The Geometry of Hamiltonian Monte Carlo

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With its systematic exploration of probability distributions, Hamiltonian Monte Carlo is a potent Markov Chain Monte Carlo technique; it is an approach, however, ultimately contingent on the choice of a suitable Hamiltonian function. By examining both the symplectic geometry underlying Hamiltonian dynamics and the requirements of Markov Chain Monte Carlo, we construct the general form of admissible Hamiltonians and propose a particular choice with potential application in Bayesian inference.

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Since its introduction by Duane, et al. [1] and development by Neal [2], Hamiltonian Monte Carlo (HMC) has proven to be a powerful Markov Chain Monte Carlo methodology. By utilizing Hamiltonian dynamics as a Markov transition kernel, HMC coherently explores the space of a target distribution and results in rapidly mixing Markov chains. Such dynamics, however, are dependent on a particular Hamiltonian function and existing applications have been limited mostly to forms common in the study of physical systems.

The feature of Hamiltonian dynamics that furnishes such efficient Markov chains is a consequence of not any particular Hamiltonian function, but rather an implicit symplectic geometry on the underlying parameter space. Particularly equipped with a symplectic geometry, and how that structure admits a flow along the cotangent bundle. The Tangent and Cotangent Bundles

A smooth, \( n \)-dimensional manifold \( M \) is defined as a topological space where the local neighborhood of any given point \( P \in M \) ‘looks like’ \( \mathbb{R}^n \). Formally, a homeomorphism \( \psi_\alpha : O_\alpha \to U_\alpha \) must exist from any open subset \( O_\alpha \subset M \) to an open subset \( U_\alpha \subset \mathbb{R}^n \) such that the map \( \psi_\beta \circ \psi^{-1}_\alpha \) is continuously differentiable for any overlapping subsets \( O_\alpha \cap O_\beta \neq \emptyset \).

Of the many possible differentiable mappings between differentiable manifolds, two of the most important are curves, which map open sets of \( \mathbb{R} \) to neighboring points on the manifold, and functions, which map each point \( P \) to \( \mathbb{R} \). The collection of all smooth curves and all smooth functions on \( M \) form differentiable manifolds in their own right, and these two manifolds naturally equip each point \( P \in M \) with two local vector spaces. Tangent vectors of all curves passing through \( P \) form an \( n \)-dimensional vector space known as the tangent space, \( T_P \); the gradients of all manifold functions in a neighborhood of point \( P \) span another \( n \)-dimensional vector space denoted the cotangent space, \( T^*_P \). These two vector spaces are dual in the sense that an element of \( T_P \) serves as a linear transformation mapping an element of \( T^*_P \) to \( \mathbb{R} \), and vice versa.

A set of \( n \) functions, \( \{ q^i(P) \} \) are coordinates on the manifold if they uniquely identify each point, and any choice of coordinate functions induces natural bases for the tangent and cotangent spaces across \( M \): the directional derivative vectors, \( \hat{e}_i \equiv \frac{\partial}{\partial q^i} \), and gradients, \( d\tilde{q}^i \), respectively. These coordinate bases provide an expansion of any element \( \bar{v} \in T_P \) or \( \bar{p} \in T^*_P \),

\[
\bar{v} = \sum_{i=1}^{n} v^i \hat{e}_i \quad \quad \quad \bar{p} = \sum_{i=1}^{n} p_i d\tilde{q}^i ,
\]

where the components \( v^i \) (resp. \( p_i \)) are manifold functions depending on \( \bar{v} \) (resp. \( \bar{p} \)) and the \( q^i \). Note that the

\[\text{1 Note that the index here, } i \in \{1, \ldots, n\}, \text{ is simply a label and need not, for example, be considered the components of a vector.}\]
components uniquely identify each element of the vector spaces: when $T_p$ and $T_p$ are treated as manifolds, the component functions $\{v^i\}$ (resp. $\{p_i\}$) serve as proper coordinate functions on $T_p$ (resp. $T^*_p$).

Collecting all of the tangent spaces across the manifold yields another 2n-dimensional manifold called the tangent bundle, $T\mathcal{M}$. A point in $T\mathcal{M}$ corresponds to a specific vector in a particular vector space $T_p$ and locally the bundle factors into a trivial product space of the base manifold $\mathcal{M}$ and the tangent space $T_p$. Coordinates on $T\mathcal{M}$ then decompose into the direct sum of coordinates on the two manifolds, $\{q^i, p_j\}$. Likewise the cotangent spaces can be collected into the cotangent bundle $T^*\mathcal{M}$ where each point is identified by the coordinates $\{q^i, p_j\}$. In analogy with physical systems, the two bundles $T\mathcal{M}$ and $T^*\mathcal{M}$ are also known as configuration space and phase space, respectively (Table I).

**The Symplectic Form**

A change of coordinates on the base manifold $\mathcal{M}$, $\{q^i\} \to \{Q^i\}$, induces a unique linear transformation on the basis one-forms $dq^i$ on $\mathcal{M}$, $\tilde{d}Q^i = \sum_{j=1}^n \frac{\partial Q^i}{\partial q^j} dq^j$, (1) and on the coordinate decomposition of a one-form $\tilde{p}$,

$$P_i = \sum_{j=1}^n \frac{\partial q^j}{\partial Q^i} p_j.$$ (2)

Note that the Jacobian and inverse Jacobian of the coordinate transformation, $\partial q^i/\partial Q^j$ and $\partial Q^i/\partial q^j$ respectively, are matrix inverses,

$$\sum_{j=1}^n \frac{\partial Q^i}{\partial q^j} \frac{\partial q^j}{\partial Q^k} = \delta^i_k.$$ 

Coordinate transformations on $\mathcal{M}$ also induce a family of transformations of the fields on $T^*\mathcal{M}$; these point transformations do not mix the $\{q^i\}$ and $\{p_i\}$ coordinates and preserve the trivial fiber structure of the manifold. Specifically, the one-forms $dq^i$ over $T\mathcal{M}$ (which are just the vertical lifts of the one-form fields $dq^i$ over $\mathcal{M}$) transform as in Eq. (1), while the coordinate functions $p_i$ transform as in Eq. (2). All of the coordinate functions, $\{q^i, p_j\}$, and their associated basis one-forms $\{dq^i, dp_j\}$ are clearly dependent on the coordinates of the base manifold.

Because the two transformations in Eq. (1) and Eq. (2) are inverses, however, there are some natural objects on $T^*\mathcal{M}$ independent of the manifold coordinates. In particular, the one-form $\theta^2$

$$\theta = \sum_{i=1}^n -p_i dq^i.$$ is coordinate independent by construction. The exterior derivative $d\theta$,

$$\omega = d\theta = \sum_i dq^i \wedge dp_i,$$ (3)

is more subtle: although the transformation of $dp_i$ involves derivatives of the Jacobian, $\omega$ is coordinate independent,

$$\omega' = \sum_j dQ^j \wedge dP_j = \sum_i dq^i \wedge dp_i = \omega.$$  

This can be seen either by explicit calculation, or more simply by noting that, because $\theta$ is coordinate independent, the exterior derivative $d\theta$ must be as well.

This *symplectic form*, $\omega$, is a two-form, or antisymmetric tensor of rank $(0, 2)$, which maps a given vector field $\vec{X}$ to a one-form $\tilde{\omega}$,

$$\tilde{\omega} \equiv \omega(\vec{X}, \cdot).$$

Because $\omega$ is non-degenerate, this linear transformation is invertible, and any one-form $\tilde{\omega}$ over phase space also defines a unique vector field $\vec{Y}$ such that $\omega(\vec{Y}, \cdot) = \tilde{\omega}$. Starting from any function $H(q, p)$ on $T^*\mathcal{M}$ one can construct a one-form via the exterior derivative, $dH$, and, from this, define the *Hamiltonian vector field* $\vec{X}_H$ associated with $H$ such that $\omega(\vec{X}_H, \cdot) = dH$.

**Hamiltonian Flow**

By specifying a direction at each point $P \in T^*\mathcal{M}$, the vector field $\vec{X}_H$ defines curves through the manifold. These curves cover the entire manifold without intersecting, mapping every point $P$ to another along the local curve and generating a *flow* of the entire cotangent bundle.

In particular, the vector field differentiates any function $f$ along the defined vector at each point, $\vec{X}_H(f) = \left(\vec{X}_H\right)^i \frac{\partial}{\partial x^i}(f)$, where $x^i = \{q^i, p_j\}$ are the coordinates of $T^*\mathcal{M}$. If the curves are parametrized by $t \in \mathbb{R}$, then the action of the vector field is simply $\vec{X}_H(f) = \frac{d}{dt}(f)$. Applying the vector field $\vec{X}_H$ to the coordinates functions.

2 The resemblance of $\theta$ and an expansion of a one-form $\tilde{p}$ on $\mathcal{M}$ is a result of ambiguous notation. Here $p_i$ are coordinate functions on $T^*\mathcal{M}$, and $dq^i$ are one-forms on $T^*\mathcal{M}$. This one-form $\theta$ (or its negation $-\theta$) is sometimes called the tautological form.
TABLE I. The tangent and cotangent bundles, and their coordinates, are often referenced in analogy to physical systems in classical mechanics.

| Manifold Name | Coordinate Functions | Coordinate Names |
|---------------|----------------------|------------------|
| $\mathcal{M}$  | Position Space       | $q^i$            |
| $T\mathcal{M}$ | Configuration Space  | $q^i, v^i$       |
| $T^*\mathcal{M}$ | Phase Space          | $q^i, p_j$       |

Consequently, the Lie derivative of the top-rank differential volume form $\Omega$

$$\Omega \equiv \omega^n \equiv \omega \wedge \omega \wedge \ldots \wedge \omega$$

also vanishes,

$$\mathcal{L}_{\vec{X}_H} \Omega = 0,$$

implying that differential volume elements of phase space are preserved under the evolution along the integral curves.

Note that, with both the Hamiltonian and the differential phase space volume preserved, the phase space density $F(H)\Omega$ for any smooth scalar function $F : \mathbb{R} \to \mathbb{R}$ is also invariant along integral curves.

$$\mathcal{L}_{\vec{X}_H} F(H)\Omega = \left( \mathcal{L}_{\vec{X}_H} F(H) \right) \Omega + F(H)\mathcal{L}_{\vec{X}_H} \Omega = F'(H) \left( \mathcal{L}_{\vec{X}_H} H \right) \Omega = 0.$$

This property is inherent to the symplectic geometry of the cotangent bundle and holds for any choice of Hamiltonian and scalar function $F.$

THE IDENTIFICATION OF FORMS AND MEASURES

A top rank form on a $n$-dimensional manifold is a tensor, independent of the manifold coordinates. Given a particular choice of coordinates $\{x^i\}$ defined across the entire manifold, however, any such top-rank form can be decomposed as

$$\phi = f(x) \, d^n x,$$

where $f(x)$ is a scalar function determined by the coordinates and $d^n x$ is the volume form of the coordinates constructed by wedging the gradients of each coordinate function together,

$$d^n x = dx^1 \wedge \cdots \wedge dx^n.$$

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3 The resulting Hamiltonian flow is often denoted Hamiltonian evolution, or Hamiltonian dynamics.

4 Local Hamiltonian flow is not always adequate: constraints of the coordinate functions, for example, require discontinuous jumps in momentum otherwise known as specular reflection (Appendix A).

5 The scalar functions considered above are geometric objects in their own right and, indeed, the Lie derivative of a scalar field agrees with the action of the vector field.

6 This geometric statement is equivalent to Liouville’s theorem in statistical mechanics [4].
Introducing the object \( f \) which evaluates to the appropriate \( f_\mathbf{x}(\mathbf{x}) \) for any given set of coordinate functions \( \{ x^i \} \), the decomposition becomes

\[
\phi = f(\mathbf{x}) \, d^n\mathbf{x}.
\]

By construction, the objects \( f(\mathbf{x}) \) and \( d^n\mathbf{x} \) in the decomposition depend on the coordinates: under a change of coordinates from \( \{ x^i \} \rightarrow \{ X^i \} \) the two terms transform by acquiring a determinant of the Jacobian matrix \( \partial \mathbf{x}/\partial \mathbf{X} \),

\[
f(\mathbf{X}) = \left| \frac{\partial \mathbf{x}}{\partial \mathbf{X}} \right|^{+1} f(\mathbf{x})
\]

\[
d^n\mathbf{X} = \left| \frac{\partial \mathbf{x}}{\partial \mathbf{X}} \right|^{-1} d^n\mathbf{x}.
\]

These objects are not tensors but rather tensor densities. In general a tensor density of weight \( w \) transforms as

\[
\rho(\mathbf{X}) = \left| \frac{\partial \mathbf{x}}{\partial \mathbf{X}} \right|^w \rho(\mathbf{x}),
\]

with \( f(\mathbf{x}) \) and \( d^n\mathbf{x} \) immediately identified as tensor densities of weight \( +1 \) and \( -1 \), respectively. Note that, when the two objects are combined, the additional Jacobian factors cancel to give a coordinate independent object as expected of the original tensor.

The topological space that forms the manifold \( M \) can also be endowed with a coordinate independent measure that, given coordinates, can be decomposed into two coordinate-dependent objects \( \mathcal{E} \). Any Borel measure \( \mu \) can be written as

\[
d\mu = f(\mathbf{x}) \, d^n\mathbf{x},
\]

where \( d^n\mathbf{x} \) is now the Lebesgue measure on the chosen coordinates and \( f(\mathbf{x}) \) is the Radon-Nikodym derivative of \( \mu \) with respect to \( d^n\mathbf{x} \). Under a coordinate transformation, these two objects acquire a factor of the Jacobian just as above,

\[
f(\mathbf{X}) = \left| \frac{\partial \mathbf{x}}{\partial \mathbf{X}} \right|^{+1} f(\mathbf{x})
\]

\[
d^n\mathbf{X} = \left| \frac{\partial \mathbf{x}}{\partial \mathbf{X}} \right|^{-1} d^n\mathbf{x}.
\]

Indeed the similarity of the two systems is no coincidence: provided that the manifold can be oriented, the Riesz representation theorem guarantees that the space of top-rank forms is locally isomorphic to the space of measures \( \mathcal{E} \), providing an identification between the form \( \phi \) and measure \( \mu \) as well as the terms in their above decompositions. If the form is everywhere positive and the integral over all of \( M \) is finite then the corresponding measure becomes a normalizable Borel measure from which one can build a probabilistic space.

Note that objects on the cotangent bundle can be endowed with respect to coordinate transformations on \( T^*M \), acquiring factors of \(|\partial(\mathbf{q},\mathbf{p})/\partial(\mathbf{Q},\mathbf{P})|\), or with respect to transformations on \( M \), picking up only factors of \(|\partial\mathbf{q}/\partial\mathbf{Q}|\). The point transformations introduced above are a special case of symplectomorphisms, which preserve the symplectic form \( \omega \) and have Jacobian determinant \( |\partial(\mathbf{q},\mathbf{p})/\partial(\mathbf{Q},\mathbf{P})| = +1 \). Therefore, any object transforming as a density with respect to \( T^*M \), such as those in the above decompositions, are actually invariant under transformations that preserve the structure of the cotangent bundle.

INTEGRAL CURVES AS MARKOV TRANSITION KERNELS

Because the volume form \( \Omega \) is nowhere zero, a symplectic manifold can always be oriented and, consequently, the form \( F(\mathbf{H}) \, \Omega \) can always be identified with a measure. Moreover, if \( F \) is restricted to positive, integrable functions,

\[
F : \mathbb{R} \rightarrow \mathbb{R}^+ \text{ s.t. } \int_M F(\mathbf{H}) \, \Omega \in \mathbb{R}^+,
\]

then the corresponding measure will be a Borel measure. Taking \( F(\mathbf{H}) = \exp(C - H) \) a given Hamiltonian uniquely defines a probability measure

\[
d\mu = \pi(\mathbf{q},\mathbf{p}) \, dq \, dp = \exp[C - H(\mathbf{q},\mathbf{p})] \, \Omega,
\]

where \( C \in \mathbb{R} \) is determined by the normalization. Hamiltonian flow maps \( \mu \) into itself and thus defines a proper Markov transition kernel for the distribution \( \pi(\mathbf{q},\mathbf{p}) \). Note that, in practical applications the dynamics must be performed numerically and the measure will not be conserved exactly \( \mathcal{E} \). Any subsequent bias, however, can be avoided by treating the flow as a Metropolis proposal function instead of the transition itself \( \mathcal{E} \).

Now if the gradients of the Hamiltonian satisfy

\[
\dot{q}^i(\mathbf{q},-\mathbf{p}) = -\dot{p}_i(\mathbf{q},\mathbf{p})
\]

\[
\dot{p}_i(\mathbf{q},-\mathbf{p}) = +\dot{q}_i(\mathbf{q},\mathbf{p})
\]

then the resulting flow is reversible: reflecting the momenta and evolving the same distance along the integral curves recovers the initial configuration. By adding such a reflection to the end of each evolution, the resulting

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7 The definition of the sign of the weight can vary within the literature; here we use the convention of \( \mathcal{E} \).

8 Other choices for \( F \) are possible, but this exponential form has a computational advantage when considering the ubiquitous distributions from the exponential family.
transition has detailed balance with respect to \( \pi(q, p) \), which then becomes the unique stationary distribution.

The augmented transitions, however, do not produce a convergent Markov chain because the evolution explores only level sets of probability density,

\[
\pi(q, p) = \pi(q_0, p_0) \propto \exp(-H(q_0, p_0)).
\]

Movement across the probability contours can be introduced by adopting a Gibbs strategy and alternating each Hamiltonian transition with transitions from any conditional distribution spanning the contours. The combined transitions guarantee ergodicity and, provided that the transitions are tuned to avoid cycles in phase space and subsequent periodicity, the resulting Markov chain will converge to \( \pi(q, p) \).

While any reversible Hamiltonian defines both a probability distribution and respective Markov chain, practical applications demand the reverse construction: what Hamiltonians, and hence well-behaved Markov chains, are consistent with a given target distribution \( \pi(x) \)?

Provided a decomposition of the random variables into positions and momenta, \( x = \{q, p\} \), the support of the target distribution could be identified with the full cotangent bundle and \( \pi(x = \{q, p\}) \) would fully define a Hamiltonian. There is no natural motivation for such a decomposition, however, and one resulting in a reversible Hamiltonian system need not even exist.\(^9\)

If we appeal to the factorization of the cotangent bundle into \( \{q^i\} \) and \( \{p_i\} \) coordinates and instead identify the random variables with the position manifold \( \mathcal{M} \), however, then \( x = q \) and the target distribution constrains only the marginal distribution of \( \pi(q, p) \),

\[
\pi(x) = \int d^n p \pi(q, p)|_{q=x}.
\]

Any joint distribution defined over the entire cotangent bundle factors,

\[
\pi(q, p) = \pi(p|q) \pi(q),
\]

and the residual freedom in the choice of conditional distribution, \( \pi(p|q) \), can be engineered to not only guarantee reversibility but also be easily sampled to ensure that the entire procedure remains computationally efficient. Once the latent variables \( p \) are marginalized out, the Markov chain generates the desired samples from \( \pi(q) \).

This final identification completes the construction of a general MCMC procedure: a given target distribution \( \pi(q) \) and the selection of an appropriate conditional distribution, \( \pi(p|q) \), defines Hamiltonian dynamics and a well-behaved transition kernel. Because the dynamics incorporate gradients of the target distribution, the transitions systematically explore the target distribution and avoid the random walk behavior typical of other MCMC techniques. Moreover, the freedom in the conditional distribution offers the potential for including more information about the target distribution and, consequently, further improving the performance of the resulting Markov chain.

### Admissible Hamiltonians

With the above considerations, the most general Hamiltonian yielding the desired Markov chain is

\[
H = -\log \pi(q, p) + C
\]

\[
= -\log \pi(p|q) \pi(q) + C
\]

\[
= -\log \pi(p|q) - \log \pi(q) + C
\]

\[
\equiv T(q, p) + V(q) + C.
\]

Note that \( T \) and \( V \) are neither scalars nor scalar densities. While the joint distribution \( \pi(q, p) \) is invariant under point transformations (and indeed all symplectomorphisms), the distributions in the decomposition are densities of opposite weight with respect to coordinate transformations on the position manifold \( \mathcal{M} \),

\[
\pi(P|Q) = \left| \frac{\partial q}{\partial Q} \right|^{-1} \pi(p|q)
\]

\[
\pi(Q) = \left| \frac{\partial q}{\partial Q} \right|^{-1} \pi(q),
\]

and the terms in the Hamiltonian must transform as

\[
T(Q, P) = T(q, p) + \log \left| \frac{\partial q}{\partial Q} \right| \tag{4}
\]

\[
V(Q) = V(q) - \log \left| \frac{\partial q}{\partial Q} \right| \tag{5}
\]

When added together the additional factors cancel to yield the scalar Hamiltonian.

While the potential energy \( V(q) \) is fully specified by the target distribution, the kinetic energy is constrained by only the defining normalization of a conditional distribution

\[
\int d^n p \exp(-T(q, p)) \in \mathbb{R}^+,
\]

i.e. a finite positive number independent of \( q \), and the demands of detailed balance,

\[
\frac{\partial T}{\partial p_i}(q, -p) = -\frac{\partial T}{\partial p_i}(q, p).
\]

Reversibility is assured for any kinetic energy of the form

\[
T(q, p) = \tau_1(q, p) + \tau_1(q, -p) + \tau_2(q),
\]

\(^9\) A trivial example being a distribution defined on an odd-dimensional space.
where the first two terms can, in general, be decomposed into a sum of completely symmetric tensors \( T_{n}^{(1)} \) of type \((n, 0)\) with \( n \) even and positive.\(^{10}\)

\[
\tau_1(q, p) + \tau_1(q, -p) = \sum_{n=2, 4, \ldots} \sum_{j_1 \ldots j_n} p_{j_1} \cdots p_{j_n} T_{n}^{(1)[j_1 \ldots j_n]}(q). 
\]

A particularly useful choice is any scalar function of a non-degenerate quadratic form in the momenta,

\[
T(q, p) = \tau \left( \sum_{ij} p_i p_j A^{ij}(q) \right) + t_2(q). 
\]

Here the tensor \( A(q) \), or more appropriately its inverse, effectively serves as a spatially-dependent linear transformation of the coordinates \( q \) — if the transformation simplifies the structure of the target distribution then the resulting Markov chain promises to explore the space much more efficiently. In particular, the incorporation of the derivatives of the potential can help to locally standardize the distribution, avoiding complications due to the narrow valleys characteristic of strong correlations.

Taking \( \tau \) to be the identity gives

\[
T(q, p) = \frac{1}{2} \sum_{ij} p_i p_j A^{ij}(q) - \frac{1}{2} \log |A(q)|, \tag{6}
\]

which results in a gaussian conditional distribution,

\[
\pi(p|q) = \mathcal{N}(p|0, A).
\]

Notice how the normalization of the conditional gaussian introduces the determinant of \( A \), which transforms as a tensor density of weight \(-2\) with respect to coordinate transformations on \( \mathcal{M} \). Under a point transformation the normalization becomes

\[
\frac{1}{2} \log |A(Q)| = \frac{1}{2} \log |\partial q/\partial Q|^{-2} |A(q)|
= \frac{1}{2} \log |A(q)| + \frac{1}{2} \log |\partial q/\partial Q|^{-2}
= \frac{1}{2} \log |A(q)| - \log |\partial q/\partial Q|,
\]

introducing exactly the necessary factor of the Jacobian to ensure the proper transformation of \( T \). The identification of measures with forms ensures consistency between the two perspectives.

If the covariance \( \Sigma = A^{-1} \) is proportional to the identity then the Hamiltonian reduces to that of classical mechanics and the form used in the first implementations of HMC.\(^{11}\) A nontrivial but constant covariance matrix allows for a global rescaling and rotation of the target distribution.\(^{2}\), and a spatially dependent covariance transforms the target distribution locally.\(^{2}\)

Because integrability requires it to be positive-definite and non-degenerate, the spatially-varying covariance can also be interpreted as a Riemannian metric and, from this perspective, the Hamiltonian evolution locally parallels geodesics of a curved manifold.\(^{2}\) This additional geometric structure embedded within the symplectic geometry creates the potential to further improve performance with the application of more tools from differential geometry. Utilizing any such possibility, however, first requires a choice of the spatially-varying covariance.

### Choices of the Covariance Matrix

The Fisher-Rao metric ubiquitous in information geometry,

\[
\Sigma_{ij} = \mathbb{E}_y \left[ \frac{\partial \log \pi(x|y)}{\partial x^i} \frac{\partial \log \pi(x|y)}{\partial x^j} \right],
\]

or given particular coordinate functions

\[
\Sigma_{ij} = \mathbb{E}_y \left[ \frac{\partial V(x|y)}{\partial x^i} \frac{\partial V(x|y)}{\partial x^j} \right],
\]

provides an obvious candidate for the covariance matrix, and its use in HMC has proven successful when the expectation can be performed analytically.\(^{2}\) While the Fisher-Rao metric does incorporate derivatives of the target distribution, however, it requires integrating over the \( y \) to ensure positive-definiteness. In a Bayesian application this necessitates expectation of the posterior over the ensemble of possible data sets; not only is the expectation contrary to the Bayesian philosophy of inference based solely on the measured data, it also washes out the local structure particular to a given data set that can prove important in posterior exploration.

The geometric perspective, however, suggests another possibility free from the unwanted marginalization. A “background” Riemannian metric \( \sigma \) defined on \( \mathcal{M} \) induces a metric on the graph of the potential \( V \),\(^{12}\)

\[
\Sigma_{ij} = \sigma_{ij}(q) + \frac{\partial V(q)}{\partial q^i} \frac{\partial V(q)}{\partial q^j}.
\]

Unfortunately, \( \Sigma \) does not transform as a proper tensor because \( V \) is not a proper scalar function. The additional structure afforded by \( \sigma \), however, admits the necessary correction: because the determinant \( |\sigma| \) is a scalar density of weight \(+2\) with respect to transformations on \( \mathcal{M} \),

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\(^{10}\) In order to satisfy the defining transformation property, the contribution from \( \tau_1(q, p) + \tau_1(q, -p) \) must be a scalar and, consequently, the \( T_{n}^{(1)} \) must be tensors. The second term \( \tau_2(q) \) is ultimately responsible for the introduction of the necessary factor of \( \log |\partial q/\partial Q| \).

\(^{11}\) Provided that \( k+l \) is even, the determinant of a rank \((k, l)\) tensor exists and transforms as a scalar density of weight \( l-k \).

\(^{12}\) The graph is an \( n \)-dimensional submanifold in the \((n + 1)\)-dimensional manifold with coordinates \((q, V(q))\).
Because the determinant of the homogeneous metric $|\sigma| \equiv \det \sigma$ is a true scalar and the modified metric also requires only $O(n)$ operations and allowing the entire Hamiltonian flow to be calculated at the same order.

Note the similarity of the outer product $(\partial \bar{V})(\partial \bar{V})$ to the argument of the expectation value in the Fisher-Rao metric: this induced metric features a similar structure without the undesired expectation. Moreover, $\Sigma$ is simply a rank-1 update of the background geometry and the metric can be efficiently inverted with the Sherman-Morrison-Woodbury formula 12.

$$\bar{\Lambda}^{ij} = \lambda^j - \frac{(\partial \bar{V})(\partial \bar{V})}{1 + (\partial \bar{V})(\partial \bar{V})},$$

where $\lambda$ is the inverse of $\sigma$ (satisfying $\lambda^{ik} \sigma_{kj} = \delta^i_j$), and $\partial^i = \lambda^{ij} \partial_j$.

If $\sigma$ is homogeneous (i.e. independent of position) then the inversions necessary at each iteration of the Hamiltonian evolution can be computed at order $O(n^2)$, significantly faster than the $O(n^3)$ required for the inversion of the dense Fisher-Rao metric. The Christoffel coefficients of the metric $\bar{\Sigma}$, which specify the Hamiltonian flow, are straightforward to calculate in this case, 13.

$$\Gamma^i_{jk} = \frac{(\partial^i \bar{V})(\partial_j \partial_k \bar{V})}{1 + (\partial^i \bar{V})(\partial_j \bar{V})}.$$

also requiring only $O(n^2)$ operations and allowing the entire Hamiltonian flow to be calculated at the same order. Note the appearance of $\partial_i \partial_j V$ in the Christoffel coefficients: while $\bar{\Sigma}$ appears to incorporate only the outer product approximation to the Hessian of $V$, the full Hessian, and all the information it contains, is included in the evolution.

Constructed from derivatives of $\bar{\Sigma}$, the Riemann curvature tensor and its contraction, the rank-2 Ricci tensor, offer the potential to include higher-order derivatives and, consequently, more information into the evolution. An explicit calculation, however, shows that, surprisingly, only second derivatives of $V$ contribute to the Riemann tensor. Further investigation is necessary to determine the full utility of including these tensors into the kinetic energy.

CONCLUSIONS AND FUTURE WORK

By considering the geometry of Hamiltonian dynamics and the basic constraints of Markov chain Monte Carlo, we have constructed the most general approach to Hamiltonian Monte Carlo (HMC).

The simplest admissible Hamiltonian given in Eq. 9 reproduces existing approaches to Hamiltonian Monte Carlo, but knowing the most general form begs further extensions. Girolami, et al., for example, have considered the kinetic energy

$$T(q, p) = \frac{\nu + n}{2 \nu} \log \left( 1 + \sum_{ij=1}^n p_i \bar{A}^{ij}(q) \right) \ln \lambda(q),$$

which gives Student’s t-distribution in place of the gaussian, but with only mixed results. Other choices of the kinetic energy may dramatically improve HMC for certain distributions, and there may still be means to improve the performance universally.

Generalizing the symplectic manifold of HMC to a Poisson manifold 10 offers even more possibilities. Without the restriction of non-degenerate forms, the Poisson manifold can accommodate distributions with spatially varying dimensionality and perhaps even admits trans-dimensional Monte Carlo.

Given the unexplored possibilities of this geometric perspective, the future of HMC is promising.

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APPENDIX A: SPECULAR REFLECTION FOR GENERAL HAMILTONIANS

The explicit incorporation of inequality constraints is often advantageous, and sometimes even necessary, in the construction of certain Markov chains. Arbitrary inequality constraints,

$$C(q) > 0,$$

can be incorporated into the Hamiltonian framework with the introduction of an infinite potential 11,

$$V(q) = \begin{cases} \infty, & C(q) \leq 0 \\ 0, & \text{else} \end{cases}.$$ 

A naïve implementation of Hamiltonian dynamics with such a potential, however, immediately fails because the gradient $dV(q)$ along the boundary is undefined.

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13 Because the determinant of the homogeneous metric $|\sigma|$ is also position independent, $\partial_i V = \partial_i V$ and the metrics coincide, $\Sigma = \bar{\Sigma}$. 


When considering the classical mechanics of a point particle, \( H = \frac{1}{2} \sum_{ij} p_i p_j \delta^{ij} + V(q) \), the difficulties around the potential barrier can be avoided by appealing to the exact result: the components of momentum perpendicular to the constraint surface reflect while preserving the value of the Hamiltonian. This \textit{specular reflection} is given by

\[
\Delta p = p' - p = -2 (p, \hat{n}) \hat{n}, \tag{7}
\]

where the unit normal along the surface of equality \((C(q) = 0)\) is

\[
\hat{n} = \frac{dC}{\sqrt{(dC, dC)}}
\]

and the inner product of one-forms is induced by the symmetric \((2,0)\) tensor \(\delta\),

\[
(a, b) \equiv \sum_{ij} a_i b_j \delta^{ij} = \sum_i a_i b_i.
\]

The reflection depends only on the direction of \(dC\) and not the undefined \(dV\). Also note that only the components of the momentum perpendicular to level sets of \(C(q)\) transform; those parallel to level sets are unaffected.

Generalizing specular reflection to a general Hamiltonian system is straightforward. The gradient \(n \equiv dC\) defines a unique one-form at the surface of constraint equality \((C(q) = 0)\), and forms a basis with the addition of \((n-1)\) one-forms \(\omega^i\), \(i \in \{1, \ldots, n-1\}\), each linearly independent of one another and \(n\). With this basis, the momentum \(p\) at a point of reflection \(q\) on the constraint boundary may be decomposed as

\[
p = p^+ n + \sum_{i=1}^{n-1} p_i^\parallel \omega^i.
\]

Because the reflection is determined entirely by the surface \(C(q) = 0\), the momentum can transform only along the one-dimensional subspace spanned by \(n\). Consequently, the \(p^\parallel\) should be invariant and a general reflection is given by

\[
p = p^+ n + \sum_{i=1}^{n-1} p_i^\parallel \omega^i \rightarrow p' = \alpha p^+ n + \sum_{i=1}^{n-1} p_i^\parallel \omega^i,
\]

along with the condition that the Hamiltonian remains invariant, \(H(q, p') = H(q, p)\).

In the case of a quadratic kinetic energy,

\[
H(q, p) = \frac{1}{2} \sum_{ij} p_i p_j \Lambda^{ij}(q) - \frac{1}{2} \log |\Lambda(q)| + V(q),
\]

conservation of the Hamiltonian requires

\[
0 = H(q, p') - H(q, p)
\]

\[
= (\alpha - 1) p^+ \left[ \frac{1}{2} (\alpha + 1) p^\parallel \sum_{ij} (dC)_i (dC)_j \Lambda^{ij} + \sum_{k=1}^{n-1} p_i^\parallel \sum_{ij} (dC)_i (\omega^k)_j \Lambda^{ij} \right],
\]

where \((dC)_i\) and \((\omega^k)_j\) are the components of the respective one-forms in an arbitrary basis.

Ignoring the \(\alpha = 1\) solution where the momentum is unchanged,

\[
\alpha = -2 \sum_{k=1}^{n-1} p_i^\parallel \sum_{ij} (dC)_i (\omega^k)_j \Lambda^{ij} - 1,
\]

or with a bit of manipulation

\[
\alpha - 1 = -2 \frac{\sum_{ij} (dC)_i p_j \Lambda^{ij}}{p^\parallel \sum_{ij} (dC)_i (dC)_j \Lambda^{ij}},
\]

implying that the change in momentum is

\[
\Delta p = (\alpha - 1) p^\parallel n = -2 \frac{\sum_{ij} (dC)_i p_j \Lambda^{ij}}{\sum_{ij} (dC)_i (dC)_j \Lambda^{ij}} n.
\]

Defining an inner product induced by the tensor \(\Lambda\),

\[
(a, b)_{\Lambda} \equiv \sum a_i b_j \Lambda^{ij},
\]

and a unit one-form under this inner product

\[
\hat{a} \equiv \frac{a}{\sqrt{(a, a)_{\Lambda}}},
\]

the generalized specular reflection becomes

\[
\Delta p = -2 (\hat{n}, p)_{\Lambda} \hat{n}. \tag{8}
\]

The resemblance of Eq. (8) to Eq. (7) is welcome. As before, the dependence of the result on only the direction of \(n\) ensures that the infinite magnitude of the potential barrier provides no difficulties. Moreover, the general result not only reduces to the classical case for \(\Lambda^{ij} = \delta^{ij}\), it also agrees with the generalization that would be expected given the interpretation of the quadratic kinetic energy resulting from a Riemannian (covariant) metric \(\Sigma_{ij}\) on the base manifold (where as before \(\Sigma = \Lambda^{-1}\)).

A straightforward calculation verifies that Eq. (8) is also a sufficient reflection solution for any kinetic energy of the form

\[
T(q, p) = \tau \left( \sum_{ij} p_i p_j \Lambda^{ij}(q) \right) + \tau_2(q).
\]
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