

Hamiltonian Monte Carlo for high dimensional problems

Tijana Radivojević and Elena Akhmatskaya

Abstract

Hamiltonian (Hybrid) Monte Carlo (HMC) method, initially proposed in High Energy Physics, is a popular tool for solving complex and intractable problems of statistical inference. We introduce a number of modifications in the original formulation of the HMC in order to enhance sampling from high-dimensional target densities. The new features include a modified Metropolis test, alternative strategies for momentum refreshment step and novel numerical integrators. All alterations have been formulated and implemented within the Generalized Shadow Hybrid Monte Carlo framework, earlier proposed by the authors for simulation of molecular systems.