Probability theory

Convergence of adaptive biasing potential methods for diffusions

Convergence de méthodes de biaisage adaptatif du potentiel dans des processus de diffusion

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A B S T R A C T

We prove the consistency of an adaptive importance sampling strategy based on biasing the potential energy function \( V \) of a diffusion process \( dX_t^0 = -\nabla V(X_t^0)dt + dW_t \); for the sake of simplicity, periodic boundary conditions are assumed, so that \( X_t^0 \) lives on the flat \( d \)-dimensional torus. The goal is to sample its invariant distribution \( \mu = Z^{-1} \exp(-V(x))dx \). The bias \( V_t - V \), where \( V_t \) is the new (random and time-dependent) potential function, acts only on some coordinates of the system, and is designed to flatten the corresponding empirical occupation measure of the diffusion \( X \) in the large-time regime. The diffusion process writes \( dX_t = -\nabla V(X_t)dt + dW_t \), where the bias \( V_t - V \) is function of the key quantity \( \overline{\pi}_t \): a probability occupation measure which depends on the past of the process, i.e. on \( \{X_{t \in [0,t]}\} \). We are thus dealing with a self-interacting diffusion. In this note, we prove that when \( t \) goes to infinity, \( \overline{\pi}_t \) almost surely converges to \( \mu \). Moreover, the approach is justified by the convergence of the bias to a limit that has an interpretation in terms of a free energy. The main argument is a change of variables, which formally validates the consistency of the approach. The convergence is then rigorously proven adapting the ODE method from stochastic approximation.

R É S U M É

Nous prouvons la convergence d’une méthode adaptative d’échantillonnage préférentiel, basée sur le biaisage du potentiel d’un processus de diffusion \( dX_t^0 = -\nabla V(X_t^0)dt + dW_t \); pour simplifier, des conditions au bord périodiques sont appliquées, si bien que \( X_t^0 \) est à valeurs dans le tore \( d \)-dimensionnel. L’objectif est d’échantillonner sa mesure invariante \( \mu = Z^{-1} \exp(-V(x))dx \). Le biais \( V_t - V \), où \( V_t \) est le nouveau potentiel (aléatoire et dépendant du temps), n’agit que sur certaines coordonnées du système, et est construit de façon à rendre la mesure d’occupation empirique correspondante uniforme en temps long. Le processus de diffusion s’écrit \( dX_t = -\nabla V(X_t)dt + dW_t \), où le biais \( V_t - V \) est fonction de la quantité \( \overline{\pi}_t \): une mesure d’occupation qui dépend du passé du processus, i.e. de \( \{X_{t \in [0,t]}\} \). Nous étudions ainsi un processus de diffusion en auto-interaction. Dans cette

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1. Introduction

Computing the average \( \mu(\varphi) = \int_D \varphi(x) \mu(dx) \) of a function \( \varphi : D \to \mathbb{R} \), with respect to a probability distribution \( \mu \) defined on \( D \subset \mathbb{R}^d \), is typically a challenging task in many applications (e.g., chemistry, statistical physics, see, e.g., [5]), since usually \( d \) is large and \( \mu \) is multimodal.

In the sequel, we assume that \( D = \mathbb{T}^d = (\mathbb{R}/\mathbb{Z})^d \) is the flat \( d \)-dimensional torus, and that \( \mu \) writes

\[
\mu(dx) = \mu_\beta(dx) = \frac{\exp(-\beta V(x))}{Z(\beta)} dx.
\]

where \( V : \mathbb{T}^d \to \mathbb{R} \) is a smooth potential function, \( \beta \in (0, +\infty) \) is the inverse temperature, \( dx \) denotes the Lebesgue measure on \( \mathbb{T}^d \) and \( Z(\beta) \) is a normalizing constant. In this context, the multimodality of \( \mu_\beta \) follows, in the case of so-called energetic barriers, from the existence of several local minima of \( V \).

A standard approach to computing \( \mu_\beta(\varphi) \) is to consider the following SDE on \( \mathbb{T}^d \) (overdamped Langevin dynamics):

\[
dX^0_t = -\nabla V(X^0_t) dt + \sqrt{2\beta^{-1}} dW_t, \quad X^0_0 = x,
\]

where \( (W(t))_{t \geq 0} \) is standard Brownian Motion on \( \mathbb{T}^d \). Indeed, it is well-known that, for any continuous function \( \varphi : \mathbb{T}^d \to \mathbb{R} \), almost surely

\[
\frac{1}{t} \int_0^t \varphi(X^0_r) dr \xrightarrow{t \to +\infty} \int_{\mathbb{T}^d} \varphi(x) \mu_\beta(dx).
\]

However, this convergence may be very slow, when \( \beta \) is large and \( V \) has several minima: the stochastic process \( X^0 \) is then metastable, and hopping from the neighborhood of one local minimum of \( V \) to another is a rare event that may have a strong influence on the estimation of averages \( \mu_\beta(\varphi) \).

Many strategies based on importance sampling techniques – self-healing umbrella-sampling [7], well-tempered meta-dynamics [1], Wang–Landau algorithms, adaptive biasing force, etc. – have been proposed and applied to improve the convergence to equilibrium of stochastic processes in order to compute approximations of \( \mu_\beta \). We refer for instance to [6] and references therein for a mathematical review.

In this work, we focus on an Adaptive Biasing Potential (ABP) method, given by the system (4). The method was designed in [4,7] for problems in chemistry, and up to our knowledge no rigorous general mathematical analysis has been performed so far. Precisely, in (2), \( V \) is replaced with a time-dependent and random potential function \( V_t \), which is modified adaptively, using the history of the process up to time \( t \): \( A_t \) depends on the values of the associated stochastic process \( X_t \) for all \( 0 \leq r \leq t \). Here, \( V_t = V - A_t \circ \xi \), where, for some \( m \in \{1, \ldots, d - 1\} \), \( A_t : \mathbb{T}^m \to \mathbb{R} \) and \( \xi : \mathbb{T}^d \to \mathbb{T}^m \) is a smooth function, referred to as the reaction coordinate mapping. In applications, usually \( m \in \{1, 2, 3\} \). To simplify further the presentation, we assume that \( \xi(x_1, \ldots, x_d) = (x_1, \ldots, x_m) \); in this case, \( z = (x_1, \ldots, x_m) = \xi(x_1, \ldots, x_d) \) (resp. \( z^* = (x_{m+1}, \ldots, x_d) \)) is interpreted as the slow (resp. fast) variable.

The dynamics of the ABP method is given by the following system

\[
\begin{aligned}
\left\{ 
\begin{array}{l}
\dX_t = -\nabla (V - A_t \circ \xi)(X_t) dt + \sqrt{2\beta^{-1}} dW(t) \\
\mu_t = \frac{\mu_0 + \int_0^t \exp(-\beta A_t(\xi(X_t)) \delta x, dr}{\int_0^t \exp(-\beta A_t(\xi(X_t)) \delta x, dr} \\
\exp(-\beta A_t(z)) = \int_{\mathbb{T}^m} K(z, \xi(x)) \mu_t(dx), \; \forall z \in \mathbb{T}^m,
\end{array}
\right.
\]

where a smooth kernel function \( K : \mathbb{T}^m \times \mathbb{T}^m \to (0, +\infty) \), such that \( \int_{\mathbb{T}^m} K(z, \zeta)dz = 1, \forall \zeta \in \mathbb{T}^m \), is introduced to define a smooth function \( A_t \) from the distribution \( \mu_t \). The unknowns in (4) are the stochastic processes \( t \mapsto X_t \in \mathbb{T}^d, t \mapsto \mu_t \in \mathcal{P}(\mathbb{T}^d) \) (the set of Borel probability distributions on \( \mathbb{T}^d \), endowed with the usual topology of weak convergence of probability distributions), and \( t \mapsto A_t \in \mathcal{C}^\infty(\mathbb{T}^m) \) (the set of infinitely differentiable functions on \( \mathbb{T}^m \)). In addition to (4), arbitrary (and deterministic, for simplicity) initial conditions \( X_{t=0} = x, \mu_{t=0} = \mu_0 \) and \( A_{t=0} = A_0 \) are prescribed.
The third equation in (4) introduces a coupling between the evolutions of the diffusion \( X_t \) and of the weighted empirical distribution \( \overline{\mu}_t \): then \( X \) can be seen as a self-interacting diffusion process, like in \([3]\).

Our main result is the consistency of the ABP approach.

**Theorem 1.1.** Almost surely, \( \overline{\mu}_t \to \mu_\beta \) in \( \mathcal{P}(\mathbb{T}^d) \).

With standard arguments, **Theorem 1.1** yields almost sure convergence of \( A_t \) in \( C^k(\mathbb{T}^m) \), for all \( k \in \mathbb{N} \).

**Corollary 1.2.** Set \( \exp(-\beta A_\infty) = \int K(\cdot, \xi(\cdot)) \exp(-\beta A_\star(\cdot, \beta)) \, d\xi \), where \( A_\star(\cdot, \beta) \) is the free energy at temperature \( \beta^{-1} \), defined by: for all \( z \in \mathbb{T}^m \)

\[
\exp(-\beta A_\infty(z)) = \int_{\mathbb{T}^d} \frac{\exp(-\beta V(z, z^\perp))}{Z(\beta)} \, dz^\perp. \tag{5}
\]

Usually, \( K(z, \xi) = K^\varepsilon((z - \xi)/\varepsilon) \), where \( \varepsilon \in (0, 1) \) and \( K : \mathbb{R}^m \to (0, +\infty) \) is symmetric, smooth, with compact support in \([1/2, 1/2]\); then \( A_\infty \) converges to \( A_\star(\cdot, \beta) \), in \( C^\infty \). Choosing \( \varepsilon \) sufficiently small, \( A_t \) almost surely approximates the free energy \( A_\star(\cdot, \beta) \) when \( t \to +\infty \), thanks to **Corollary 1.2**.

Equation (5) means that \( \exp(-\beta A_\star(z, \beta)) \, dz \in \mathcal{P}(\mathbb{T}^m) \) is the image \( \mu_\beta(z^{-1}(\cdot)) \) of \( \mu_\beta \) by \( \xi \). The free energy gives an effective potential along \( \xi \), which is chosen in practice such that \( (\xi(X_0^d))|_{t \geq 0} \) is metastable; this is related to \( \mu_\beta(z^{-1}(\cdot)) \) being metastable, for instance when \( A_\star(\cdot, \beta) \) has several local minima.

This is why, in many applications, computing free-energy differences \( A_\star(z_1, \beta) - A_\star(z_2, \beta) \) is essential, see \([6]\). The free-energy function also theoretically provides efficient importance sampling algorithms; however, these algorithms can only be implemented if \( A_\star \) is explicitly known, and adaptive strategies allow us to circumvent this practical difficulty. Define biased probability distribution and dynamics

\[
\mu^*_\beta = \frac{\exp(-\beta [V(x) - A_\star(\xi(x), \beta)])}{Z(\beta)} \, dx \tag{6}
\]

\[
dX^*_\beta = -\nabla[V - A_\star(\xi(\cdot), \beta)](X^*_\beta) \, dt + \sqrt{2\beta^{-1}} \, dW(t).
\]

by replacing the original potential function \( V \) with the biased potential function \( V - A_\star(\xi(\cdot), \beta) \) in (1) and (2). Note that \( \mu^*_\beta \) is the unique invariant distribution of \( X^* \). By construction, it is easy to check that the image by \( \xi \) of \( \mu^*_\beta \) is the uniform distribution on \( \mathbb{T}^m \), i.e. the associated free energy is equal to 0.

Now define (unweighted) empirical distributions associated with (2) and (6) respectively:

\[
\rho^0_t = \frac{1}{t} \int_0^t \delta_{X^*_\beta} \, dr, \quad \rho^*_t = \frac{1}{t} \int_0^t \delta_{X^*_\beta} \, dr.
\]
Then, by (3), the image by $\xi$ of $\rho_0^\mu$, resp. $\rho^\mu$, converges almost surely in $\mathcal{P}(\mathbb{T}^m)$, to $\exp(-\beta A_*(z, \beta))dz$, resp. $dz$. Thus the dynamics in (6) reaches asymptotically a flat histogram property in the $z = \xi(x)$ direction; the exploration of $\mathbb{T}^m$ is thus faster for $\xi(X^*)$ than for $\xi(X^0)$, and in turn the convergence of $X^*$ to $\mu^*_\beta$ is expected to be faster than the convergence of $X^0$ to $\mu_\beta$.

Finally, the construction of the ABP method (4), in particular the use of weighted empirical distributions $\overline{\mu}_t$, is motivated by the following almost sure convergence: for any continuous $\varphi: \mathbb{T}^d \to \mathbb{R}$,

$$\frac{1}{\sqrt{t}} \int_0^t \exp(-\beta A_*(\xi(X^*_s), \beta))\varphi(X^*_s) \, ds \to_{t \to +\infty} \mu^*_\beta(\varphi \exp(-\beta A_*(\xi(\cdot), \beta))) = \mu_\beta(\varphi).$$

Theorem 1.1 thus extends this consistency property from a non-adaptive (6) to an adaptive dynamics (4).

3. Proof of Theorem 1.1

In this section, we provide the main ideas of the proof of Theorem 1.1. Some technical arguments are skipped, and will be fully detailed in [2], in a more general framework. We first state an important property of $A_t$, and then introduce a change of variables, which helps us identify a more standard form for self-interacting diffusion processes. We then adapt in our context arguments from [3] to establish the consistency of the ABP approach thanks to the ODE method from stochastic approximation theory.

3.1. Properties of the ABP dynamics (4)

Our first task in the study of the ABP dynamics is to study the well-posedness of the equation, i.e. the existence of a unique global solution $t \mapsto (X_t, \overline{\mu}_t, A_t) \in \mathbb{T}^d \times \mathcal{P}(\mathbb{T}^d) \times C^\infty(\mathbb{T}^m)$. In order to apply a standard fixed point/Picard iteration strategy, it is essential to control the Lipschitz constant of $\nabla (A_t \circ \xi)$ (first equation in (4)). This key stability property is ensured as follows. Let $m = \min_{z \in \mathbb{T}^m} K(z, \xi)$, and $M^{(n)} = \max_{z \in \mathbb{T}^m} \{ |\partial^n_x K(z, \xi) | \}$ for $n \in [0, 1]$, where $\partial^n_x$ denotes the differential of order $n$, and introduce

$$A = \left\{ A \in C^\infty(\mathbb{T}^m) \mid \min_{z \in \mathbb{T}^m} e^{-\beta A(z)} \geq m, \max_{z \in \mathbb{T}^m} |\partial^n_x e^{-\beta A(z)}| \leq M^{(n)}, n = 0, 1 \right\}.$$ 

Then $A$ is left invariant by the evolution $t \mapsto A_t$, i.e. $A_0 \in A$ implies $A_t \in A$ for all $t \geq 0$, almost surely.

3.2. Change of variables

The stochastic process $t \mapsto \overline{\mu}_t$, with values in $\mathcal{P}(\mathbb{T}^d)$, is the unique solution of the random Ordinary Differential Equation (ODE), interpreted in a weak sense (considering continuous bounded test functions):

$$\frac{d\overline{\mu}_t}{dt} = \frac{\theta'(t)}{1 + \theta(t)} (\delta_{X_t} - \overline{\mu}_t),$$

where $\theta(t) = \int_0^t \exp(-\beta A_t(\xi(X_s))) \, ds$. The random function $\theta: [0, +\infty) \to [0, +\infty)$ is a $C^1$-diffeomorphism: indeed, for all $t \geq 0$, almost surely $\theta'(t) = \exp(-\beta A_t(\xi(X_t))) \in [m, M]$. This fundamental property allows us to apply the following change of variables:

$$s = \theta(t) , \quad t = \theta^{-1}(s) ; \quad Y_s = X_t , \quad \overline{V}_s = \overline{\mu}_t , \quad B_s = A_t .$$

Observe that almost surely $s = \theta(t) \to +\infty$ and that $t = \theta^{-1}(s) \to +\infty$. Instead of studying the asymptotic behavior of $\overline{\mu}_t$ when $t \to +\infty$, it is thus equivalent to study the asymptotic behavior of $\overline{V}_s$ when $s \to +\infty$. In the new variables (9), the ABP dynamics (4) writes

$$\begin{cases}
   dY_s = -\nabla (V - B_s \circ \xi)(Y_s) e^{\beta B_s(\xi(Y_s))} \, ds + \sqrt{2\beta^{-1} e^{\beta B_s(\xi(Y_s))}} \, dW(s) \\
   d\overline{V}_s = \frac{\overline{V}_0 + \int_0^s \delta_y \, ds}{1 + s} - \int_0^s \exp(-\beta B_s(z)) \, d\overline{V}_s(\mathbb{I})(dx) ,
\end{cases}$$

where $W$ is a new standard Brownian motion on $\mathbb{T}^d$, defined from $W$ and $\theta$. Notice that $\overline{V}_s$ is a nonweighted empirical distribution and that $s \mapsto \overline{V}_s$ satisfies the simpler random ODE

$$\frac{d\overline{V}_s}{ds} = \frac{1}{1 + s} (\delta_{\overline{V}_s} - \overline{V}_s).$$

The change of variable (9) removes both $\theta(t)$ from (8) and weights $\exp(-\beta A_t(\xi(X_t))) = \theta'(t)$ from (4).

Thanks to Equation (10), an analogy with the framework of [3] can now be made. Even though we cannot directly apply the results therein, due to the specific form of the dynamics on $Y$, we follow the same strategy for the analysis of $\overline{V}_s$ when $s \to +\infty$: we use the ODE method.
3.3. Application of the ODE method and sketch of proof of Theorem 1.1

The guideline of the so-called ODE approach we wish to apply is as follows: there is an asymptotic time-scale separation between the (fast) evolution of \( Y_s \) and the (slow) evolution of \( \overline{Y}_s \) (and of \( B_s \)). The asymptotic behavior of \( \overline{Y}_s \) is then determined by a so-called limit ODE, where \( \delta Y_s \) is replaced in (11) with the unique invariant probability distribution of the following SDE on \( \mathbb{T}^d \),

\[
dY^B_s = -\nabla (V - B \circ \xi) (Y_s) e^{\beta B (\xi (Y_s))} \, ds + \sqrt{2 \beta^{-1} e^{\beta B (\xi (Y_s))}} dW(s),
\]

i.e. the first (fast) equation of (10) where the slowly varying variable \( B_s \) is frozen at an arbitrary value \( B \in A \). In fact, we have the following fundamental result: the invariant distribution of (12) does not depend on \( B \).

**Proposition 3.1.** For any smooth \( B : \mathbb{T}^m \rightarrow \mathbb{R} \), the unique invariant distribution of (12) is \( \mu_\beta \).

**Proposition 3.1.** is essential and its proof is very simple. Indeed, introduce the generator \( \mathcal{L}_X^B \), resp. the unique invariant distribution \( \mu_\beta (dx) = Z^B (\beta)^{-1} \exp (-\beta (V - B \circ \xi))(x) \, dx \), of \( X^B \), where \( dX^B_s = -\nabla (V - B \circ \xi) (Y_s) \, dt + \sqrt{2 \beta^{-1}} dW(t) \). Then the generator \( \mathcal{L}_Y^B \) of \( Y^B \) defined by (12) is equal to \( \exp (\beta B \circ \xi) \mathcal{L}_X^B \). **Proposition 3.1** is a consequence of the following identity: for any smooth \( \phi, \psi : \mathbb{T}^d \rightarrow \mathbb{R} \),

\[
\mathcal{L}_Y^B \phi (y) \psi (y) \mu_\beta (dy) = \int \phi (x) \mathcal{L}_X^B \psi (x) \mu_\beta (dx) = 0.
\]

We now outline the end of the proof of Theorem 1.1, adapting the arguments from [3] in our original case; details in a more general setting are given in [2]. The ODE method suggests us to define \( \Gamma (\sigma, s, \nu) = \Gamma_{\sigma - s} (\nu) \), for any \( \sigma \geq s \) and \( \nu \in \mathcal{P}(\mathbb{T}^d) \), where \( \Gamma_{\sigma} (\nu) = e^{-\sigma} \nu + (1 - e^{-\sigma}) \mu_\beta \xrightarrow{\sigma \rightarrow +\infty} \mu_\beta \) is the solution of \( \frac{d\nu}{ds} = \mu_\beta - \Gamma \nu \), with \( \Gamma \nu = \nu \). To state (without proof) our last technical result, we recall that weak convergence in \( \mathcal{P}(\mathbb{T}^d) \) is associated with the following metric

\[
d(\mu^1, \mu^2) = \sum_{n=1}^{+\infty} \frac{1}{2^n} \min (1, | \int f_n d\mu^1 - f_n d\mu^2 |).
\]

for a given family \( (f_n)_{n \geq 1} \) of \( \mathcal{C}^1 \) functions, which is dense in \( \mathcal{C}^0(\mathbb{T}^d) \).

**Proposition 3.2.** For any \( S \geq 0 \), almost surely \( \Delta (s, S) = \sup_{\sigma \in [0, S]} \| \Gamma (\sigma, s, \tau_s) \| \rightarrow 0 \), i.e. almost surely \( s \mapsto \tau_s \) is an asymptotic pseudo-trajectory of the semi-flow \( \Gamma \).

We refer to [3] for a proof of a similar result in a different context, and to [2] for a detailed proof in a more general context; the main difference between the two situations is the use of a specific Poisson equation related to the generator of (12).

To conclude, observe that \( d(\tau_{\exp (s)}, \mu_\beta) \leq \Delta (s - S, S) + d(\Gamma (S, \tau_{\exp (s)}), \mu_\beta) \). Letting first \( s \), then \( S \), go to +\infty, **Proposition 3.2** implies the main result of this paper, Theorem 1.1.

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