Magnetic HMC: Project Proposal

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1 Problem Statement

Hamiltonian Monte Carlo (HMC) uses the properties of Hamiltonian dynamics to use information on the gradients of the target density to generate efficient proposals. However, HMC struggles to cross low-density regions in multimodal densities due to its proposal mechanism and fails to give efficient samples for such problems. A standard solution discussed in the literature to solve this problem is to generalize the Hamiltonian equations by adding external forces to make the system non-canonical and exploiting the mechanics to force the sampler to cross the low-density regions (Vishwanath and Tak (2024)).

Magnetic HMC (Tripuraneni et al. (2017)) uses a generalized version of the Hamiltonian equations to sample efficiently from multimodal systems. These represented in 3-D resemble the motion of a particle moving in a charged field, which gives the algorithm its name. They also describe a symplectic leapfrog-like integrator that allows easy implementation of MHMC for any target.

The crucial problem most such algorithms face is that they introduce new tuning parameters, which are hard to interpret for different target densities. This becomes an issue during most implementations as tuning these parameters becomes increasingly difficult with an increase in dimensions and the complexity of the target. Algorithms like NUTS (Hoffman et al. (2014)) try to solve this problem by dual averaging.

2 Aim

The project aims to devise a theoretically sound problem-agnostic implementation of MHMC that allows the user to enter the desired target and the algorithm to sample from the same efficiently. It also aims to explain how this tuning can be interpreted theoretically and intuitionally, allowing an average algorithm user to understand its functioning without much background. This implementation would be inspired by the dual-averaging scheme (Nesterov (2009)).

References

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