Sampling of singular Gibbs measures

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Gibbs measure

Gas of $N \gg 1$ particles, temperature $T = \beta^{-1}$, in domain $D \subset \mathbb{R}^3$.

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Hamiltonian :

$$H(x, y) = U(x) + \frac{|y|^2}{2}.$$

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Goal :

$$\mu_\beta(f) = \mathbb{E}(f(X)), \quad X \sim \mu_\beta.$$

Example

Lennard-Jones potential :

$$U(x) = \sum_{1 \leqslant i \neq j \leqslant N} U_i(|x_i - x_j|), \quad U_i(r) = 4\varepsilon \left(\frac{\sigma}{r^{12}} - \frac{\sigma}{r^6} \right).$$

Argon : $\varepsilon = 1.66 * 10^{-21} J$, $\sigma = 3.405 \mathring{A}$.

Pressure :

$$P = \mu_\beta(f), \qquad f(x, y) = \frac{1}{3|D|} \sum_{i=1}^{N} \left(\frac{y_i^2}{m} - x_i \cdot \nabla_{x_i} U(x) \right).$$

Gabriel Stoltz, *An introduction to Computational Statistical Physics*.

Langevin Process

d=3N

$$U : \mathbb{R}^d \to [0, \infty].$$

$$\begin{cases} \mathrm{d}X_t = Y_t \mathrm{d}t, \\ \mathrm{d}Y_t = -\nabla U(X_t)\mathrm{d}t - \gamma Y_t \mathrm{d}t + \sqrt{2\gamma\beta^{-1}}\mathrm{d}B_t. \end{cases}$$

Ergodic [1]

$$\lim_{t\to\infty} \mathbb{E}\left(f(X_t, Y_t)\right) = \mu_\beta(f).$$

Simulation of a large number of (X_t, Y_t) :

$$\frac{1}{n}\sum_{k=1}^{n} f(X_t^k, Y_t^k) \approx \mathbb{E}\left(f(X_t, Y_t)\right) \approx \mu(f).$$

1. D.-P. Herzog and J.-C. Mattingly. Ergodicity and Lyapunov functions for Langevin dy-namics with singular potentials.Comm. Pure Appl. Math., 72(10) :2231–2255, 2019

A simpler model

$$\mathrm{d}Z_t = b(Z_t)\mathrm{d}t + \mathrm{d}B_t,$$

b smooth, derivative of all order bounded, $z \cdot b(z) \leqslant -\beta|z|^2$ outside some compact set.

Euler-Maruyama scheme :

$$\bar{Z}_{n+1} = \bar{Z}_n + \delta b(Z_n) + \sqrt{\delta} G_n.$$

Proposition

Z admits an invariant measure ν.
$\bar{Z}$ admits an invariant measure ν_δ for all $0 < \delta < \delta_0$.

A simpler model

Theorem Talay-Tubaro 90'

$\forall f \in \mathcal{P}$, $t \geqslant 0$, $\exists (C_i(t))_i$ explicit such that :

$$\mathbb{E}_z(f(\bar{Z}_n)) = \mathbb{E}_z(f(Z_t)) + C_1(t)\delta + \cdots + C_k(t)\delta^k + O(\delta^{k+1}),$$

where $n\delta = t$.
$\exists (D_i)_i$ of explicit real numbers such that :

$$\nu_\delta(f) = \nu(f) + D_1\delta + \cdots + D_k\delta^k + O(\delta^{k+1}).$$

$$2\mathbb{E}_z\left(f\left(\bar{Z}_{2n}^{\delta/2}\right)\right) - \mathbb{E}_z\left(f\left(\bar{Z}_n^{\delta}\right)\right) = \mathbb{E}_z(f(Z_t)) + O(\delta^2).$$

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- D. Talay. Stochastic Hamiltonian systems : exponential convergence to the invariant measure, and discretization by the implicit Euler scheme. Markov Process. Related Fields,8(2) :163–198, 2002.
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Context

$$\begin{cases} dX_t = Y_t dt, \\ dY_t = -\nabla U(X_t)dt - \gamma Y_t dt + \sqrt{2\gamma\beta^{-1}} dB_t. \end{cases}$$

Process defined on :

$$\mathcal{D} = \left\{ x \in \mathbb{R}^d | U(x) < \infty \right\}, \qquad \mathcal{X} = \mathcal{D} \times \mathbb{R}^d.$$

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Hypothesis

- $\int_{\mathcal{D}} e^{-\beta U(x)} \mathrm{d}x < \infty.$
- $\lim\limits_{x \to \mathcal{D}^c} \frac{|\nabla^2 U(x)|}{|\nabla U(x)|^2} = 0.$
- $\exists \eta_0 \in \mathbb{R} \setminus [-1, 0],\ \eta_\infty > 1$:
  $c_\infty U^{2-\frac{2}{\eta_\infty}} + d_\infty \leqslant |\nabla U|^2 \leqslant c_0 U^{2+\frac{2}{\eta_0}} + d_0.$
- $\forall \alpha \in \mathbb{N}^{2d}$: $|\partial^\alpha U| \leqslant U^{k_\alpha} + C_\alpha.$

Lyapunov function

Lyapunov function :

$$LV \leqslant -\alpha V + \alpha K,$$

with L the generator

$$L = y \cdot \nabla_x - \nabla U \cdot \nabla_y - \gamma y \cdot \nabla_y + \gamma \beta^{-1} \Delta_y.$$

For all $0 < b < \beta$, $\exists$ Lyapunov function

$$V(x,y) = exp(bH(x,y) + o(H(x,y))).$$

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Allowed function :

$$\mathcal{F} = \left\{ f : \mathcal{C}^\infty(\mathcal{X}), \forall \alpha \in \mathbb{N}^{2d}, |\partial^\alpha f| \leqslant C_{\alpha,f} e^{c_{\alpha,f} H}, c_{\alpha,f} < \beta \right\}.$$

Theorem

$\forall f \in \mathcal{F}$, $\exists C, q, b > 0$ such that :

$$|\partial^\alpha (P_t f - \mu(f))| \leqslant C e^{-qt} e^{bH}.$$

Proof based on hypocoercivity in Sobolev spaces [2].

$$\|h\|^2_{mH^k} = \int_{\mathcal{X}} h^2 V_k \mathrm{d}\mu + \int_{\mathcal{X}} \sum_{p=1}^{r} \left(\sum_{i=0}^{p-1} \omega_{i,p} |\nabla_x^i \nabla_y^{p-i} h|^2 + \omega_{p,p} | \left(\nabla_x^p - \xi \nabla_x^{p-1} \nabla_y \right) h|^2 \right) (1 + \varepsilon_p V_{k-p}) \, \mathrm{d}\mu.$$

2. F. Baudoin, M. Gordina, and D.-P. Herzog. Gamma calculus beyond Villani and explicit convergence estimates for Langevin dynamics with singular potentials.Arch. Ration.Mech. Anal., 241(2) :765–804, 2021

Numerical scheme

Simplectic Euler-Scheme :

$$\begin{cases} \tilde{X}_{n+1} = \tilde{X}_n + \delta \tilde{Y}_{n+1}, \\ \tilde{Y}_{n+1} = \tilde{Y}_n - \delta \nabla U(\tilde{X}_n) - \delta\gamma \tilde{Y}_n + \sqrt{2\gamma\beta^{-1}\delta}\, G_n. \end{cases}$$

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$\forall \varepsilon > 0$:

$$\mathbb{E}\left(e^{\varepsilon H(\tilde{X}_n, \tilde{Y}_n)}\right) = \infty, \quad \forall n \geqslant 1.$$

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Stopped Scheme :

$$\begin{cases} \bar{X}_{n+1} = \bar{X}_n + \mathbb{1}_{E_\delta(\bar{X}_n, \bar{Y}_n, G_n) \in \mathcal{H}_d} \delta \bar{Y}_{n+1}, \\ \bar{Y}_{n+1} = \bar{Y}_n + \mathbb{1}_{E_\delta(\bar{X}_n, \bar{Y}_n, G_n) \in \mathcal{H}_d} \left(-\delta \nabla U(\bar{X}_n) - \delta\gamma \bar{Y}_n + \sqrt{2\gamma\beta^{-1}\delta}\, G_n \right). \end{cases}$$

$$\mathcal{H}_d = \left\{ H \leqslant \delta^{-l} \right\},$$

$$E_\delta(x, y, g) = \begin{pmatrix} x + \delta \left(y - \delta \nabla U(x) - \delta\gamma y + \sqrt{2\gamma\beta^{-1}\delta}\, g \right) \\ y - \delta \nabla U(x) - \delta\gamma y + \sqrt{2\gamma\beta^{-1}\delta}\, g \end{pmatrix}.$$

Proposition

$\forall 0 < b < \beta$,

$$\exists V_b = exp(bH(x,y) + o(H(x,y))),$$

and $\alpha, K > 0$ such that $\forall 0 < \delta < \delta_0$, $(x,y) \in \mathcal{H}_d$:

$$\mathbb{E}_{(x,y)}\left(V_b(\bar{X}_1, \bar{Y}_1)\right) \leqslant (1-\alpha\delta)V_b(x,y) + \alpha\delta K.$$

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For all $0 < b < \beta$:

$$\sup_{0<\delta<\delta_0} \sup_{n\in\mathbb{N}} \mathbb{E}_z\left(e^{bH\left(\bar{X}_n, \bar{Y}_n\right)}\right) < \infty.$$

For all $a > 0$:

$$\mathbb{P}_{(x,y)}\left(H(\bar{X}_n, \bar{Y}_n) \geqslant a\right) \leqslant Ce^{-ca}.$$

Proposition

$\forall 0 < b < \beta$,

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and $\alpha, K > 0$ such that $\forall 0 < \delta < \delta_0$, $(x,y) \in \mathcal{H}_d$:

$$\mathbb{E}_{(x,y)}\left(V_b(\bar{X}_1, \bar{Y}_1)\right) \leqslant (1 - \alpha\delta) V_b(x,y) + \alpha\delta K.$$

Proposition

$\forall 0 < \delta < \delta_0$, $\exists$ invariant measure $\mu_{\beta,\delta}$, $\forall f \in \mathcal{F}$:

$$\lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \mathbb{E}_{(x,y)}\left(f\left(\bar{X}_k, \bar{Y}_k\right)\right) = \mu_{\beta,\delta}(f).$$

Method

$$t = n\delta,\ u(t,x,y) = P_t f(t,x,y),\ \bar{Z}_n = \left(\bar{X}_n, \bar{Y}_n\right) :$$

$$\begin{aligned}\mathbb{E}_z\left(f\left(\bar{Z}_n\right)\right) - \mathbb{E}_z\left(f\left(Z_t\right)\right) &= \mathbb{E}_z\left(u\left(0, \bar{Z}_n\right) - u\left(n\delta, z\right)\right) \\ &= \sum_{p=0}^{n-1} \mathbb{E}_z\left(u\left(p\delta, \bar{Z}_{n-p}\right) - u\left((p+1)\delta, \bar{Z}_{n-(p+1)}\right)\right).\end{aligned}$$

$$\begin{aligned}&\mathbb{E}_z\left(u\left(k\delta, \bar{Z}_{n-p}\right) - u\left((p+1)\delta, \bar{Z}_{n-(p+1)}\right)\right) \\ &\qquad = 0 + \delta^2 \mathbb{E}\left(\psi\left(p\delta, \bar{Z}_{n-p}\right)\right) + \delta^3 R^{\delta}_{n-p},\end{aligned}$$

where

$$R^{\delta}_{n-p} \leqslant C\left(1 + \mathbb{E}\left(e^{bH\left(\bar{Z}_{n-p}\right)}\right)\right).$$

Theorem

$\forall f \in \mathcal{F}$, $t \geqslant 0$, $\exists (C_i)_i$ explicit such that :

$$\mathbb{E}_{(x,y)}\left(f\left(\bar{X}_n, \bar{Y}_n\right)\right) = \mathbb{E}_{(x,y)}\left(f\left(X_t, Y_t\right)\right) + C_1\delta + \cdots + C_k\delta^k + O\left(\delta^{k+1}\right).$$

There exists a family $(D_i)_i$ of explicit real numbers such that :

$$\mu_{\beta,\delta}(f) = \mu_\beta(f) + D_1\delta + \cdots + D_k\delta^k + O(\delta^{k+1}).$$

THANK YOU FOR YOUR ATTENTION