Discussion of the article ‘Geodesic Monte Carlo on Embedded Manifolds’
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Geodesic Monte Carlo on Embedded Manifolds

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ABSTRACT. Markov chain Monte Carlo methods explicitly defined on the manifold of probability distributions have recently been established. These methods are constructed from diffusions across the manifold and the solution of the equations describing geodesic flows in the Hamilton–Jacobi representation. This paper takes the differential geometric basis of Markov chain Monte Carlo further by considering methods to simulate from probability distributions that themselves are defined on a manifold, with common examples being classes of distributions describing directional statistics. Proposal mechanisms are developed based on the geodesic flows over the manifolds of support for the distributions, and illustrative examples are provided for the hypersphere and Stiefel manifold of orthonormal matrices.

Key words: directional statistics, geodesic, Hamiltonian Monte Carlo, Riemannian manifold, Stiefel manifold

1. Introduction

Markov chain Monte Carlo (MCMC) methods that originated in the physics literature have caused a revolution in statistical methodology over the last 20 years by providing the means, now in an almost routine manner, to perform Bayesian inference over arbitrary non-conjugate prior and posterior pairs of distributions (Gilks et al., 1996).

A specific class of MCMC methods, originally known as hybrid Monte Carlo (HMC), was developed to more efficiently simulate quantum chromodynamic systems (Duane et al., 1987). HMC goes beyond the random walk Metropolis or Gibbs sampling schemes and overcomes many of their shortcomings. In particular, HMC methods are capable of proposing bold long distance moves in the state space that will retain a very high acceptance probability and thus improve the rate of convergence to the invariant measure of the chain and reduce the autocorrelation of samples drawn from the stationary distribution of the chain. The HMC proposal mechanism is based on simulating Hamiltonian dynamics defined by the target distribution (see Neal (2011) for a comprehensive tutorial). For this reason, HMC is now routinely referred to as Hamiltonian Monte Carlo. Despite the relative strengths and attractive properties of HMC, it has largely been bypassed in the literature devoted to MCMC and Bayesian statistical methodology with very few serious applications of the methodology being published.

More recently, Girolami & Calderhead (2011) defined a Hamiltonian scheme that is able to incorporate geometric structure in the form a Riemannian metric. The Riemannian manifold Hamiltonian Monte Carlo (RMHMC) methodology makes proposals implicitly via Hamiltonian dynamics on the manifold defined by the Fisher–Rao metric tensor and the corresponding Levi-Civita connection. The paper has raised an awareness of the differential geometric foundations of MCMC schemes such as HMC and has already seen a number of methodological and algorithmic developments as well as some impressive and challenging applications exploiting these geometric MCMC methods (Konukoglu et al., 2011; Martin et al., 2012; Raue et al., 2012; Vanlier et al., 2012).

In contrast to Girolami & Calderhead (2011), in this particular paper, we show how Hamiltonian Monte Carlo methods may be designed for and applied to distributions defined...