

Probabilistic sampling for physics: finding needles in a field of high-dimensional haystacks

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Barrier Hamiltonian Monte Carlo

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This talk introduces Barrier Hamiltonian Monte Carlo (BHMC), a version of HMC which aims at sampling from a Gibbs distribution π on a manifold M , endowed with a Hessian metric g derived from a self-concordant barrier. Like Riemannian Manifold HMC, our method relies on Hamiltonian dynamics which comprise g . It incorporates the constraints defining M and is therefore able to exploit its underlying geometry. We first introduce c -BHMC (continuous BHMC), for which we assume that the Hamiltonian dynamics can be integrated exactly, and show that it generates a Markov chain for which π is invariant. Secondly, we design n -BHMC (numerical BHMC), a Metropolis-Hastings algorithm which combines an acceptance filter including a “reverse integration check” and numerical integrators of the Hamiltonian dynamics. Our main results establish that n -BHMC generates a reversible Markov chain with respect to π . This is in contrast to existing algorithms which extend the HMC method to Riemannian manifolds, as they do not deal with asymptotic bias. Our conclusions are supported by numerical experiments where we consider target distributions defined on polytopes.

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Classification de Session: Challenge and Perspective