Sampling of singular Gibbs measure

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Contribution [1]

We show **weak error expansion** of a numerical scheme with rejection for the **Langevin process** in the case of a **singular potential**. In order to achieve this, we provide estimates on the associated semi-group of the process. The class of admissible potentials includes the Lennard-Jones interaction with confinement, which is an important potential in molecular dynamics and served as the primary motivation for this study.

Motivation

Hamiltonian:

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

Gibbs measure:

$$\mu_\beta(\mathrm{d}x,\mathrm{d}y) = Z^{-1}e^{-\beta H(x,y)}\mathrm{d}x\mathrm{d}y.$$

Goal: compute

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

Kinetic sampler:

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

Splitting scheme with rejection:

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

If $H(X,Y) \leqslant \delta^{-l}$,

- $(\bar{X}_{n+1},\bar{Y}_{n+1}) = (X,Y)$,

else,

- $(\bar{X}_{n+1},\bar{Y}_{n+1}) = (\bar{X}_n,\bar{Y}_n)$.

Assumptions

Assumptions on U:

- $\int_{\mathcal{D}} e^{-\beta U(x)}\mathrm{d}x < \infty$.
- $\lim_{U\to\infty} \frac{|\nabla^2 U(x)|}{|\nabla U(x)|^2} = 0$.
- $\exists \eta_0 \in \mathbb{R}\setminus[-1,0]$, $\eta_\infty > 1$:

$$c_\infty U^{2-\frac{2}{\eta_\infty}} + d_\infty \leqslant |\nabla U|^2 \leqslant c_0 U^{2+\frac{2}{\eta_0}} + d_0.$$

- $\forall \alpha \in \mathbb{N}^{2d}$: $|\partial^\alpha U| \leqslant U^{k_\alpha} + C_\alpha$.

Assumptions on f: $f \in \mathcal{F}$ *iff*

- $f \in \mathcal{C}^\infty(\{U < \infty\})$.
- $|\partial^\alpha f| \leqslant C_{\alpha,f}e^{c_{\alpha,f}H}$, $c_{\alpha,f} < \beta$.

Example from **statistical physics**: Lennard-Jones:

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

Pressure:

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

Semi-group estimates

Semi-group: $P_t f(x,y) = \mathbb{E}_{x,y}(f(X_t,Y_t))$

Theorem 1. *$\forall f \in \mathcal{F}$, $\exists C, q$, $0 < b < \beta$ such that:*

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

Idea of proof: For all $0 < b < \beta$, $\exists$ Lyapunov function

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

Hypocoercivity in Sobolev spaces:

$$\|h\|_{mH^k}^2 = \int_{\mathcal{X}} h^2 V_0 \mathrm{d}\mu + \int_{\mathcal{X}}\sum_{p=1}^r\left(\sum_{i=0}^{p-1}\omega_{i,p}|\nabla_x^i\nabla_y^{p-i}h|^2\right)(1+\varepsilon_p V_p)\,\mathrm{d}\mu + \int_{\mathcal{X}}\sum_{p=1}^r \omega_p|\left(\nabla_x^p - \xi\nabla_x^{p-1}\nabla_y\right)h|^2(1+\varepsilon_p V_p)\,\mathrm{d}\mu.$$

H^1 case done in [2].

Lemma 2. $\forall h \in \mathcal{C}^\infty(\{U < \infty\})$,

$$\langle h, Lh\rangle_{mH^k}^2 \leqslant -c\|h\|_{mH^k}^2.$$

Proof based on generalised **Gamma calculus**.

Cv of the numerical scheme

Why rejection ? If $(\tilde{X}_n,\tilde{Y}_n)$ scheme without rejection:

$$\mathbb{E}\left(f\left(\tilde{X}_n,\tilde{Y}_n\right)\right) = \infty,$$

for $f \in \mathcal{F}\setminus L^1_{loc}$.

Lemma 3. $\forall 0 < b < \beta$,

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

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

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

Lemma 4. *$\forall 0 < \delta < \delta_0$, $\exists$ invariant measure $\mu_{\beta,\delta}$, $\forall f \in \mathcal{F}$:*

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

Theorem 5. *$\forall f \in \mathcal{F}$, $t \geqslant 0$, $\exists (C_i)_i$ explicit such that:*

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

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

$$\mu_{\beta,\delta}(f) = \mu_\beta(f) + \sum_{p=1}^p D_p\delta^p + O(\delta^{k+1}).$$

See also [3, 4, 5].

Numerical experiments

Toy model:

$$U(x) = \frac{1}{x} + x^2,\ \beta^{-1} = 15.0,\ \gamma = 1.$$

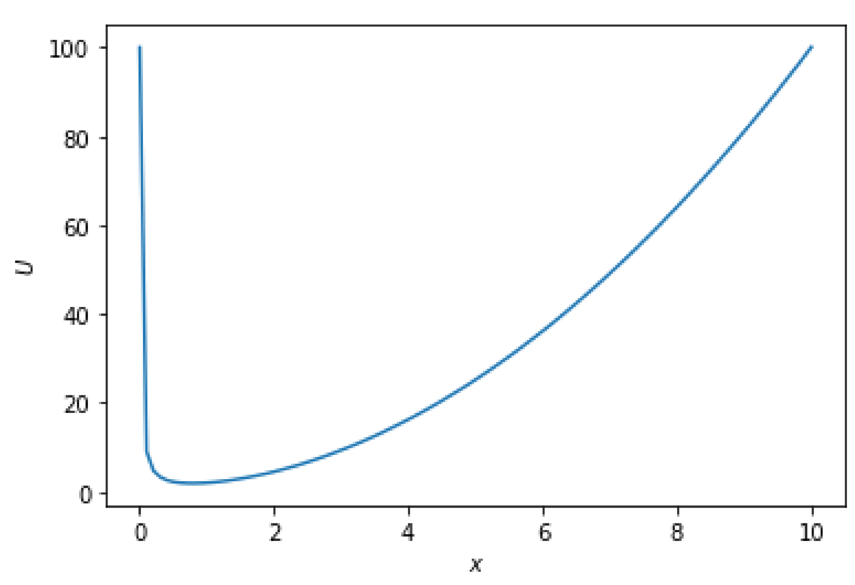

Figure 1: The potential.

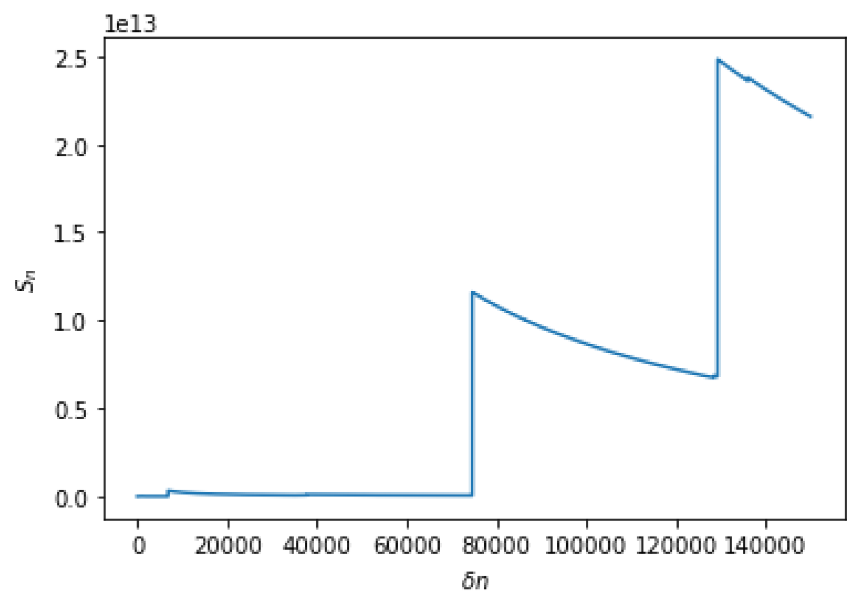

Figure 2: Typical trajectory of the empirical average without rejection for $\delta = 10^{-2}$.

Fix $K = 1000$, $T = 150000$, compute K independent copies of

$$S_n = \frac{1}{n}\sum_{k=1}^n U(X_k),$$

with $n = \lfloor T/\delta \rfloor$. The following graph represents the proportion of copies that have more then 1% error.

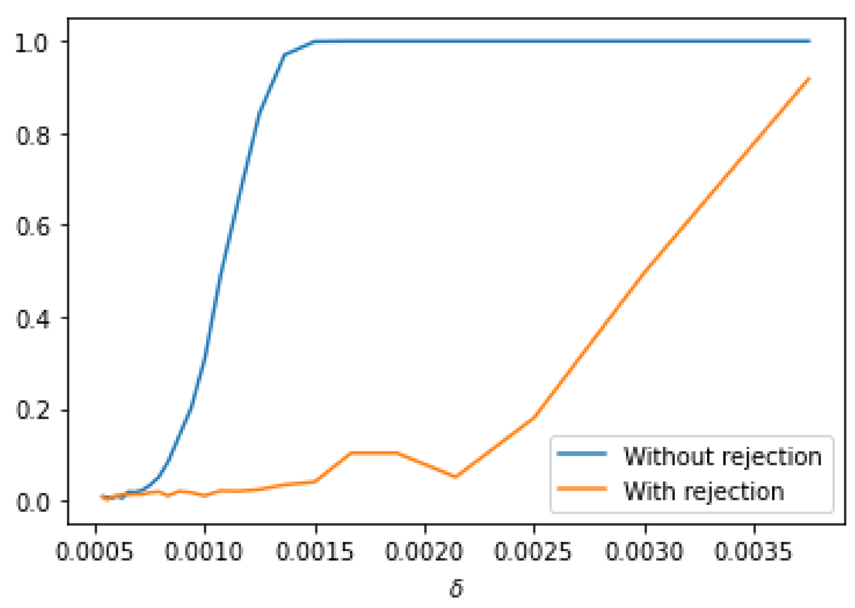

Figure 3: Failure probability.

References

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