Exploiting Algebraic and Geometric Structure in Time-Integration Methods

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Energy-preserving splitting integration for Hamiltonian Monte Carlo method with adaptive tuning

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Splitting schemes provide a promising alternative to the classical Stormer-Verlet method in Hamiltonian Monte Carlo (HMC) methodology. Within the family of one-parameter second-order splitting procedures, we demonstrate that using a designated function of the free parameter to select the step size ensures stability and Hamiltonian preservation when sampling from Gaussian distributions. This guarantees no sample rejections in the HMC process, a key factor for superior performance compared to recent similar methods. The effectiveness of the proposed approach for sampling from general non-Gaussian distributions is assessed, incorporating a simple adaptive selection technique for the free parameter to improve HMC performance. Benchmark examples from literature and experiments, including the Log-Gaussian Cox process and Bayesian Logistic Regression, highlight the effectiveness of the approach.

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