Some Remarks on Preconditioning Molecular Dynamics

Houssam AlRachid, MAPMO, Université d'Orléans

We consider a Preconditioned Overdamped Langevin algorithm that does not alter the invariant distribution and ask whether preconditioning improves the standard model in terms of reducing the asymptotic variance and of accelerating convergence to equilibrium. We present a detailed study of the dependence of the asymptotic variance on preconditioning in some elementary toy models related to molecular simulation.

The most commonly employed algorithms in molecular simulation are based on discretising the Langevin equation, but for the sake of simplicity we will focus on the overdamped Langevin equation,

$$dX_t = -\nabla E_N(X_t)dt + \sqrt{2}dW_t, \tag{1}$$

where E_N is, e.g., a potential energy and W_t is a N-dimensional standard Brownian motion. Thus, given an observable $f \in L^1(\mu)$, we are interested in quantifying the convergence

$$\epsilon_T(f) := \frac{1}{T}\int_0^T f(X_t)dt \to \mu(f) \qquad \text{for } \mu\text{-a.e } X_0. \tag{2}$$

For a (fixed) preconditioner $P \in \mathbb{R}^{N\times N}$, symmetric positive definite, we consider the preconditioned Overdamped Langevin dynamics (P-Langevin),

$$dX_t^P = -P^{-1}\nabla E_N(X_t^P)dt + \sqrt{2}P^{-1/2}dW_t. \tag{3}$$

The preconditioner does not affect the invariance property of the diffusion process, i.e., the target measure μ is still invariant for the P-Langevin process (3). Moreover, we also obtain

$$\epsilon_T^P(f) := \frac{1}{T}\int_0^T f(X_t^P)dt \to \mu(f), \qquad \text{for } \mu\text{-a.e } X_0. \tag{4}$$

and analogously to the standard Langevin dynamics, a central limit theorem characterizes the asymptotic distribution of the fluctuations,

$$\sqrt{t}\left(\epsilon_t^P(f) - \mu(f)\right) \xrightarrow{D} \mathcal{N}(0, \sigma_{f,P}^2), \tag{5}$$

where $\sigma_{f,P}^2$ is the asymptotic variance of f under P-Langevin dynamics.

The main aim of our paper is to present several simplified but still realistic examples at which we can observe *whether or not* preconditioning accelerates sampling in the sense that it achieves a reduction in the asymptotic variance, i.e., $\sigma_{f,P}^2 \ll \sigma_{f,I}^2$.

Références

[1] H. AlRachid, L. Mones and C. Ortner, *Some Remarks on Preconditioning Molecular Dynamics*, submitted, Arxiv: 1612.05435 (2017).

Houssam AlRachid, MAPMO, Universit d'Orléans, 6 Avenue du Parc Floral, 45100 Orléans
houssam.alrachid@univ-orleans.fr