Robustness of the Adaptive Biasing Force Method

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Abstract

We propose a study of the Adaptive Biasing Force method's robustness when the interaction force between particles can either be conservative or non-conservative.

ABF method

N particles. Momenta $p \in \mathbb{R}^{dN}$ are distributed according to a Gaussian measure. As for positions $q \in \mathcal{D} \subset \mathbb{T}^{dN}$, they are distributed according to the *Boltzmann-Gibbs measure*

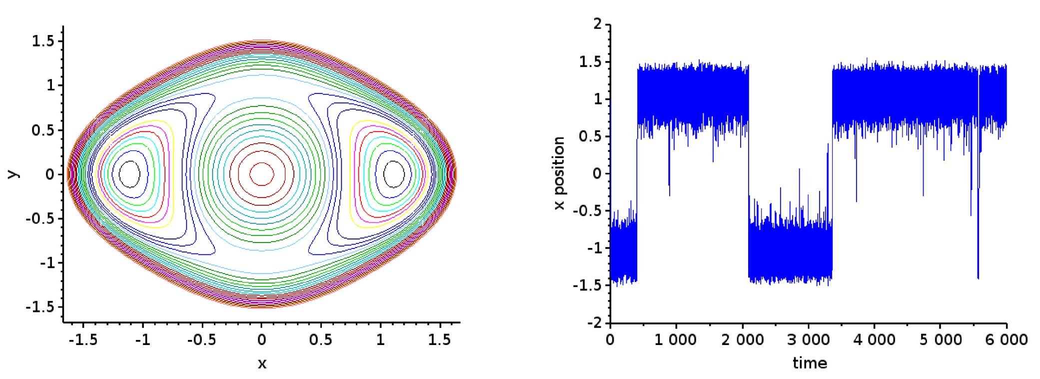
$$\mu(\mathrm{d}x) = Z_\mu^{-1} e^{-\beta V(x)} \mathrm{d}x \qquad (1)$$

where V is a potential function. Sampling (1) with the *overdamped Langevin dynamics*:

$$\mathrm{d}X_t = -\nabla V(X_t)\,\mathrm{d}t + \sqrt{\frac{2}{\beta}}\mathrm{d}W_t. \qquad (2)$$

$(X_t)_{t\geq 0}$ is ergodic: $\lim_{\tau\to+\infty} \frac{1}{\tau}\int_0^\tau \psi(X_t)\,\mathrm{d}t = \mathbb{E}_\mu[\psi]$

Metastability



- *Transition coordinate* $\xi : \mathcal{D} \to \mathcal{M}, \quad \mathcal{M} \subset \mathbb{T}$
- *Free energy derivative*

$$A'(z) = \mathbb{E}[F(X)|\xi(X) = z] \qquad (3)$$

where F is the *local mean force*, given by:

$$F = \left(\frac{\nabla V \cdot \nabla \xi}{|\nabla \xi|^2} - \frac{1}{\beta}\mathrm{div}\left(\frac{\nabla \xi}{|\nabla \xi|^2}\right)\right) \qquad (4)$$

Adaptive Biasing Force algorithm

$$\begin{cases} \mathrm{d}X_t = \left(-\nabla V + A'_t \circ \xi\right)(X_t)\,\mathrm{d}t + \sqrt{\frac{2}{\beta}}\mathrm{d}W_t \\ A'_t(z) = \mathbb{E}[F(X_t)\,|\,\xi(X_t) = z]. \end{cases} \qquad (5)$$

- $A'_t \longrightarrow A'$ and the law of (5), μ_V converges towards $\mu_{\infty,V} \propto e^{-\beta(V - A\circ\xi)}$.

References

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Our model

- $x \in \mathbb{T}^n$, $y \in \mathbb{T}^{d-n}$ and $\xi(x, y) = x$.
- $\mathcal{F}$ is an interaction force that can be either *conservative* or *non-conservative*.

Setting

$$\begin{cases} \mathrm{d}X_t = & \mathcal{F}_1(X_t, Y_t)\mathrm{d}t + B_t(X_t)\mathrm{d}t + \sqrt{\frac{2}{\beta}}\mathrm{d}W_t^1 \\ \mathrm{d}Y_t = & \mathcal{F}_2(X_t, Y_t)\mathrm{d}t + \sqrt{\frac{2}{\beta}}\mathrm{d}W_t^2 \end{cases} \qquad (6)$$

where G_t is the averaged local mean force:

$$G_t(x) = \mathbb{E}[-\mathcal{F}_1(X_t, Y_t)\,|\,X_t = x] \qquad \forall x \in \mathbb{T}^n.$$

and the bias B_t is either:

- G_t (ABF)
- $\nabla H_t = \mathsf{P}_{L^2(\lambda)}(G_t)$ (Projected ABF)

where $\mathsf{P}_{L^2(\nu)}(G)$ is the Helmholtz projection in $L^2(\nu)$ of the vector field G.

Associated Fokker-Planck equation

$$\partial_t \pi_t = \beta^{-1}\Delta \pi_t - \nabla \cdot ((\mathcal{F} + B_t)\pi_t)\,. \qquad (7)$$

Q1: In the conservative case $\mathcal{F} = -\nabla V$, does the PABF method converges like the ABF one?

Q2: Does the process converge in the non-conservative case?

Q3: What are the conditions required for the existence of an equilibrium measure for dynamics (6)?

- *Relative entropy*:

$$\mathcal{H}(\mu|\nu) = \begin{cases} \int \ln(\frac{\mathrm{d}\mu}{\mathrm{d}\nu})\mathrm{d}\mu & \text{if } \mu \ll \nu \\ +\infty & \text{else.} \end{cases}$$

Assumptions

Assumption 1 *There exist $s > d/2$ and $C > 0$ such that, for all $t \geqslant 0$ and any indices $(i_1, \dots, i_\alpha)$ with $\alpha \in [\![1, s]\!]$, $G_t - B_t \in \mathcal{C}^s(\mathbb{T}^d)$ and $\|\partial_{x_{i_1}} \dots \partial_{x_{i_\alpha}}(G_t - B_t)\|_\infty \leqslant C$.*

Proposition 1 *For both the ABF and PABF algorithms, the law π_t^ξ of $\xi(X_t, Y_t)$ converges to the Lebesgue measure λ as $t \to \infty$. More precisely,*

$$\mathcal{H}(\pi_t^\xi|\lambda) \leqslant e^{-8\beta^{-1}\pi^2 t}\mathcal{H}(\pi_0^\xi|\lambda)\,.$$

Assumption 2 ***(i)*** *There exists a fixed point $\pi_\infty \in \mathcal{P}(\mathbb{T}^d)$ of the non-linear equation (7), and it satisfies a log-Sobolev inequality of constant $R > 0$.*

(ii) *There exists $M > 0$ such that for all $y \in \mathbb{T}^{d-n}$, $x \mapsto \mathcal{F}_1(x, y)$ is M-Lipschitz.*

(iii) *There exists $\rho > 0$ such that, for all $x \in \mathbb{T}^n$, the conditional density $y \mapsto \pi_\infty(x, y)/\pi_\infty^\xi(x) = \pi_{\infty,x}(y)$ satisfies a log-Sobolev inequality of constant ρ.*

Convergence result

Theorem 1 *For both the ABF and PABF algorithms, under both Assumptions 1 and 2, suppose moreover that $\mathcal{F} = -\nabla V$ with $V \in \mathcal{C}^2(\mathbb{T}^d)$. Then, there exists $C > 0$ such that*

$$\mathcal{H}(\pi_t|\pi_\infty) \leqslant Ce^{-\Lambda t}\,,$$

where Λ is an explicitely known constant, which depends on the problem's parameters.

Theorem 2 *For both the ABF and PABF algorithms, under both Assumptions 1 and 2, suppose moreover that $M < 2\rho\beta^{-1}$. Then*

$$\mathcal{H}(\pi_t|\pi_\infty) \leqslant e^{-\Lambda t}\mathcal{H}(\pi_0|\pi_\infty)\,.$$

where Λ is an explicitely known constant, which depends on the problem's parameters.

⇝ Relying on the decomposition of the entropy $E(t) = \mathcal{H}(\pi_t|\pi_\infty)$ as the sum of the microscopic entropy $E_m(t) = \int_{\mathbb{T}} e_m(t, x)\,\mathrm{d}x = \int_{\mathbb{T}} \mathcal{H}(\pi_{t,x}|\pi_{\infty,x})\,\mathrm{d}x$ and of the macroscopic entropy $E_M(t) = \mathcal{H}(\pi^\xi(t,.)|\pi^\xi_\infty)$.

⇝ Entropy inequalities as found in [3].

⇝ Theorem 1: by-passing technical difficulties of the proof found in [2].

⇝ Theorem 2: using results on the *carré du champ* operator combined with entropy inequalities.

Existence

Theorem 3 *For the PABF algorithm, in the case where $n = 1$, there exists $\varepsilon_0 > 0$ such that if $\|\mathcal{F} + \nabla v\|_\infty \leq \varepsilon_0$, then there exists an unique equilibrium measure π_∞ for dynamics (6), to which is associated a bias B_∞. Furthermore, if $\pi_{\infty,V}$ denotes the equilibrium measure of dynamics (6) with bias B_∞ and $-\nabla V$ instead of $\mathcal{F}$, then there exists a constant $K > 0$ such that:*

$$\|\pi_\infty - \pi_{\infty,V}\|_{TV} \leq K\varepsilon_0.$$

⇝ Schauder's fixed point theorem.

⇝ Bounds on the equilibrium measure's density, obtained by comparison with the conservative case [4].

Conclusion

▲ Robustness of ABF and PABF in both conservative and non-conservative case.

▼ Assumption A-1 is very strong and necessary only for the PABF case using a multidimensional reaction coordinate.

⇝ What about the convergence of the ABF method for the Langevin dynamics?

⇝ Implementation of ABF in Tinker ?