NOTE ON THE GEODESIC MONTE CARLO

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Abstract. Geodesic Monte Carlo (gMC) comprises a powerful class of algorithms for Bayesian inference on non-Euclidean manifolds. The original gMC algorithm was cleverly derived in terms of its progenitor, the Riemannian manifold Hamiltonian Monte Carlo (RMHMC). Here, it is shown that an alternative, conceptually simpler derivation is available which clarifies the algorithm when applied to manifolds embedded in Euclidean space.

1. Introduction

Bayesian inference is hard. Bayesian inference on non-Euclidean manifolds is harder. Prior to the publication of [1], a statistician required great ingenuity to compute the posterior distribution for any model with non-Euclidean parameter space, and the algorithmic details might change significantly depending on the prior, the likelihood, and the constraints implied by the non-Euclidean geometry. A good example of this approach is found in [2], where the posterior distribution over the Stiefel manifold of orthonormal matrices is computed by way of column-at-a-time Gibbs updates that rely on model specifications.

It is preferable, rather, that the same algorithm work for many different kinds of models. This is one of the strengths of Hamiltonian Monte Carlo [3] and its Riemannian extension, RMHMC [4], which augments the posterior distribution \( \pi(q) \) by the random Gaussian momentum \( p \sim N(0, G(q)) \), where \( G(q) \) is the metric tensor pertaining to the Riemannian manifold over which the model is defined. RMHMC simulates from the posterior distribution by simulating the augmented canonical distribution with Hamiltonian

\[
H(q, p) = U(q) + K(q, p) \propto -\log \pi(q) + \frac{1}{2} \log |G(q)| + \frac{1}{2} p^T G(q)^{-1} p,
\]

i.e., \( U(q) \) is the negative log-posterior and \( K(q, p) \) is the negative logarithm of the probability density function of Gaussian momentum \( p \). Since the kinetic energy is not separable in \( q \) and \( p \), the system is not integrable using Euler’s method, so, in most cases, implicit integration methods are required [4]. However, [1] point out that, for certain manifolds with known geodesics, it is beneficial to split the Hamiltonian into two parts and simulate the two systems iteratively. Here, the first Hamiltonian \( H^{[1]} = -\log \pi(q) + \frac{1}{2} \log |G(q)| \) renders the equations

\[
\dot{q} = 0
\]

\[
\dot{p} = \nabla_q (\log \pi(q) - \frac{1}{2} \log |G(q)|),
\]

and, crucially, the second Hamiltonian \( H^{[2]} = \frac{1}{2} p^T G(q)^{-1} p \) renders the geodesic dynamics for the Riemannian metric’s Levi-Civita connection. Thus, the entire
system may be simulated by iterating between (1) perturbing the momentum and (2) advancing along the manifold geodesics.

2. gMC on Embedded Manifolds

[1] extends the RMHMC formalism to posterior inference on manifolds embedded in Euclidean space. In the following, this extension is referred to as the embedding geodesic Monte Carlo (egMC). To maintain the RMHMC formalism, the authors begin by considering the inference problem on the intrinsic manifold, where the Hausdorff measure

\[ \mathcal{H}^d(dq) = \sqrt{|G(q)|} \lambda^d(dq), \]

and not the Lebesgue measure \( \lambda^d(dq) \), is the base measure with respect to which the posterior distribution is defined[1]. Here, the RMHMC Hamiltonian (1.1) may be written

\[ H(q, p) = -\log \pi_H(q) + \frac{1}{2} p^T G(q)^{-1} p, \]

for

\[ \log \pi_H(q) = \log \pi(q) - \frac{1}{2} \log |G(q)| \]

the log-posterior with respect to the Hausdorff base measure. Now, a clever change of variables occurs using an isometric embedding as a tool. An isometric embedding of a manifold \( Q \) into Euclidean space is a map \( x : Q \rightarrow \mathbb{R}^d \) satisfying

\[ G_{ij}(q) = \sum_{l=1}^d \frac{\partial x_l(q)}{\partial q_i}(q) \frac{\partial x_l(q)}{\partial q_j}(q), \quad \text{or} \quad G(q) = J_x(q)^T J_x(q) \]

for \( J_x(q) \) the Jacobian of the map \( x \) evaluated at \( q \in Q \). [1] use the isometric embedding to make gMC practical on certain manifolds. This is accomplished by the change of variables \( (q, p) \mapsto (x(q), Mp) \), with

\[ M = J_x(q)(J_x(q)^T J_x(q))^{-1} = J_x(q)G(q)^{-1}. \]

If \( v = Mp \), then the Hamiltonian \( H(q, p) \) becomes ([1], Equation (9))

\[ H(x, v) = -\log \pi_H(x) + \frac{1}{2} v^T \Pi_q v \]
\[ = -\log \pi_H(x) + \frac{1}{2} v^T v \]

for \( \Pi_q \) the projection matrix of the tangent space of the embedded manifold (at point \( q \)) conceived of as a subspace of the ambient Euclidean space. The authors point out that “the target density \( \pi_H(x) \) is still defined with respect to the Hausdorff measure of the manifold, and so no additional log-Jacobian term is introduced,” and invite the reader to

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[1] Whereas the ensuing derivation is extremely clever, it is unfortunate that it relies on an intrinsic conception of the inference problem, which, we will argue, causes confusion when the object of interest is a priori defined on the embedded manifold.
[n]ote that by working entirely in the embedded space, we completely avoid the coordinate system $q$ and the related problems where no single global coordinate system exists. The Riemannian metric $G$ only appears in the Jacobian determinant term of the density: in certain examples, this can also be removed, for example by specifying the prior distribution as uniform with respect to the Hausdorff measure...

Indeed, this latter situation occurs for compact manifolds such as the Stiefel manifold and its special cases, the sphere and the orthogonal group.

But how should one approach the more common scenario where the prior is defined a priori with respect to the Lebesgue measure of the embedded manifold? On the sphere, for example, such priors include the uniform and Bingham-Von Mises-Fisher distributions. Here, one suspects that the log-Jacobian term should never be necessary, and this turns out to be the case.

3. An alternative derivation

Let $\pi(x)$ denote a target posterior density defined directly on the embedded manifold. For the unit sphere, this means that $x^T x = 1$; for the Stiefel manifold of $d \times s$ orthonormal matrices, this means that $x^T x = I_s$, for $I_s$ the identity matrix of the given dimension $s$. Let $\Pi_x$ be the orthogonal projection onto the tangent space of the embedded manifold at point $x$. For example, for the sphere, this projection is given by

$$\Pi_x = I - xx^T;$$

for the Stiefel manifold, the matrix is (see Appendix A)

$$\Pi_x = I_{ds} - \frac{1}{2}(I_{s^2} \otimes x)(P + I_{ds})(I_{s^2} \otimes x^T),$$

for $\otimes$ the Kronecker product and $P$ the $ds \times ds$ permutation matrix for which $P \text{vec}(x) = \text{vec}(x^T)$ for any matrix $x$. For simplicity, we take the sphere as our prime example and leave the Stiefel manifold case for the appendix.

Let momentum $p$ follow a degenerate Gaussian distribution on the tangent space to the sphere at $x$, i.e. $p \sim N(0, \Pi_x M \Pi_x)$, where $M$ is some positive semi-definite matrix. Then at any point $x$, the density of $p$ is proportional to

$$\text{Det}^{-1/2}(\Pi_x M \Pi_x) \exp \left(-\frac{1}{2}p^T(\Pi_x M \Pi_x)^+ p \right),$$

where $\text{Det}(A)$ is the pseudo determinant and $A^+$ is the pseudo inverse of matrix $A$. Then the Hamiltonian is given by

$$H(x, p) = -\log \pi(x) + \frac{1}{2} \log \text{Det}(\Pi_x M \Pi_x) + \frac{1}{2}p^T(\Pi_x M \Pi_x)^+ p,$$

for any pair $x$ and $p$. Similarly to the original gMC algorithm, we split $H(x, p)$ into two Hamiltonians

$$H^{[1]}(x, p) = -\log \pi(x) + \frac{1}{2} \log \text{Det}(\Pi_x M \Pi_x)$$

and

$$H^{[2]}(x, p) = \frac{1}{2}p^T(\Pi_x M \Pi_x)^+ p.$$
Using some matrix calculus and the fact that $\nabla \text{Det}(A) = \text{Det}(A) A^+$ (see the recent note on the derivative of the pseudo determinant [3]), the first system gives the equations

$$\dot{x} = 0$$
$$\dot{p} = \nabla_x \log \pi(x) - (\Pi_x M \Pi_x)^+ \Pi_x M x .$$

Since the gradient $\nabla_x \log \pi(x)$ does not necessarily belong to the tangent space, we perform the change of variables $v = (\Pi_x M \Pi_x)^+ p$. The equations now read

\begin{equation}
\dot{x} = 0 \tag{3.1}
\end{equation}
$$\dot{v} = (\Pi_x M \Pi_x)^+ (\nabla_x \log \pi(x) - (\Pi_x M \Pi_x)^+ \Pi_x M x) .$$

Velocity $v$ stays on the tangent space at $x$ because $(\Pi_x M \Pi_x)^+ = \Pi_x (\Pi_x M \Pi_x)^+ \Pi_x$ in general. The second system may also be written in terms of $v$:

\begin{align*}
H^{[2]}(x, p) &= \frac{1}{2} p^T (\Pi_x M \Pi_x)^+ p \\
&= \frac{1}{2} p^T (\Pi_x M \Pi_x)^+ (\Pi_x M \Pi_x) (\Pi_x M \Pi_x)^+ p \\
&= \frac{1}{2} v^T (\Pi_x M \Pi_x) v \\
&= \frac{1}{2} \tilde{v}^T \tilde{v} := H^{[2]}(x, v),
\end{align*}

where $\tilde{v} = (\Pi_x M \Pi_x)^{1/2} v$. The system corresponding to $H^{[2]}$ is solved by the geodesic with initial conditions $(x, \tilde{v})$. Thus the system corresponding to $H$ may be integrated by iteratively integrating according to (3.1) and the spherical geodesics. The accept/reject step is easy since the Hamiltonian is given explicitly.

The formulas greatly simplify when $M$ is the identity matrix. Since the pseudo determinant is equal to unity on projection matrices, the Hamiltonian reduces to

$$H(x, v) = -\log \pi(x) + \frac{1}{2} v^T v .$$

This is the same as Formula (2.1), but with $\pi(x)$ replacing $\pi_H(x)$, the posterior with respect to the Hausdorff measure. Hence, by working completely on the embedded manifold, we are able to derive a Hamiltonian that does not depend on any notion of intrinsic geometry whatsoever and thus avoids the log-Jacobian calculation of the embedding. The resulting details are given by Algorithm 1.

4. Discussion

We have proposed an alternative derivation to the geodesic Monte Carlo for embedded manifolds [1]. This derivation is conceptually simpler, as it does not rely on a notion of intrinsic manifold geometry and thus clarifies the algorithm. Specifically, it becomes clear that the inclusion of the log-Jacobian of the embedding in the Hamiltonian is unnecessary in any case where the target distribution is defined with respect to embedding coordinates. The resulting class of algorithms are symplectic and completely explicit (do not require implicit integration). The algorithm also allows for non-trivial mass matrix as an added benefit. Finally, the exposition hints how Metropolis adjustments may be incorporated into geometric Langevin algorithms such as [6].
Algorithm 1 Embedding geodesic Monte Carlo with non-trivial mass matrix

Let $x = x^{(k)}$ be the $k$th state of the Markov chain. The next sample is generated according to the following procedure.

(a) Generate proposal state $x^*$:

1: $v \sim N(0, (\Pi_x M \Pi_x)^\dagger)$
2: $e \leftarrow -\log \pi(x) + \frac{1}{2} \log \text{Det}(\Pi_x M \Pi_x) + \frac{1}{2}v^T(\Pi_x M \Pi_x)v$
3: $x^* \leftarrow x$
4: for $\tau = 1, \ldots, T$ do
5: $v \leftarrow v + \frac{1}{2}(\Pi_x M \Pi_x)^\dagger(\nabla_{x^*} \log \pi(x^*) - (\Pi_x M \Pi_x)^\dagger\Pi_x x^*)$
6: $\tilde{v} \leftarrow (\Pi_x M \Pi_x)^{1/2}v$
7: Progress $(x^*, \tilde{v})$ along the geodesic flow for time $\epsilon$.
8: $v \leftarrow (\Pi_x M \Pi_x)^{-1/2}\tilde{v}$
9: $v \leftarrow v + \frac{1}{2}(\Pi_x M \Pi_x)^\dagger(\nabla_{x^*} \log \pi(x^*) - (\Pi_x M \Pi_x)^\dagger\Pi_x x^*)$
10: end for
11: $e^* \leftarrow -\log \pi(x^*) + \frac{1}{2} \log \text{Det}(\Pi_x M \Pi_x^*) + \frac{1}{2}v^T(\Pi_x M \Pi_x^*)v$

(b) Accept proposal with probability $\min\{1, \exp(e) / \exp(e^*)\}$:

1: $u \sim U(0, 1)$
2: if $u < \exp(e - e^*)$ then
3: $x \leftarrow x^*$
4: end if

(c) Assign value $x$ to $x^{(k+1)}$, the $(k+1)$th state of the Markov chain.

References

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Appendix A. Projection matrix for the Stiefel manifold

When modeling an element $x \in S(d, s)$ of the Stiefel manifold, for $d \times s$ momentum matrix we write the degenerate Gaussian distribution

$$\det^{-1/2}(\Pi_x M \Pi_x) \exp \left( -\frac{1}{2} \text{vec}(p)^T(\Pi_x M \Pi_x)^\dagger \text{vec}(p) \right),$$
Π_\text{x} \text{ and } M \text{ are } ds \times ds \text{ matrices. To get the form for } \Pi_\text{x}, \text{ we note that the orthogonal projection of a matrix } v \text{ onto the tangent space at } x \text{ is }
\Pi_\text{x}(v) = v - \frac{1}{2} x (v^T x + x^T v).

Applying the vec operator gives
\text{vec}(\Pi_\text{x}(v)) = \text{vec}(v) - \frac{1}{2} \text{vec}(x (v^T x + x^T v))
\hspace{1cm} = \text{vec}(v) - \frac{1}{2} (I_{s^2} \otimes x) \text{vec}(v^T x + x^T v)
\hspace{1cm} = \text{vec}(v) - \frac{1}{2} (I_{s^2} \otimes x) \text{vec}(v^T x) + \text{vec}(x^T v)
\hspace{1cm} = \text{vec}(v) - \frac{1}{2} (I_{s^2} \otimes x) P \text{ vec}(x^T) + x^T v
\hspace{1cm} = \text{vec}(v) - \frac{1}{2} (I_{s^2} \otimes x)(P + I_{ds}) \text{vec}(x^T v)
\hspace{1cm} = \text{vec}(v) - \frac{1}{2} (I_{s^2} \otimes x)(P + I_{ds})(I_{s^2} \otimes x^T) \text{vec}(v)
\hspace{1cm} = (I_{ds} - \frac{1}{2} (I_{s^2} \otimes x)(P + I_{ds})(I_{s^2} \otimes x^T)) \text{vec}(v)
\hspace{1cm} = \Pi_\text{x} v

Hence
\Pi_\text{x} = I_{ds} - \frac{1}{2} (I_{s^2} \otimes x)(P + I_{ds})(I_{s^2} \otimes x^T).