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Optimizing the diffusion for sampling with overdamped Langevin dynamics Gabriel Stoltz (CERMICS ,Ecole des Ponts and Matherials, Inria Paris)

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Overdamped Langevin dynamics are stochastic differential equations, where gradient dynamics are perturbed by noise in order to sample high dimensional probability measures such as the ones appearing in computational statistical physics and Bayesian inference. By varying the diffusion coefficient, there are in fact infinitely many overdamped Langevin dynamics which preserve the target probability measure at hand. This suggests to optimize the diffusion coefficient in order to increase the convergence rate of the dynamics, as measured by the spectral gap of the generator associated with the stochastic differential equation. We analytically study this problem here, obtaining in particular necessary conditions on the optimal diffusion coefficient. We also derive an explicit expression of the optimal diffusion in some homogenized limit. Numerical results, both on discretizations of the spectral gap problem and Monte Carlo simulations of the stochastic dynamics, demonstrate the increased quality of the sampling arising from an appropriate choice of the diffusion coefficient.

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Classification de Session: Challenge and Perspective