SEMINARIO

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Adaptive splitting integrators for enhancing sampling efficiency of shadow Hamiltonian Monte Carlo methods

Abstract: The idea to sample with modified or shadow Hamiltonians in Hybrid Monte Carlo (HMC) methods was first proposed by Izaguirre and Hampton in 2004 [1]. It has originated the competitive importance sampling method for molecular simulation Generalized Shadow Hybrid Monte Carlo (GSHMC) [2] and its successor for statistics Mix & Match Hybrid Monte Carlo (MMHMC) [3]. The methods are proved to be successful in solving high dimensional problems and often outperforming in sampling efficiency the standard techniques such as molecular dynamics and Hybrid/Hamiltonian Monte Carlo (HMC). The GSHMC algorithm was originally formulated for the leapfrog integrator. However, more sophisticated numerical schemes can be employed.

Recently, a novel adaptive splitting integrator named Adaptive Integration Approach (AIA) has been formulated for the original HMC method [4]. AIA nominates an integrator from a family of splitting schemes which, given a step size and a simulation problem, guarantees the best conservation of Hamiltonians and thus the highest proposal acceptance rates.

Following the same strategy, we propose the analogous new approach which we call MAIA - a Modified Adaptive Integration Approach - specifically derived for shadow Hamiltonian Monte Carlo methods.

In this talk we summarize the main features of GSHMC and MMHMC and show how they can be combined with splitting schemes. The MAIA method is introduced as an extension of the original AIA. Some results of simulations of realistic applications are also presented.

References

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