^d}\right)^{\lfloor\overline{m}\rfloor+1}. \end{aligned} \tag{4.19}$$

The terms E_{ml} for $l < m$ can be dealt with using the following lemma, the proof of which is postponed to the end of this section.

Lemma 4.4. *Let A_m, B_m and $\mathcal{G}_k$ be given by (4.6), (4.15) and (4.8). For $0 \leqslant l < m$, one has*

$$\mathbb{P}(A_0^c\cap\ldots\cap A_{m-1}^c\cap B_0^c\cap\ldots\cap B_{l-1}^c\cap B_l|\mathcal{G}_k) \leqslant Cd\rho_l(1-p)^{m-1}.$$

This lemma ensures that for $l < m$, $E_{ml} \leqslant Cd((1-\gamma_{T_k})^{-(m+1)d} - 1)(1-p)^{m-1}\rho_l$. By Fubini's theorem (the terms of the sums below are non-negative) and a reasoning similar to the one used above to estimate the sum $\sum_{m\in\mathbb{N}} E_{mm}$, we obtain

$$\begin{aligned} \frac{1}{Cd}\sum_{m\in\mathbb{N}}\sum_{l=0}^{m-1} E_{ml} \leqslant & \sum_{l\in\mathbb{N}}\rho_l \sum_{m\geqslant l+1}((1-\gamma_{T_k})^{-(m+1)d} - 1)(1-p)^{m-1} \\ = & \sum_{l\in\mathbb{N}}\rho_l\left(\frac{(1-\gamma_{T_k})^{-d}((1-\gamma_{T_k})^{-d}(1-p))^l}{p+(1-\gamma_{T_k})^d-1} - \frac{(1-p)^l}{p}\right) \\ \leqslant & Y_k^{1/2(d-1)}\left(\frac{1}{(p+(1-\gamma_{T_k})^d-1)^2} - \frac{1}{p^2}\right) + \frac{1}{(p+(1-\gamma_{T_k})^d-1)^2}\left(\frac{1-p}{(1-\gamma_{T_k})^d}\right)^{\lfloor\overline{m}\rfloor+1}. \end{aligned} \tag{4.20}$$

Since $T_k \geqslant k$, and $\lim_{n\to\infty} \gamma_n = 0$ by A3a, there exists a deterministic constant $\underline{k}$ such that for $k \geqslant \underline{k}$, $(1-\gamma_{T_k})^d \geqslant 1-\frac{p}{2}$ and $\ln(1+\gamma_{T_k}(1-Y_k)) \geqslant \frac{\gamma_{T_k}}{2}(1-Y_k)$. In view of (4.18)-(4.19)-(4.20), the definition of $\overline{m}$ and $\ln\left(\frac{1+\gamma_{T_k}}{1-\gamma_{T_k}}\right) \leqslant \frac{2\gamma_{T_k}}{1-\gamma_{T_k}}$, there exists a finite constant K such that, for $k \geqslant \underline{k}$ and $Y_k \leqslant 1/4d^2$,

$$\mathbb{E}\big(v(Y_{k+1})\big|\mathcal{G}_k\big) - v(Y_k) \leqslant -\frac{\gamma_{T_k}}{2}(1-Y_k) \\ + K\left(\gamma_{T_k} Y_k^{1/2(d-1)} + \exp\left(\frac{(1-\gamma_{T_k})\ln\left(\frac{1-p}{1-p/2}\right)\ln(4d^2Y_k)}{4d(d-1)\gamma_{T_k}}\right)\right).$$

This implies that there exists $\bar{y} \in (0, 1/4d^2]$ such that, for all $k \geqslant \underline{k}$,

$$Y_k \leqslant \bar{y} \Rightarrow \mathbb{E}(v(Y_{k+1})|\mathcal{G}_k) \leqslant v(Y_k),$$

which concludes the proof of Lemma 4.3. $\square$

Proof of Lemma 4.4. Let us first consider the case when $l \geqslant 1$. By Lemma 4.2,

$$\mathbb{P}(A_0^c \cap \ldots \cap A_{m-1}^c \cap B_0^c \cap \ldots \cap B_{l-1}^c \cap B_l|\mathcal{G}_k) \\ \leqslant (1-p)^{m-1-l}\mathbb{E}\left(\mathbb{1}_{\{A_0^c\cap\ldots\cap A_{l-1}^c\}}\mathbb{1}_{\{B_{l-1}^c\}}\mathbb{P}(B_l|\mathcal{F}_{T_k+ld})\Big|\,\mathcal{G}_k\right).$$

To conclude, it is therefore enough to check that $\mathbb{1}_{\{B_{l-1}^c\}}\mathbb{P}(B_l|\mathcal{F}_{T_k+ld}) \leqslant Cd\rho_l$. Now,

$$\mathbb{1}_{\{B_{l-1}^c\}}\mathbb{P}(B_l|\mathcal{F}_{T_k+ld}) \leqslant \mathbb{1}_{\{X_{T_k+ld}\notin\mathsf{X}(k)\}}P_{\theta_{T_k+ld}}(X_{T_k+ld}, \mathsf{X}(k)) \\ + \sum_{n=1}^{d-1}\mathbb{P}(X_{T_k+ld+1} \notin \mathsf{X}(k), \ldots, X_{T_k+ld+n} \notin \mathsf{X}(k), X_{T_k+ld+n+1} \in \mathsf{X}(k)|\mathcal{F}_{T_k+ld}) \\ \leqslant \sum_{n=0}^{d-1}\mathbb{E}(\mathbb{1}_{\{X_{T_k+ld+n}\notin\mathsf{X}(k)\}}P_{\theta_{T_k+ld+n}}(X_{T_k+ld+n}, \mathsf{X}(k))|\mathcal{F}_{T_k+ld}),$$

where $\mathbb{1}_{\{X_{T_k+ld+n}\notin\mathsf{X}(k)\}}P_{\theta_{T_k+ld+n}}(X_{T_k+ld+n}, \mathsf{X}(k)) \leqslant C\rho_l$ by (4.12) and (4.16).

For the case $l = 0$, we use again Lemma 4.2 to obtain

$$\mathbb{P}(A_0^c \cap \ldots \cap A_{m-1}^c \cap B_0|\mathcal{G}_k) \leqslant (1-p)^{m-1}\mathbb{P}(B_0|\mathcal{G}_k).$$

The second factor is still bounded from above by $Cd\rho_l$ since $X_{T_k} \notin \mathsf{X}(k)$, which gives the claimed result. $\square$

4.2.4 Adaptation of the stability result to the standard Wang-Landau update (2.8)

Proposition 4.1 and therefore Theorem 3.2 still hold when the update (2.5) of the weights is replaced by the standard Wang-Landau update (2.8). Indeed, to adapt the proof of (4.2), it is enough to

- modify the definition (4.5) of i_m into $i_m = \max\{i \leqslant d : \theta_{T_k+md}((i)_m) \leqslant \underline{\theta}_{T_k+md}(1+\gamma_1)\}$ to guarantee, using the simplified evolution of ratios of weights

$$\frac{\theta_{n+1}(i)}{\theta_{n+1}(j)} = \frac{\theta_n(i)}{\theta_n(j)} \times \frac{1+\gamma_{n+1}\mathbb{1}_{\mathsf{X}_i}(X_{n+1})}{1+\gamma_{n+1}\mathbb{1}_{\mathsf{X}_j}(X_{n+1})}$$

under the standard Wang-Landau update, that (4.7) still holds.

- replace accordingly the factor $\frac{1-\gamma_1}{1+\gamma_1}$ by $\frac{1}{1+\gamma_1}$ in the definition (4.10) of p in the proof of Lemma 4.2.

To adapt the proof of (4.3), it is enough to

- replace the factor $(1+\gamma_{T_k}(1-Y_k))$ by $\frac{1+\gamma_{T_k}}{1+\gamma_{T_k}Y_k}$ in (4.11) which causes no complication in the remaining of the proof of Lemma 4.3 since one still has $\ln\left(\frac{1+\gamma_{T_k}}{1+\gamma_{T_k}Y_k}\right) = \ln\left(1+\frac{\gamma_{T_k}(1-Y_k)}{1+\gamma_{T_k}Y_k}\right) \geqslant \frac{\gamma_{T_k}}{2}(1-Y_k)$ for k large enough. Notice that since for $x \geqslant 0$, $\frac{1}{1+x} \geqslant 1-x$, one can keep the product in (4.11) unchanged.

- replace (4.13) by $\displaystyle\prod_{i=1}^{d-1} \frac{\theta_{T_k}((i+1)_0)}{\theta_{T_k}((i)_0)} = \frac{\max_i \theta_{T_k}(i)(1+\gamma_{T_k}Y_k)}{Y_k(1+\gamma_{T_k})} \geqslant \frac{1}{2dY_k}$.

4.3 Proof of Theorem 3.3

We start by proving that the function V defined in (3.7) is a Lyapunov function for the mean-field h given by (3.2).

Proposition 4.5. *Under A1,*

a) V is non-negative and continuously differentiable on Θ.

b) h is continuous on Θ and given by

$$h(\theta) = \left(\sum_{i=1}^{d} \frac{\theta_\star(i)}{\theta(i)}\right)^{-1} (\theta_\star - \theta) \ . \tag{4.21}$$

c) for any $M > 0$, $\{\theta \in \Theta,\ V(\theta) \leqslant M\}$ is a compact subset of Θ.

d) for any $\theta \in \Theta$, $\langle \nabla V(\theta), h(\theta)\rangle \leqslant 0$. In addition, $\{\theta \in \Theta,\ \langle \nabla V(\theta), h(\theta)\rangle = 0\} = \{\theta_\star\}$.

Proof. (a) It is trivial to check that V is C^1 on Θ. By Jensen's inequality,

$$V(\theta) = -\sum_{i=1}^{d} \theta_\star(i) \log\left(\frac{\theta(i)}{\theta_\star(i)}\right) \geqslant -\log\left(\sum_{i=1}^{d} \theta(i)\right) = 0 \ .$$

(b) For any $i \in \{1,\ldots,d\}$, we have by (2.7) and (3.2),

$$h_i(\theta) = \int_{\mathsf{X}} H_i(x,\theta)\, \pi_\theta(x)\, \lambda(dx) = \theta(i) \int_{\mathsf{X}_i} \pi_\theta(x)\, \lambda(dx) - \theta(i) \sum_{k=1}^{d} \theta(k) \int_{\mathsf{X}_k} \pi_\theta(x)\ \lambda(dx) \ .$$

The property (4.21) now follows upon noting that, by definition of π_θ (see (2.4)),

$$\int_{\mathsf{X}_k} \pi_\theta(x)\,\lambda(dx) = \left(\sum_{i=1}^d \frac{\theta_\star(i)}{\theta(i)}\right)^{-1} \frac{\theta_\star(k)}{\theta(k)}\ .$$

(c) Set $M' \stackrel{\text{def}}{=} M - \sum_{i=1}^d \theta_\star(i)\log\theta_\star(i)$. Observe that, by A1, $M' > M > 0$. By definition of V (see (3.7)),

$$\{V \leqslant M\} = \left\{\theta \in \Theta,\ -\sum_{i=1}^d \theta_\star(i)\log\theta(i) \leqslant M'\right\} \subseteq \bigcap_{j=1}^d \{\theta\in\Theta,\ \theta(j) \geqslant m\}\ .$$

with $m \stackrel{\text{def}}{=} \exp(-M'/\inf_k \theta_\star(k))$. Therefore, for any $M>0$, there exists $m>0$ such that

$$\{V \leqslant M\} \subset \left\{\theta\in\Theta,\ m \leqslant \inf_i \theta(i) \leqslant \sup_i \theta(i) \leqslant 1\right\}\ .$$

Since V is continuous, $\{V \leqslant M\}$ is a compact subset of Θ.

(d) By definition of V and h (see (3.7) and (4.21)), a simple computation shows that

$$\begin{aligned}\langle \nabla V(\theta), h(\theta)\rangle &= -\left(\sum_{i=1}^d \frac{\theta_\star(i)}{\theta(i)}\right)^{-1} \sum_{i=1}^d \frac{\theta_\star(i)}{\theta(i)}(\theta_\star(i)-\theta(i)) \\ &= -\left(\sum_{i=1}^d \frac{\theta_\star(i)}{\theta(i)}\right)^{-1} \sum_{i=1}^d \frac{(\theta_\star(i)-\theta(i))^2}{\theta(i)} \leqslant 0\ ,\end{aligned}$$

where we have used $\sum_{i=1}^d(\theta_\star(i)-\theta(i)) = 0$ to obtain the second equality. It is also clear from the above expression that the scalar product is null if and only if $\theta = \theta_\star$. □

We now wish to prove that the increment $\gamma_{n+1}\,(H(X_{n+1},\theta_n) - h(\theta_n))$ in (3.6) vanishes in an appropriate sense. To this end, we need some preliminary results and we rewrite the update of the weights as

$$\frac{\theta_{n+1}(i)}{\theta_n(i)} = 1 + \gamma_{n+1} Y_{n+1}(i)\ , \tag{4.22}$$

where $Y_{n+1}(i) \stackrel{\text{def}}{=} \mathbb{1}_{\mathsf{X}_i}(X_{n+1}) - \theta_n(I(X_{n+1}))$ satisfies $|Y_{n+1}(i)| \leqslant 1$. This key formula says that the difference $\theta_{n+1}(i)-\theta_n(i)$ is not simply of order of the step-size γ_{n+1} but of order $\theta_n(i)\gamma_{n+1}$ which permits to circumvent the explosive behavior of the various estimates obtained in the next lemmas as $\min_{1\leqslant i\leqslant d}\theta(i)$ tends to 0.

Lemma 4.6. *For any $\theta, \theta' \in \Theta$,*

$$\|\pi_\theta d\lambda - \pi_{\theta'} d\lambda\|_{\mathrm{TV}} \leqslant 2(d-1)\sum_{i=1}^d \left|1 - \frac{\theta'(i)}{\theta(i)}\right|\ .$$

Proof. By definition of π_θ (see (2.4)),

$$\pi_\theta(x) = \sum_{i=1}^d \frac{[\theta_\star(i)/\theta(i)]}{\sum_{j=1}^d [\theta_\star(j)/\theta(j)]}\ \frac{\pi(x)}{\theta_\star(i)}\ \mathbb{1}_{\mathsf{X}_i}(x)\ .$$

Hence,

$$\|\pi_\theta d\lambda - \pi_{\theta'} d\lambda\|_{\mathrm{TV}} \leqslant \frac{\sum_{j=1}^d \sum_{i=1}^d \theta_\star(i)\theta_\star(j)\,|1/[\theta(i)\theta'(j)] - 1/[\theta'(i)\theta(j)]|}{\sum_{k=1}^d[\theta_\star(k)/\theta(k)] \quad \sum_{l=1}^d[\theta_\star(l)/\theta'(l)]}\,.$$

We denote by $N(\theta,\theta')$ the numerator of the expression of the right-hand side of the previous inequality. Then,

$$\begin{aligned}
N(\theta,\theta') &= \sum_{j=1}^d \sum_{i\neq j} \theta_\star(i)\theta_\star(j)\ \frac{|\theta'(i)\theta(j) - \theta(i)\theta'(j)|}{\theta(i)\theta'(i)\theta(j)\theta'(j)} \\
&\leqslant \sum_{j=1}^d \sum_{i\neq j} \theta_\star(i)\theta_\star(j)\ \left|\frac{\theta(j)-\theta'(j)}{\theta(i)\theta(j)\theta'(j)}\right| + \sum_{j=1}^d \sum_{i\neq j} \theta_\star(i)\theta_\star(j)\ \left|\frac{\theta(i)-\theta'(i)}{\theta(i)\theta'(i)\theta(j)}\right|\,.
\end{aligned}$$

For the denominator, we use the lower bound

$$\forall i,j \in \{1,\ldots,d\}, \qquad \sum_{k=1}^d[\theta_\star(k)/\theta(k)] \quad \sum_{l=1}^d[\theta_\star(l)/\theta'(l)] \geqslant \frac{\theta_\star(i)\theta_\star(j)}{\theta(i)\theta'(j)}.$$

Therefore,

$$\|\pi_\theta d\lambda - \pi_{\theta'} d\lambda\|_{\mathrm{TV}} \leqslant 2\sum_{j=1}^d \sum_{i\neq j} \left|\frac{\theta(j)-\theta'(j)}{\theta(j)}\right| \leqslant 2(d-1)\sum_{j=1}^d \frac{|\theta(j)-\theta'(j)|}{\theta(j)}\,,$$

which gives the claimed result. □

Lemma 4.7. *For any $\theta,\theta' \in \Theta$ and any $x \in \mathsf{X}$ such that $\pi_\theta(x) \leqslant \pi_{\theta'}(x)$,*

$$\|P_\theta(x,\cdot) - P_{\theta'}(x,\cdot)\|_{\mathrm{TV}} \leqslant 2\ \left(2 \sup_{i\in\{1,\ldots,d\}} \left|1 - \frac{\theta(i)}{\theta'(i)}\right| + \sup_{i\in\{1,\ldots,d\}} \left|1 - \frac{\theta'(i)}{\theta(i)}\right|\right)\,.$$

Proof. For any $x \in \mathsf{X}_j$ and $y \in \mathsf{X}_k$, we have by definition of π_θ (see (2.4))

$$\frac{\pi_\theta(x)\pi_{\theta'}(y)}{\pi_\theta(y)\pi_{\theta'}(x)} = \frac{\theta(k)}{\theta(j)}\frac{\theta'(j)}{\theta'(k)}\,, \qquad \frac{\pi_\theta(x)}{\pi_{\theta'}(x)} = \frac{\theta'(j)}{\theta(j)}\,. \tag{4.23}$$

Since P_θ is a Metropolis kernel, for any bounded measurable function f,

$$\begin{aligned}
|P_\theta f(x) - P_{\theta'} f(x)| &= \left|\int_{\mathsf{X}} q(x,y)\,(\alpha_\theta(x,y) - \alpha_{\theta'}(x,y))\,(f(y)-f(x))\,\lambda(dy)\right|\,, \\
&\leqslant 2\sup_{\mathsf{X}}|f|\ \sup_{\mathsf{X}^2}|\alpha_\theta - \alpha_{\theta'}|\ ,
\end{aligned}$$

with $\alpha_\theta(x,y) = 1 \wedge (\pi_\theta(y)/\pi_\theta(x))$. Let us distinguish all the cases:

- $\pi_\theta(y) \leqslant \pi_\theta(x)$ and $\pi_{\theta'}(y) \leqslant \pi_{\theta'}(x)$. Then,

$$\begin{aligned}
|\alpha_\theta(x,y) - \alpha_{\theta'}(x,y)| &= \left|\frac{\pi_\theta(y)}{\pi_\theta(x)} - \frac{\pi_{\theta'}(y)}{\pi_{\theta'}(x)}\right| \leqslant \frac{|\pi_\theta(y) - \pi_{\theta'}(y)|}{\pi_\theta(x)} + \frac{|\pi_\theta(x) - \pi_{\theta'}(x)|}{\pi_\theta(x)} \\
&\leqslant \frac{|\pi_\theta(y) - \pi_{\theta'}(y)|}{\pi_\theta(y)} + \frac{|\pi_\theta(x) - \pi_{\theta'}(x)|}{\pi_\theta(x)} \\
&\leqslant 2\sup_{\mathsf{X}}\left|1 - \frac{\pi_{\theta'}}{\pi_\theta}\right| = 2\sup_{i\in\{1,\ldots,d\}}\left|1 - \frac{\theta(i)}{\theta'(i)}\right|\,,
\end{aligned}$$

where we used (4.23) in the last equality.

- $\pi_\theta(y) \leqslant \pi_\theta(x)$ and $\pi_{\theta'}(x) \leqslant \pi_{\theta'}(y)$. Since $\pi_\theta(x) \leqslant \pi_{\theta'}(x) \leqslant \pi_{\theta'}(y)$, it holds

$$|\alpha_\theta(x,y) - \alpha_{\theta'}(x,y)| = 1 - \frac{\pi_\theta(y)}{\pi_\theta(x)} \leqslant 1 - \frac{\pi_\theta(y)}{\pi_{\theta'}(y)} \leqslant \sup_{\mathsf{X}} \left|1 - \frac{\pi_\theta}{\pi_{\theta'}}\right| = \sup_{i \in \{1,\ldots,d\}} \left|1 - \frac{\theta'(i)}{\theta(i)}\right| .$$

- $\pi_\theta(x) \leqslant \pi_\theta(y)$ and $\pi_{\theta'}(x) \leqslant \pi_{\theta'}(y)$. Then, $|\alpha_\theta(x,y) - \alpha_{\theta'}(x,y)| = 0$.
- $\pi_\theta(x) \leqslant \pi_\theta(y)$ and $\pi_{\theta'}(y) \leqslant \pi_{\theta'}(x)$. Then, using again (4.23),

$$\begin{aligned}|\alpha_\theta(x,y) - \alpha_{\theta'}(x,y)| &= 1 - \frac{\pi_{\theta'}(y)}{\pi_{\theta'}(x)} \leqslant 1 - \frac{\pi_{\theta'}(y)}{\pi_{\theta'}(x)}\frac{\pi_\theta(x)}{\pi_\theta(y)} = \frac{\pi_{\theta'}(x) - \pi_\theta(x)}{\pi_{\theta'}(x)} + \frac{\pi_\theta(x)}{\pi_{\theta'}(x)}\frac{\pi_\theta(y) - \pi_{\theta'}(y)}{\pi_\theta(y)} \\ &\leqslant \sup_{i \in \{1,\ldots,d\}} \left|1 - \frac{\theta'(i)}{\theta(i)}\right| + \sup_{i \in \{1,\ldots,d\}} \left|1 - \frac{\theta(i)}{\theta'(i)}\right| .\end{aligned}$$

This concludes the proof. □

As a corollary of Lemmas 4.6 and 4.7, we obtain the following result.

Corollary 4.8. *Under A3a and A3c,*

$$\|\pi_{\theta_n} d\lambda - \pi_{\theta_{n+1}} d\lambda\|_{\mathrm{TV}} \leqslant 2d(d-1)\,\gamma_{n+1}, \forall n \geqslant 0 \tag{4.24}$$

and for any $N \geqslant 0$

$$\sup_{x \in \mathsf{X}} \|P_{\theta_n}(x,\cdot) - P_{\theta_{n+1}}(x,\cdot)\|_{\mathrm{TV}} \leqslant 4\left(1 + \frac{1}{1 - \sup_{n \geqslant N} \gamma_{n+1}}\right)\,\gamma_{n+1}, \quad \forall n \geqslant N \ .$$

Proof. The inequality (4.24) immediately follows from Lemma 4.6, (4.22) and the upper bound $|Y_{n+1}(i)| \leqslant 1$. In addition, by Lemma 4.7,

$$\begin{aligned}\|P_{\theta_{n+1}}(x,\cdot) - P_{\theta_n}(x,\cdot)\|_{\mathrm{TV}} &\leqslant 4\left(\sup_i \left|1 - \frac{\theta_{n+1}(i)}{\theta_n(i)}\right| + \sup_i \left|1 - \frac{\theta_n(i)}{\theta_{n+1}(i)}\right|\right) \\ &\leqslant 4\gamma_{n+1}\left(\sup_i |Y_{n+1}(i)| + \sup_i \frac{|Y_{n+1}(i)|}{|1 + \gamma_{n+1}Y_{n+1}(i)|}\right) .\end{aligned}$$

The proof is concluded upon noting that $|Y_{n+1}(i)| \leqslant 1$ and $1 - \gamma_{n+1} \geqslant 1 - \sup_{n \geqslant N} \gamma_{n+1}$. □

Lemma 4.9. *Assume A1 and A2. Then, for any $\theta \in \Theta$, there exists a function $\widehat{H}_\theta$ solving the Poisson equation $\widehat{H}_\theta - P_\theta \widehat{H}_\theta = H(\cdot,\theta) - \pi_\theta(H(\cdot,\theta)) = H(\cdot,\theta) - h(\theta)$. In addition,*

$$\sup_{\theta \in \Theta, x \in \mathsf{X}} \left|\widehat{H}_\theta(x)\right| < \infty ,$$

and there exists a constant $C > 0$ such that for any $\theta, \theta' \in \Theta$,

$$\sup_{\mathsf{X}} \left\{\left|\widehat{H}_\theta - \widehat{H}_{\theta'}\right| + \left|P_\theta \widehat{H}_\theta - P_{\theta'} \widehat{H}_{\theta'}\right|\right\} \leqslant C \frac{|\theta - \theta'|}{\inf_{i \in \{1,\ldots,d\}} \{\theta(i) \wedge \theta'(i)\}} .$$

Proof. Since $\sup_{\theta \in \Theta} \sup_{x \in \mathsf{X}} |H(x,\theta)| \leqslant 1$, the results of Proposition 3.1 show that $\widehat{H}_\theta$ exists for any $\theta \in \Theta$ and (see *e.g.* [28, Section 17.4.1])

$$\sup_{\theta \in \Theta} \sup_{x \in \mathsf{X}} \left| \widehat{H}_\theta(x) \right| \leqslant \sup_{\theta \in \Theta} \sup_{x \in \mathsf{X}} \sum_{n \geqslant 0} |P_\theta^n H(\cdot,\theta)(x) - \pi_\theta(H(\cdot,\theta))| \leqslant \frac{2}{\rho} \, . \tag{4.25}$$

In addition, in view of Proposition 3.1 and [12, Lemma 4.2.], there exists a constant C such that, for any $\theta, \theta' \in \Theta$,

$$\begin{aligned} &\sup_{\mathsf{X}} \left| P_\theta \widehat{H}_\theta - P_{\theta'} \widehat{H}_{\theta'} \right| + \sup_{\mathsf{X}} \left| \widehat{H}_\theta - \widehat{H}_{\theta'} \right| \\ &\qquad \leqslant C \left(\sup_{\mathsf{X}} \left| H(\cdot,\theta) - H(\cdot,\theta') \right| + \sup_{x \in \mathsf{X}} \| P_\theta(x,\cdot) - P_{\theta'}(x,\cdot) \|_{\mathrm{TV}} + \| \pi_\theta d\lambda - \pi_{\theta'} d\lambda \|_{\mathrm{TV}} \right) \, . \end{aligned}$$

By definition of H (see (2.7)), there exists a constant C' such that for any $\theta, \theta' \in \Theta$,

$$\sup_{\mathsf{X}} \left| H(\cdot,\theta) - H(\cdot,\theta') \right| \leqslant C' |\theta - \theta'| \, .$$

The proof is then concluded by Lemmas 4.6 and 4.7. □

Proposition 4.10. *Assume A1, A2 and A3. Then, almost-surely,*

$$\limsup_{k \to \infty} \sup_{\ell \geqslant k} \left| \sum_{n=k}^{\ell} \gamma_{n+1} \left(H(X_{n+1}, \theta_n) - h(\theta_n) \right) \right| = 0 \, .$$

Proof. We decompose the increment into a martingale term and two remainders, using the function $\widehat{H}_\theta$ defined in Lemma 4.9:

$$H(X_{n+1}, \theta_n) - h(\theta_n) = \widehat{H}_{\theta_n}(X_{n+1}) - P_{\theta_n} \widehat{H}_{\theta_n}(X_{n+1}) = M_{n+1} + R^{(1)}_{n+1} + R^{(2)}_{n+1} \, ,$$

with

$$\begin{aligned} M_{n+1} &= \widehat{H}_{\theta_n}(X_{n+1}) - P_{\theta_n} \widehat{H}_{\theta_n}(X_n) \, , \\ R^{(1)}_{n+1} &= P_{\theta_n} \widehat{H}_{\theta_n}(X_n) - P_{\theta_{n+1}} \widehat{H}_{\theta_{n+1}}(X_{n+1}) \, , \\ R^{(2)}_{n+1} &= P_{\theta_{n+1}} \widehat{H}_{\theta_{n+1}}(X_{n+1}) - P_{\theta_n} \widehat{H}_{\theta_n}(X_{n+1}) \, . \end{aligned}$$

Observe that $(M_n)_{n \geqslant 1}$ is a martingale-increment such that $\sum_n \gamma_n^2 \mathbb{E}\left[|M_n|^2 \right] < \infty$ by A3c and Lemma 4.9. Hence (see *e.g.* [13, Corollary 2.2]) $\limsup_k \, \sup_{\ell \geqslant k} \left| \sum_{n=k}^{\ell} \gamma_{n+1} M_{n+1} \right| = 0$ almost surely.

Consider now $\sum_{n=k}^{\ell} \gamma_{n+1} R^{(1)}_{n+1}$. Note that $R^{(1)}_{n+1}$ is a telescopic sum. We therefore resort to Abel's transform, and obtain

$$\sum_{n=k}^{\ell} \gamma_{n+1} R^{(1)}_{n+1} = \gamma_{k+1} P_{\theta_k} \widehat{H}_{\theta_k}(X_k) - \gamma_{\ell+1} P_{\theta_{\ell+1}} \widehat{H}_{\theta_{\ell+1}}(X_{\ell+1}) + \sum_{n=k+1}^{\ell} \left(\gamma_{n+1} - \gamma_n \right) P_{\theta_n} \widehat{H}_{\theta_n}(X_n) \, .$$

In view of Lemma 4.9 and A3a, there exists a constant C such that for any $\ell \geqslant k$,

$$\left| \sum_{j=k}^{\ell} \gamma_{j+1} R^{(1)}_{j+1} \right| \leqslant C \left(\sup_{j \geqslant k} \gamma_{j+1} + \sum_{j=k+1}^{\ell} |\gamma_{j+1} - \gamma_j| \right) \leqslant 2C \gamma_{k+1} \, .$$

Assumption A3a then implies that $\limsup_k \sup_{\ell \geqslant k} \left| \sum_{n=k}^{\ell} \gamma_{n+1} R_{n+1}^{(1)} \right| = 0$ almost surely.

We finally turn to $\sum_{n=k}^{\ell} \gamma_{n+1} R_{n+1}^{(2)}$. Lemma 4.9 combined with assumption A2 imply, after manipulations similar to the ones used in the proof of Corollary 4.8, that there exists a constant C'' such that for any $j \geqslant 0$,

$$\sup_{\mathsf{X}} \left| P_{\theta_{j+1}} \widehat{H}_{\theta_{j+1}} - P_{\theta_j} \widehat{H}_{\theta_j} \right| \leqslant C'' \gamma_{j+1} .$$

Then, by assumption A3c, $\sum_n \gamma_n \left| R_n^{(2)} \right|$ exists almost-surely, which implies that

$$\mathbb{P}\left(\limsup_k \sup_{\ell \geqslant k} \left| \sum_{n=k}^{\ell} \gamma_{n+1} R_{n+1}^{(2)} \right| = 0 \right) = 1 .$$

This gives the claimed result. $\square$

The proof of Theorem 3.3 is now concluded by resorting to [1, Theorems 2.2 and 2.3.]. Theorem 3.2 and Propositions 4.5 and 4.10 prove that the assumptions of these theorems hold.

4.4 Proof of Theorem 3.4

Proof of (3.8). The proof is based on [12, Theorem 2.1]. We successively check the assumptions required to apply this result. First, the condition A1 of [12] holds since $\pi_\theta P_\theta = \pi_\theta$ by assumption A2.

We now turn to condition A2 in [12]. Fix $\varepsilon > 0$. By Proposition 3.1,

$$\mathbb{E}\left[\| P_{\theta_{n-r_\varepsilon}}^{r_\varepsilon}(X_{n-r_\varepsilon}) - \pi_{\theta_{n-r_\varepsilon}} \, d\lambda \|_{\mathrm{TV}} \right] \leqslant \varepsilon$$

by choosing $r_\varepsilon > \ln(\varepsilon/2)/\ln(1-\rho)$. The constant sequence $r_\varepsilon(n) = r_\varepsilon$ is non-increasing and obviously satisfies $r_\varepsilon(n)/n \to 0$. Furthermore, by Corollary 4.8, there exists a constant C (independent of ε) such that

$$\begin{aligned} &\sum_{j=1}^{r_\varepsilon - 1} \mathbb{E}\left[\sup_{x \in \mathsf{X}} \| P_{\theta_{n-r_\varepsilon+j}}(x,\cdot) - P_{\theta_{n-r_\varepsilon}}(x,\cdot) \|_{\mathrm{TV}} \right] \\ &\qquad \leqslant \sum_{j=1}^{r_\varepsilon - 1} \sum_{\ell=0}^{j-1} \mathbb{E}\left[\sup_{x \in \mathsf{X}} \| P_{\theta_{n-r_\varepsilon+\ell+1}}(x,\cdot) - P_{\theta_{n-r_\varepsilon-\ell}}(x,\cdot) \|_{\mathrm{TV}} \right] \leqslant C \sum_{j=1}^{r_\varepsilon - 1} \sum_{\ell=0}^{j-1} \gamma_{n-r_\varepsilon+\ell+1} \underset{n\to\infty}{\longrightarrow} 0 \end{aligned}$$

since the last sum is composed of a finite number of terms, each of them going to 0 in view of assumption A3a This ensures that condition A2 in [12] holds.

Finally, Theorem 3.3 and Lemma 4.6 imply that $\lim_n \int_{\mathsf{X}} f(x) \pi_{\theta_n}(x) \, \lambda(dx) = \int_{\mathsf{X}} f(x) \pi_{\theta_\star}(x) \, \lambda(dx)$ almost-surely. $\square$

Proof of (3.9). We check the conditions of [12, Theorem 2.7]. First, the condition A3 of [12] holds with $V = 1$ (with the notation of [12]) in view of Proposition 3.1. Observe indeed that since $V = 1$, $P_\theta V(x) = 1 = c + (1-c)$ for any $c \in (0,1)$ thus showing the drift inequality. In addition, by Proposition 3.1, $P_\theta(x, A) \geqslant \rho \int_A \pi_\theta(x) \, \lambda(dx)$ for any $x \in \mathsf{X}, A \in \mathcal{X}$: this implies

(i) the minorization condition on the kernel P_θ; (ii) $\pi_\theta \, d\lambda$ is an irreducible measure and P_θ is psi-irreducible; (iii) and P_θ is strongly aperiodic since X is small for P_θ (see [28, Section 5.4.3]).

In addition, by Corollary 4.8, there exists a constant C such that

$$\sum_{k \geqslant 1} \frac{1}{k} \sup_{x \in \mathsf{X}} \|P_{\theta_k}(x, \cdot) - P_{\theta_{k-1}}(x, \cdot)\|_{\mathrm{TV}} \leqslant C \sum_{k \geqslant 1} \frac{\gamma_k}{k} \leqslant C \sum_{k \geqslant 1} \left(\gamma_k^2 + \frac{1}{k^2} \right) < \infty$$

by A3c. This shows that the condition A4 of [12] holds. Finally, the condition A5 of [12] is trivially satisfied in the case under consideration (since $V = 1$ with the notation of [12]). $\square$

4.5 Proof of Theorem 3.5

Proof of (3.10). We write

$$\mathbb{E}\left[\sum_{i=1}^d \theta_n(i) \; f(X_n) \; \mathbb{1}_{\mathsf{X}_i}(X_n)\right] = \mathbb{E}\left[\sum_{i=1}^d \{\theta_n(i) - \theta_\star(i)\} \; f(X_n) \; \mathbb{1}_{\mathsf{X}_i}(X_n)\right] + \sum_{i=1}^d \theta_\star(i) \, \mathbb{E}\left[f(X_n) \; \mathbb{1}_{\mathsf{X}_i}(X_n)\right] \; .$$

Theorem 3.3 and the dominated convergence theorem imply that the first term in the right-hand side converges to zero. By Theorem 3.4, the second term converges to

$$\sum_{i=1}^d \theta_\star(i) \int_{\mathsf{X}_i} f \, \pi_{\theta_\star} \, d\lambda = \frac{1}{d} \sum_{i=1}^d \theta_\star(i) \int_{\mathsf{X}_i} f \frac{\pi}{\theta_\star(i)} \, d\lambda = \frac{1}{d} \int_{\mathsf{X}} f \, \pi \, d\lambda \; ,$$

which gives the claimed result. $\square$

Proof of (3.11). We write

$$\frac{1}{d} \mathcal{I}_n(f) = \frac{1}{n} \sum_{i=1}^d \left(\theta_n(i) - \theta_\star(i)\right) \sum_{k=1}^n f(X_k) \mathbb{1}_{\mathsf{X}_i}(X_k) + \sum_{i=1}^d \theta_\star(i) \left[\frac{1}{n} \sum_{k=1}^n f(X_k) \mathbb{1}_{\mathsf{X}_i}(X_k)\right] \; .$$

We have

$$\frac{1}{n} \left| \sum_{i=1}^d \; \left(\theta_n(i) - \theta_\star(i)\right) \; \sum_{k=1}^n f(X_k) \mathbb{1}_{\mathsf{X}_i}(X_k) \right| \leqslant \sup_{\mathsf{X}} |f| \; \sum_{i=1}^d \; |\theta_n(i) - \theta_\star(i)|$$

and the right-hand side converges to zero almost-surely by Theorem 3.3. In addition, by Theorem 3.4,

$$\frac{1}{n} \sum_{k=1}^n f(X_k) \mathbb{1}_{\mathsf{X}_i}(X_k) \xrightarrow{\text{a.s.}} \int_{\mathsf{X}_i} f \, \pi_{\theta_\star} \, d\lambda = \frac{1}{d \; \theta_\star(i)} \int_{\mathsf{X}_i} f \, \pi \, d\lambda \; .$$

This concludes the proof. $\square$

4.6 Proof of Theorem 3.6

We write $H(X_{n+1}, \theta_n) = h(\theta_n) + e_{n+1} + r_{n+1}$ with

$$e_{n+1} \stackrel{\text{def}}{=} \widehat{H}_{\theta_n}(X_{n+1}) - P_{\theta_n}\widehat{H}_{\theta_n}(X_n) \;, \qquad r_{n+1} \stackrel{\text{def}}{=} P_{\theta_n}\widehat{H}_{\theta_n}(X_n) - P_{\theta_n}\widehat{H}_{\theta_n}(X_{n+1}) \;.$$

The result follows from [10, Theorem 1.1]. We check below the various conditions necessary to apply this theorem, and finally establish the expression of the limiting variance. Notice that, in our context, the event $\{\lim_q \theta_q = \theta_\star\}$ has probability 1 (by Theorem 3.3), and thus, the multiplicative factor $\mathbb{1}_{\{\lim_q \theta_q = \theta_\star\}}$ which appears in all the conditions in [10, Theorem 1.1] can be omitted below.

Condition C1. The vector $\theta_\star$ is a zero of the mean field h in view of (4.21), and h is twice continuously differentiable in a neighborhood of $\theta_\star$ under A1. From (4.21), it is easily checked that $\nabla h(\theta_\star) = -d^{-1}\mathrm{I}$, so that $\nabla h(\theta_\star)$ is a Hurwitz matrix. This gives condition C1 of [10]. □

Condition C2. By definition, $\{e_n, n \geqslant 0\}$ is a martingale increment and by Lemma 4.9, it is bounded, so that conditions C2a and C2b of [10] follow with $\mathbb{1}_{\mathcal{A}_{m,k}} = \mathbb{1}_{\mathcal{A}_m}$ equal to the constant function $\mathbb{1}$. We now consider C2c. A simple computation shows that $\mathbb{E}\left[e_{k+1}e_{k+1}^T|\mathcal{F}_k\right] = \Xi(X_k, \theta_k)$ with

$$\Xi(x,\theta) \stackrel{\text{def}}{=} \int_{\mathsf{X}} P_\theta(x,dy)\ \widehat{H}_\theta(y)\widehat{H}_\theta(y)^T - \left(\int_{\mathsf{X}} P_\theta(x,dy)\widehat{H}_\theta(y)\right)\left(\int_{\mathsf{X}} P_\theta(x,dy)\widehat{H}_\theta(y)\right)^T \;.$$

We introduce the function $\widehat{\Xi}_\theta$ solution of the Poisson equation

$$\widehat{\Xi}_\theta(x) - P_\theta\widehat{\Xi}_\theta(x) = \Xi(x,\theta_\star) - \int_{\mathsf{X}} \Xi(x,\theta_\star)\,\pi_\theta(x)\,\lambda(dx) \;.$$

Since $\sup_x |\Xi(x,\theta_\star)| \leqslant \sup_{\theta,x}\left|\widehat{H}_\theta(x)\right|^2 < \infty$ (see Lemma 4.9), by Proposition 3.1 and [28, Section 17.4.1], such a function exists and $\sup_{\theta\in\Theta, x\in\mathsf{X}}\left|\widehat{\Xi}_\theta(x)\right| < \infty$. Using the previous equality with x replaced by X_k and θ replaced by θ_{k-1}, we obtain

$$\begin{aligned}\Xi(X_k,\theta_k) - \int_{\mathsf{X}} \Xi(x,\theta_\star)\,\pi_{\theta_\star}(x)\lambda(dx) &= \{\Xi(X_k,\theta_k) - \Xi(X_k,\theta_\star)\} \\ &+ \left(\int_{\mathsf{X}} \Xi(x,\theta_\star)\,\pi_{\theta_{k-1}}(x)\lambda(dx) - \int_{\mathsf{X}} \Xi(x,\theta_\star)\,\pi_{\theta_\star}(x)\lambda(dx)\right) \\ &+ \left(\widehat{\Xi}_{\theta_{k-1}}(X_k) - P_{\theta_k}\widehat{\Xi}_{\theta_k}(X_k)\right) + \left(P_{\theta_k}\widehat{\Xi}_{\theta_k}(X_k) - P_{\theta_{k-1}}\widehat{\Xi}_{\theta_{k-1}}(X_k)\right) .\end{aligned}$$

The terms on the right-hand side should be small. This motivates therefore the following decomposition: $\mathbb{E}\left[e_{k+1}e_{k+1}^T|\mathcal{F}_k\right] = U_\star + D_k^{(1)} + D_k^{(2)}$ with

$$U_\star \stackrel{\text{def}}{=} \int_{\mathsf{X}} \Xi(x,\theta_\star)\,\pi_{\theta_\star}(x)\lambda(dx) \;, \qquad D_k^{(2)} \stackrel{\text{def}}{=} \widehat{\Xi}_{\theta_{k-1}}(X_k) - P_{\theta_k}\widehat{\Xi}_{\theta_k}(X_k),$$

and

$$\begin{aligned}D_k^{(1)} = \left(\Xi(X_k,\theta_k) - \Xi(X_k,\theta_\star)\right) &+ \int_{\mathsf{X}} \Xi(x,\theta_\star)\left(\pi_{\theta_{k-1}}(x) - \pi_{\theta_\star}(x)\right)\lambda(dx) \\ &+ \left(P_{\theta_k}\widehat{\Xi}_{\theta_k}(X_k) - P_{\theta_{k-1}}\widehat{\Xi}_{\theta_{k-1}}(X_k)\right) .\end{aligned} \tag{4.26}$$

We first prove that

$$\lim_{n\to\infty} \gamma_n \, \mathbb{E}\left[\left|\sum_{k=1}^n D_k^{(2)}\right|\right] = 0 \; . \tag{4.27}$$

To this end, we decompose this sum as

$$\begin{aligned}\sum_{k=1}^n D_k^{(2)} &= \sum_{k=1}^n \left\{\widehat{\Xi}_{\theta_{k-1}}(X_k) - P_{\theta_{k-1}}\widehat{\Xi}_{\theta_{k-1}}(X_{k-1})\right\} + \sum_{k=1}^n \left\{P_{\theta_{k-1}}\widehat{\Xi}_{\theta_{k-1}}(X_{k-1}) - P_{\theta_k}\widehat{\Xi}_{\theta_k}(X_k)\right\} \\ &= \sum_{k=1}^n \left\{\widehat{\Xi}_{\theta_{k-1}}(X_k) - P_{\theta_{k-1}}\widehat{\Xi}_{\theta_{k-1}}(X_{k-1})\right\} + P_{\theta_0}\widehat{\Xi}_{\theta_0}(X_0) - P_{\theta_n}\widehat{\Xi}_{\theta_n}(X_n) \; .\end{aligned}$$

Since $\sup_{\theta\in\Theta, x\in\mathsf{X}} \left|\widehat{\Xi}_\theta(x)\right| < \infty$, the last two terms on the right-hand side of the above equality are such that $\gamma_n \mathbb{E}\left[\left|P_{\theta_0}\widehat{\Xi}_{\theta_0}(X_0) - P_{\theta_n}\widehat{\Xi}_{\theta_n}(X_n)\right|\right] \to 0$. The first term is the sum of bounded martingale increments: by [13, Theorem 2.10], there exists a constant C such that

$$\begin{aligned}&\sup_n \mathbb{E}\left[\left|\sum_{k=1}^n \left\{\widehat{\Xi}_{\theta_{k-1}}(X_k) - P_{\theta_{k-1}}\widehat{\Xi}_{\theta_{k-1}}(X_{k-1})\right\}\right|\right] \\ &\qquad\qquad \leqslant \sup_n \left(\mathbb{E}\left[\left|\sum_{k=1}^n \left\{\widehat{\Xi}_{\theta_{k-1}}(X_k) - P_{\theta_{k-1}}\widehat{\Xi}_{\theta_{k-1}}(X_{k-1})\right\}\right|^2\right]\right)^{1/2} \leqslant C\sqrt{n} \; .\end{aligned}$$

Since $\lim_n \gamma_n \sqrt{n} = 0$, this concludes the proof of (4.27). We now prove that

$$D_k^{(1)} \xrightarrow{\text{a.s.}} 0 \; . \tag{4.28}$$

We start with the first term in the definition (4.26) of $D_k^{(1)}$. Under A1, there exist $\eta > 0$ and a random variable N, almost surely finite, such that

$$\inf_{n\geqslant N} \inf_i \{\theta_n(i) \wedge \theta_\star(i)\} \geqslant \eta \qquad \text{a.s.} \tag{4.29}$$

By Lemma 4.7 and the property $\sup_{\theta\in\Theta, x\in\mathsf{X}} \left|\widehat{H}_\theta(x)\right| < \infty$ (see Lemma 4.9), there exists a constant C such that for any $x \in \mathsf{X}$, $\theta, \theta' \in \Theta$,

$$\left|\Xi(x,\theta) - \Xi(x,\theta')\right| \leqslant C \left(\sup_{y\in\mathsf{X}} \left|\widehat{H}_\theta(y) - \widehat{H}_{\theta'}(y)\right| + \frac{|\theta - \theta'|}{\inf_i \theta(i) \wedge \theta'(i)}\right) \; . \tag{4.30}$$

By (4.29) and Lemma 4.9, there exists a random variable Z almost-surely finite such that

$$\sup_{x\in\mathsf{X}} |\Xi(x,\theta_k) - \Xi(x,\theta_\star)| \leqslant Z\,|\theta_k - \theta_\star|, \qquad \text{a.s.}$$

and the right-hand side converges to zero almost surely. For the second term in the definition (4.26) of $D_k^{(1)}$, we use Lemma 4.6, (4.29) and the bound $\sup_{\theta\in\Theta, x\in\mathsf{X}} |\Xi(x,\theta)| < \infty$ to obtain the existence of a random variable Z almost-surely finite such that for any $k \geqslant 1$,

$$\begin{aligned}\left|\int_{\mathsf{X}} \Xi(x,\theta_\star)\;\{\pi_{\theta_k}(x) - \pi_{\theta_\star}(x)\}\,\lambda(dx)\right| &\leqslant \sup_{\theta\in\Theta, x\in\mathsf{X}} |\Xi(x,\theta)|\;\|\pi_{\theta_k} d\lambda - \pi_{\theta_\star} d\lambda\|_{\mathrm{TV}} \\ &\leqslant Z\,|\theta_k - \theta_\star| \qquad \text{a.s.}\end{aligned}$$

The right-hand side converges to zero almost surely. Finally, for the third term in the definition (4.26) of $D_k^{(1)}$, by Lemma 4.9, it can be proved that there exists a random variable Z almost-surely finite such that for any $k \geqslant 1$,

$$\sup_{x \in \mathsf{X}} \left| P_{\theta_k} \widehat{\Xi}_{\theta_k}(x) - P_{\theta_{k-1}} \widehat{\Xi}_{\theta_{k-1}}(x) \right| \leqslant Z \left| \theta_k - \theta_{k-1} \right| \qquad \text{a.s.}$$

and the right-hand side converges to zero almost surely. This concludes the proof of (4.28) and the proof of the condition C2c of [10]. $\square$

Condition C3. We write $r_{n+1} = r_{n+1}^{(1)} + r_{n+1}^{(2)}$ with

$$r_{n+1}^{(1)} \stackrel{\text{def}}{=} P_{\theta_{n+1}} \widehat{H}_{\theta_{n+1}}(X_{n+1}) - P_{\theta_n} \widehat{H}_{\theta_n}(X_{n+1}) \;, \quad r_{n+1}^{(2)} \stackrel{\text{def}}{=} P_{\theta_n} \widehat{H}_{\theta_n}(X_n) - P_{\theta_{n+1}} \widehat{H}_{\theta_{n+1}}(X_{n+1}) \;.$$

By Lemma 4.9 and (4.29), there exists a random variable Z almost-surely finite such that $|r_{n+1}^{(1)}| \leqslant Z \left| \theta_{n+1} - \theta_n \right| \leqslant Z \gamma_{n+1}$ almost-surely. Moreover,

$$\sqrt{\gamma_n}\, \mathbb{E}\left[\left| \sum_{k=1}^{n} r_k^{(2)} \right| \right] \leqslant \sqrt{\gamma_n}\, \mathbb{E}\left[\left| P_{\theta_0} \widehat{H}_{\theta_0}(X_0) - P_{\theta_n} \widehat{H}_{\theta_n}(X_n) \right| \right] \leqslant 2 \sqrt{\gamma_n} \sup_{x,\theta} \left| \widehat{H}_\theta(x) \right| \;,$$

where the supremum in the right-hand side is finite by Lemma 4.9. This concludes the proof of condition C3 of [10]. $\square$

Condition C4. This condition is precisely assumptions A3b-c and A4. $\square$

Limiting variance. In case (i) of assumption A4, the limiting variance Σ solves the equation $\Sigma \nabla h(\theta_\star)^T + \nabla h(\theta_\star) \Sigma = -U_\star$. Since $\nabla h(\theta_\star) = -d^{-1}\mathrm{Id}$, it holds $\Sigma = (d/2) U_\star$. In case (ii), the limiting variance solves the equation $\Sigma(\mathrm{Id} + 2\gamma_\star \nabla h(\theta_\star)^T) + (\mathrm{Id} + 2\gamma_\star \nabla h(\theta_\star))\Sigma = -2\gamma_\star U_\star$, so that $(d - 2\gamma_\star)\Sigma = -\gamma_\star d\, U_\star$. $\square$

Acknowledgements

We thank Prof. Eric Moulines for stimulating discussions. This work is supported by the French National Research Agency under the grants ANR-09-BLAN-0216-01 (MEGAS) and ANR-08-BLAN-0218 (BigMC).

References

[1] C. Andrieu, E. Moulines, and P. Priouret, *Stability of stochastic approximation under verifiable conditions*, SIAM J. Control Optim. **44** (2005), 283–312.

[2] Y. F. Atchade and J. S. Liu, *The Wang-Landau algorithm for Monte Carlo computation in general state spaces*, Stat. Sinica **20** (2010), no. 1, 209–233.

[3] V. Babin, C. Roland, and C. Sagui, *Adaptively biased molecular dynamics for free energy calculations*, J. Chem. Phys. **128** (2008), 134101.

[4] A. Benveniste, M. Métivier, and Priouret P., *Adaptive Algorithms and Stochastic Approximations*, Springer-Verlag, 1987.

[5] L. Bornn, P. Jacob, P. Del Moral, and A. Doucet, *An Adaptive Interacting Wang-Landau Algorithm for Automatic Density Exploration*, J. Comput. Graph. Stat. (2012).

[6] H. Chen, L. Guo, and A. Gao, *Convergence and robustness of the Robbins-Monro algorithm truncated at randomly varying bounds*, Stoch. Proc. Appl. **27** (1988), 217–231.

[7] N. Chopin, T. Lelièvre, and G. Stoltz, *Free energy methods for efficient exploration of mixture posterior densities*, Stat. Comput. **22** (2012), no. 4, 897–916.

[8] E. Darve and A. Pohorille, *Calculating free energies using average force*, J. Chem. Phys. **115** (2001), no. 20, 9169–9183.

[9] B. Dickson, F. Legoll, T. Lelièvre, G. Stoltz, and P. Fleurat-Lessard, *Free energy calculations: An efficient adaptive biasing potential method*, J. Phys. Chem. B **114** (2010), 5823–5830.

[10] G. Fort, *Central Limit Theorems for Stochastic Approximation with Controlled Markov chain Dynamics*, arXiv:1309.3116

[11] G. Fort, B. Jourdain, E. Kuhn, T. Lelièvre and G. Stoltz, *Efficiency of the Wang-Landau algorithm: a simple test case*, in preparation.

[12] G. Fort, E. Moulines, and P. Priouret, *Convergence of adaptive and interacting Markov chain Monte Carlo algorithms*, Ann. Statist. **39** (2012), no. 6, 3262–3289.

[13] P. Hall and P.P. Heyde, *Martingale limit theory and its application*, Academic Press, 1980.

[14] W. K. Hastings, *Monte Carlo sampling methods using Markov chains and their applications*, Biometrika **57** (1970), 97–109.

[15] J. Hénin and C. Chipot, *Overcoming free energy barriers using unconstrained molecular dynamics simulations*, J. Chem. Phys. **121** (2004), no. 7, 2904–2914.

[16] P. E. Jacob and R. J. Ryder, *The Wang-Landau algorithm reaches the Flat Histogram criterion in finite time*, Ann. Appl. Probab. (2012)

[17] B. Jourdain, T. Lelièvre, and R. Roux, *Existence, uniqueness and convergence of a particle approximation for the adaptive biasing force process*, Math. Model. Numer. Anal. **44** (2010), no. 5, 831–865.

[18] H. Kushner and G. Yin, *Stochastic Approximation Algorithms and Applications*, Application of Mathematics, Springer-Verlag, 1997.

[19] T. Lelièvre and K. Minoukadeh, *Longtime convergence of an adaptive biasing force method: The bi-channel case*, Arch. Ration. Mech. Anal. **202** (2011), no. 1, 1–34.

[20] T. Lelièvre, M. Rousset, and G. Stoltz, *Computation of free energy profiles with adaptive parallel dynamics*, J. Chem. Phys. **126** (2007), 134111.

[21] T. Lelièvre, M. Rousset, and G. Stoltz, *Long-time convergence of an Adaptive Biasing Force method*, Nonlinearity **21** (2008), 1155–1181.

[22] T. Lelièvre, M. Rousset, and G. Stoltz, *Free-Energy Computations: A Mathematical Perspective*, Imperial College Press, 2010.

[23] J. Lelong, *Almost sure convergence for randomly truncated stochastic algorithms under verifiable conditions*, Statist. Probab. Lett. **78** (2008), no. 16, 2632–2636.

[24] F. Liang, *A general Wang-Landau algorithm for Monte Carlo computation*, J. Am. Stat. Assoc. **100** (2005), 1311–1327.

[25] F. Liang, C. Liu, and R. J. Carroll, *Stochastic approximation in Monte Carlo computation*, J. Am. Stat. Assoc. **102** (2007), 305–320.

[26] S. Marsili, A. Barducci, R. Chelli, P. Procacci, and V. Schettino, *Self-healing Umbrella Sampling: A non-equilibrium approach for quantitative free energy calculations*, J. Phys. Chem. B **110** (2006), no. 29, 14011–14013.

[27] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, *Equations of State Calculations by Fast Computing Machines*, J. Chem. Phys. **21** (1953), no. 6, 1087–1091.

[28] S. Meyn and R.L. Tweedie, *Markov Chains and Stochastic Stability*, Cambridge, 2009.

[29] K. Minoukadeh, C. Chipot, and T. Lelièvre, *Potential of mean force calculations: a multiple-walker adaptive biasing force approach*, J. Chem. Th. Comput. **6** (2010), no. 4, 1008–1017.

[30] H. Robbins and S. Monro, *A stochastic approximation method*, Ann. Math. Statist. **22** (1951), no. 3, 400–407.

[31] F.G. Wang and D.P. Landau, *Determining the density of states for classical statistical models: A random walk algorithm to produce a flat histogram*, Phys. Rev. E **64** (2001), 056101.

[32] F.G. Wang and D.P. Landau, *Efficient, multiple-range random walk algorithm to calculate the density of states*, Phys. Rev. Lett. **86** (2001), no. 10, 2050–2053.