CURVATURE AND CONCENTRATION OF HAMILTONIAN MONTE CARLO IN HIGH DIMENSIONS

SUSAN HOLMES, SIMON RUBINSTEIN-SALZEDO, AND CHRISTOF SEILER

ABSTRACT. In this article, we analyze Hamiltonian Monte Carlo by placing it in the setting of Riemannian geometry using the Jacobi metric, so that each step corresponds to a geodesic on a suitable Riemannian manifold. We then combine the notion of curvature of a Markov chain due to Joulin and Ollivier with the classical sectional curvature from Riemannian geometry to derive error bounds for HMC in important cases, where we have positive curvature. These cases include several classical distributions such as multivariate Gaussians, and also distributions arising in the study of Bayesian image registration. The theoretical development suggests the sectional curvature as a new diagnostic tool for convergence for certain Markov chains.

1. INTRODUCTION

Approximating integrals is central to most statistical endeavors. Here, we investigate an approach drawing from probability theory, Riemannian geometry, and physics that has applications in MCMC generation of posterior distributions for biomedical image analyses.

We take a measure space $\mathcal{X}$, a function $f : \mathcal{X} \rightarrow \mathbb{R}$, and a probability distribution $\pi$ on $\mathcal{X}$, and we aim to approximate

$$I = \int_{\mathcal{X}} f(x) \pi(dx).$$

One way to do so is to pick a number $T$, choose points $x_1, x_2, \ldots, x_T \in \mathcal{X}$ sampled according to $\pi$, and estimate $I$ by

$$\hat{I} = \frac{1}{T} \sum_{i=1}^{T} f(x_i).$$

However, difficulties quickly arise. How do we sample from $\pi$? How do we select $T$ so that the error is below an acceptable threshold without having to choose $T$ so big that computation is prohibitively time-consuming? And how do we bound the error? In this article, we address these issues.

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1.1. Main Contribution. The goal of this article is to compute error bounds for $E((I-\hat{I})^2)$ or $\mathbb{P}(|I-\hat{I}| \geq r)$ when points $x_1, x_2, \ldots, x_T \in \mathcal{X}$ are approximately sampled from $\pi$ using Hamiltonian Monte Carlo (see §4). Our bounds are applications of theorems of Joulin and Ollivier in [JO10] using a special notion of curvature. Our main contribution is the combined use of the Jacobi metric [Pin75] (see §5) with the curvature approach introduced by [JO10], [Oll09] and Joulin [Jou07] following work of Sturm [Stu06a, Stu06b].

Our results specifically target the high-dimensional setting in which there is no underlying low-dimensional model. We can show that, in important classes of distributions, $T$ depends only polynomially on the dimension and error tolerance. This is relevant for the modern world where there are multiple sources of high-dimensional data. For instance, medical imaging, for which we provide an example in §7.3, produces high-dimensional data, as points in one region of an image are essentially independent of those in other regions.

1.2. Background. The idea of constructing a Markov chain whose stationary distribution is $\pi$ appeared originally in a five-author paper [MRR+53] which introduced the incremental random walk proposal, generalized by Hastings to include independent proposals [Has70]. A recent overview of the subject can be found in [Dia09].

Unfortunately, questions about error bounds are more difficult, and in practice, the Metropolis-Hastings algorithm can converge slowly. One reason being that the algorithm uses minimal information, considering only the probabilities of the proposal distribution and a comparison of probabilities of the target distribution. In particular, it does not use any geometric information. It stands to reason that an algorithm that sees more of the structure of the problem ought to perform better.

We are going to explore a different generation method inspired from physics called Hamiltonian Monte Carlo. We imagine an object moving around on $\mathcal{X}$ continuously. From time to time, we measure the position $x_i$ of the object, with the aim of using these discrete measurements $x_i$ in (1.1). We can imagine using $\pi$ to determine the time between measurements, thereby “distorting time” based on $\pi$. In regions of high density, we increase the measurement frequency, so that we obtain many samples from these regions. In regions of low density, we decrease the measurement frequency, so that we obtain few samples there.

An equivalent approach, which will make the link with Riemannian and differential geometry, is to think of $\pi$ as stretching and shrinking the space $\mathcal{X}$ so that regions of high density are physically larger, and regions of low density are physically smaller. These two approaches are in fact the same, as shrinking a region while keeping the time between measurements fixed has the same effect as keeping space uniform while varying the time between measurements.

The idea of stretching and shrinking space is nothing new in probability and statistics; for instance, inverse transform sampling for a distribution on $\mathbb{R}$, samples a point $p$ from a distribution with cumulative distribution function $F$ by picking a random number $x \in [0,1]$ and letting $p$ be the largest number so that $F(p) \leq x$, as in Figure 1. Here, we are shrinking the regions of low density so that they are less likely to be selected.

Example 1.1. Consider the Cauchy distribution, which has cumulative distribution function $F(p) = \frac{1}{2} + \frac{1}{\pi} \arctan(p)$. Its inverse function is $F^{-1}(x) = \tan \left( \pi x - \frac{\pi}{2} \right) =$
Inverse transform sampling

Figure 1. Inverse transform sampling of a standard Cauchy distribution.

$-\cot(\pi x)$. To sample from this distribution, we pick $x \in [0, 1]$ uniformly, and then we let $p = F^{-1}(x)$. Then $p$ is a Cauchy-random variable. This method is illustrated in Figure 1.

In order to start the process, we put the particle in an initial position and start moving it. We allow the particle to move for a certain amount of time before we begin recording so that its starting point does not have an overriding influence. Thus, we typically use

$$\hat{I} = \frac{1}{T} \sum_{i=T_0+1}^{T_0+T} f(x_i)$$

in place of (1.1). The number $T_0$ is called the burn-in time. The starting point plays a role in determining $T_0$: if the particle starts in a spot near all the high density regions, then $T_0$ can be fairly small; on the other hand, if the particle starts far from the high density regions, we will need a larger $T_0$, lest the low-density region near the starting point be heavily overrepresented. We make precise statements in §6, and in particular Theorems 6.5, 6.6 and 6.7.

In §5, we define a notion of curvature for Markov chains, in §6, we use it to deduce error bounds for general Markov chains following [JO10], and in §7, we show new error bounds related to Markov chains motivated by the aforementioned physics analogy for three examples.

This article fulfills two goals. On the one hand, we produce new results on mixing times and error bounds, which we believe to be of theoretical interest. On the other hand, we hope that it can serve as a user’s guide for researchers in other areas of statistics hoping to access new tools from Riemannian geometry. We have
made every effort to keep our presentation as concrete as possible. We include a theoretical analysis of the multivariate Gaussian distribution in §7.1 and a real world example from medical image registration in §7.3.

This article extensively extends an early short version published as a conference article in the proceedings at NIPS [SRSH14a]. We present new introductory and background material, detailed mathematical developments of the proofs, and two new examples: the multivariate $t$ distribution and medical image registration.

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2. Markov Chain Monte Carlo

Our goal in this article is to quantify the approximation error made when approximating

$$I = \int_{X} f d\pi \quad \text{by} \quad \hat{I} = \frac{1}{T} \sum_{i=1}^{T} f(x_i),$$

where $x_i$ are sampled using a special Markov chain whose stationary distribution is $\pi$. The standard Metropolis-Hastings algorithm [MRR+53, Has70] uses a proposal distribution $P_x$ starting at $x \in X$ and has an acceptance probability $\alpha$ computed from the target and proposal.

Remark 2.1. Using the Metropolis-Hastings algorithm replaces the task of sampling one point from $\pi$ directly with the task of sampling many times from the (potentially much simpler) proposal distribution $\{P_x\}_{x \in X}$. All $P_x$ have the same shape but are centered at different points $x \in X$.

The Metropolis-Hastings algorithm does not tell us the number of steps needed to get close to $\pi$. However, it does give us great flexibility in how to choose $P$. In practice, it is common to let $P_x$ be a Gaussian distribution centered at $x$, or a uniform distribution on a ball centered at $x$. It is necessary to compromise between high acceptance probabilities $\alpha$ and large variances of $P$. In order to force $\alpha \approx 1$, we can take very tiny steps, so that $P_x(\cdot)$ is highly concentrated near $x$. However, it then takes many steps to explore $X$ thoroughly. On the other hand, we could choose $P$ so as to move quickly, at the cost of rarely accepting.

Example 2.2 ([GRG96]). Gelman, Roberts, and Gilks show that, in the case in which the target distribution is the independent multivariate normal distribution $\mathcal{N}(0, I_d)$ and the proposal distributions are spherically symmetric, the optimal proposal distribution has standard deviation roughly $2.38/\sqrt{d}$ and acceptance probability roughly $0.234$ as $d \to \infty$. Since the step size goes to 0 as $d \to \infty$, it takes many steps to sample in large dimensions.

There are several potential problems with the Metropolis-Hastings algorithm: the acceptance probability may be very low, particularly in the high-dimensional setting. The chain may get trapped in a low-density region, even if the acceptance probability is usually high.
Example 2.3 ([Rob99]). Suppose that $\pi$ is the exponential distribution with parameter 1, i.e. $\pi(x) = e^{-x}$. Let $\lambda > 1$, and suppose we take $P_x(y) = \lambda e^{-\lambda y}$ to be our proposal distribution, independently of $x$. Since $\lambda > 1$, the tail of the target distribution $\pi$ is larger than that of the proposal. The acceptance probability for a transition from $x$ to $y$ is

$$\min \left( \frac{e^{-y} e^{-\lambda x}}{e^{-x} e^{-\lambda y}}, 1 \right) = \min(e^{-(\lambda-1)(x-y)}, 1).$$

Therefore, if $x$ is larger, the acceptance probability is very low and tends to 0 as $x$ increases. Thus, while it is difficult to reach large values of $x$, it is even more difficult to leave if we are ever unfortunate enough to get there.

In §4, we introduce Hamiltonian Monte Carlo, a variant of the Metropolis-Hastings algorithm that allows us to overcome these issues. In later sections, we will analyze it theoretically and see that it performs well under suitable assumptions. We first present an appropriate setting for Hamiltonian Monte Carlo, which involves some Riemannian geometry.

3. Riemannian Manifolds

We introduce what we need for §4 from differential and Riemannian geometry, saving ideas about curvature for manifolds and probability measures for §5. We go through the necessary material here rather quickly and we invite the interested reader to consult [dC92] or a similar reference for a more thorough exposition.

Definition 3.1. Let $\mathcal{X}$ be a $d$-dimensional manifold, and let $x \in \mathcal{X}$ be a point. Then the tangent space $T_x\mathcal{X}$ consists of all $\gamma'(0)$, where $\gamma : (-\varepsilon, \varepsilon) \to \mathcal{X}$ is a smooth curve and $\gamma(0) = x$. (See Figure 2.) The tangent bundle $T\mathcal{X}$ of $\mathcal{X}$ is the manifold whose underlying set is the disjoint union $\bigsqcup_{x \in \mathcal{X}} T_x\mathcal{X}$.  

Remark 3.2. We can stitch $T_x\mathcal{X}$ and $T\mathcal{X}$ into manifolds. The details of that construction can be found in [dC92]. For us, it suffices to note that $T_x\mathcal{X}$ is a vector space of dimension $d$, and $T\mathcal{X}$ is a manifold of dimension $2d$.

Definition 3.3. A Riemannian manifold is a pair $(\mathcal{X}, \langle \cdot, \cdot \rangle)$, where $\mathcal{X}$ is a manifold and $\langle \cdot, \cdot \rangle$ is a smoothly varying positive definite bilinear form on the tangent space $T_x\mathcal{X}$, for each $x \in \mathcal{X}$. We call $\langle \cdot, \cdot \rangle$ the (Riemannian) metric.
The Riemannian metric allows us to measure distances between two points on \( X \). We define the length of a curve \( \gamma : [a, b] \to X \) to be

\[
L(\gamma) = \int_a^b \langle \gamma'(t), \gamma'(t) \rangle \, dt,
\]

and the distance \( \rho(x, y) \) to be

\[
\rho(x, y) = \inf_{\gamma(0)=x, \gamma(1)=y} L(\gamma).
\]

A geodesic on a Riemannian manifold is a curve \( \gamma : [a, b] \to X \) that locally minimizes distance, in the sense that if \( \tilde{\gamma} : [a, b] \to X \) is another path with \( \tilde{\gamma}(a) = \gamma(a) \) and \( \tilde{\gamma}(b) = \gamma(b) \) with \( \tilde{\gamma}(t) \) and \( \gamma(t) \) sufficiently close together for each \( t \in [a, b] \), then \( L(\gamma) \leq L(\tilde{\gamma}) \).

Example 3.4. On \( \mathbb{R}^d \) with the standard metric, geodesics are exactly the line segments, since the shortest path between two points is along a straight line. On \( S^d \), the geodesics are exactly segments of great circles.

In this article, we are primarily concerned with the case of \( X = \mathbb{R}^d \). However, it will be essential to think in terms of Riemannian manifolds, as our metric on \( X \) will vary from the standard metric. In \( \S 5 \), we will see how to choose a metric, the Jacobi metric, that is nicely tailored to a probability distribution \( \pi \) on \( X \).

4. Hamiltonian Mechanics

Physicists [DKPR87] proposed a MC sampling scheme that uses Hamiltonian dynamics to improve convergence rates. They proposed to mimic the movement of a body under potential and kinetic energy changes to avoid diffusive behavior. The stationary probability will be linked to the potential energy. The reader is invited to read [Nea11] for an elegant survey of the subject.

The setup is as follows: let \( X \) be a manifold, and let \( \pi \) be a target distribution on \( X \). As with the Metropolis-Hastings algorithm, we start at some point \( q_0 \in X \). However, we use an analogue of the laws of physics to tell us where to go for future steps. In this section, we will work on Euclidean spaces \( X = \mathbb{R}^d \) with standard Euclidean metric, but in the next section we will use a special metric induced by \( \pi \).

In physics, we have (at least) two types of energy: potential energy and kinetic energy. The potential energy is a function solely of the position of a particle, whereas the kinetic energy depends not just on the position but also its motion, and in particular its velocity; both the position and the velocity are elements of \( \mathbb{R}^d \). In a more abstract setting, we can define a potential energy function \( V : \mathbb{R}^d \to \mathbb{R} \) and a kinetic energy function \( K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R} \). Both \( V \) and \( K \) should be smooth functions. We typically write a point in \( \mathbb{R}^d \times \mathbb{R}^d \) as \( (q, p) \), where \( q, p \in \mathbb{R}^d \). We call \( q \) the position and \( p \) the momentum. We will sometimes write \( \mathbb{R}^d_{\text{pos}} \) for the space of positions and \( \mathbb{R}^d_{\text{vel}} \) for the space of velocities to avoid confusion.

The position and momentum play different roles. The position space is the state space. The momentum, on the other hand, is only an auxiliary variable which helps us update the position and is of interest in its own right.

We define the Hamiltonian function \( H : \mathbb{R}^d_{\text{pos}} \times \mathbb{R}^d_{\text{vel}} \to \mathbb{R} \) by \( H(q, p) = V(q) + K(q, p) \). This represents the total energy of a particle with position \( q \) and momentum \( p \).
According to the laws of Hamiltonian mechanics, as a particle with position \( q(t) \) and momentum \( p(t) \) travels, \( q \) and \( p \) satisfy the Hamilton equations

\[
\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q},
\]

where if \( d > 1 \) this means that these equations hold in each coordinate, i.e.

\[
\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}.
\]

A simple consequence of the Hamilton equations is the following proposition (see §2.2 of [Nea11]).

**Proposition 4.1 (Conservation of energy).** The Hamiltonian is constant along any trajectory \((q(t), p(t))\) satisfying (4.1).

The Hamilton equations (4.1) tell us how the position and momentum of a particle evolve over time, given a starting position and momentum. As a result, we can compute \( q(1) \) and \( p(1) \), its position and momentum after one second.

**Remark 4.2.** In regions with higher potential energy, the Hamiltonian tends to be larger. As a result, trajectories starting at regions with large Hamiltonians are expected to be able to travel more quickly in a given period of time than those starting at smaller Hamiltonians.

Running Hamiltonian Monte Carlo is similar to the classical MCMC in that we propose a new point in \( \mathcal{X} \) based on the current point, and then either accept or reject it. However, the method of proposal differs from the classical method. In Hamiltonian Monte Carlo, to choose \( q_{i+1} \) from \( q_i \), we select a momentum vector \( p_i \) from \( \mathbb{R}^d_{vel} \), chosen according to a \( N(0, I_d) \) distribution. We then solve the Hamilton equations (4.1) with initial point \( q(0) = q_i \) and \( p(0) = p_i \), and let \( q_{i+1}^* = q(1) \) and \( p_{i+1}^* = p(1) \). We accept and make \( q_{i+1} = q_{i+1}^* \) with probability

\[
\alpha = \min(1, \exp(-H(q_{i+1}^*, p_{i+1}^*) + H(q_i, p_i)))
\]

and reject and let \( q_{i+1} = q_i \) otherwise. However, by Proposition 4.1, the exponential term is 1, i.e. theoretically, we should always accept.

**Remark 4.3.** In practice, we may occasionally reject, as it will be necessary to solve the Hamilton equations numerically, thereby introducing numerical errors. In truly high dimensional settings, the acceptance probability should be tuned around 0.65 [BPSSS11] by varying the stepsize in the numerical integration procedure.

Note that at every step, we pick a fresh momentum vector, independent of the previous one.

In order to make the stationary distribution of the \( q_n \)’s be \( \pi \), we choose \( V \) and \( K \) following Neal in [Nea11]; we take

\[
V(q) = -\log \pi(q) + C, \quad K(p) = \frac{1}{2} ||p||^2,
\]

where \( C \) is a convenient constant. Note that \( V \) only depends on \( q \) and \( K \) only depends on \( p \), \( V \) is larger when \( \pi \) is smaller, and so by Remark 4.2, trajectories are able to move more quickly starting from lower density regions than out of higher density regions.
Remark 4.4. The Hamiltonian is separable in the case of a distribution on Euclidean space, meaning that it can be expressed as the sum of a function of $q$ alone and a function of $p$ alone. However, we write $K(q, p)$ as a function of both $q$ and $p$, because tangent vectors should not be thought of as being detachable from the underlying manifold.

Remark 4.5. It is possible to choose other distributions for the momentum. Doing so changes $K$ accordingly. See [Nea11, §3.1] for a discussion of how to relate $K$ and the distribution of $p$.

Example 4.6. If $\pi = \mathcal{N}(0, \Sigma)$ is a multivariate Gaussian distribution, then, by choosing $C$ to be a suitable normalizing constant, we can take
\[
V(q) = \frac{1}{2} q^T \Sigma^{-1} q, \quad K(p) = \frac{1}{2} \|p\|^2.
\]
Taking $\pi = \mathcal{N}(0, 1)$ to be the standard univariate normal, we can see the trajectory of HMC explicitly. Suppose we choose a terrible starting point $q_0 = 1000$ and $p_0 = 1$, so that we are initially moving away from the high-density region. We quickly recover, the Hamilton equations become
\[
\frac{dq}{dt} = p, \quad \frac{dp}{dt} = -q.
\] Solving these equations with our initial conditions, we find that $q(t) = 1000 \cos(t) + \sin(t)$, so that when $t = 1$, we have $q(1) = 1000 \cos(1) + \sin(1) \approx 541$. Hence, in only one step, we have already made a substantial recovery. On the other hand, if we start at $q_0 = 1.5$, again with $p = 1$, then after one second, we reach $q(1) = 1.5 \cos(1) + \sin(1) \approx 1.65$, so we stay in a sensible location.

There are several reasons to expect Hamiltonian Monte Carlo to perform better than classical MCMC. For one thing, there are no (or at least very few) rejections. Also, since the potential energy is greater in regions of $\mathcal{X}$ with lower $\pi$-density, the Hamiltonian trajectory moves more quickly starting at such a point, allowing a rapid escape; on the other hand, the trajectory moves more slowly away from a region of high density, encouraging the chain to spend more time there. Furthermore, an unfortunate tendency of classical MCMC is random walk behavior, in which we move back and forth for several steps in a row; this behavior is less likely in the HMC setting, since the potential energy dictating the step size changes at every step. Finally, we expect it to perform better because the Hamiltonian trajectory adjusts continuously to the local shape of $\mathcal{X}$, rather than taking discrete steps that may not detect the fine structure of the space.

In practice, we have found that HMC outperforms MCMC as did Neal in [Nea11, §3.3] who performed simulations that demonstrate HMC’s advantage over MCMC.

5. Curvature

We can associate a notion of curvature to a Markov chain, an idea introduced by Ollivier in [Oll09] and Joulin in [Jou07]. We apply this notion of curvature to the HMC chain whose stationary distribution is our target distribution (not to its state space). This will allow us in §7 to obtain error bounds for numerical integration, using Hamiltonian Monte Carlo, in the cases when HMC has positive curvature.

In order to bring the geometry and the probability closer together, we will deform our space state space $\mathcal{X}$ to take the probability distribution into account, in a manner reminiscent of the inverse transform method mentioned in the introduction. Formally, this amounts to putting a suitable Riemannian metric on our $\mathcal{X}$. 
Here $\mathcal{X}$ is a Riemannian manifold: the Euclidean space $\mathbb{R}^d$ with the extra Riemannian metric. Given a probability distribution $\pi$ on $\mathcal{X} = \mathbb{R}^d$, we now define a metric on $\mathcal{X}$ that is tailored to $\pi$ and the Hamiltonian it induces (see §4). This construction is originally due to Jacobi, but our treatment follows Pin in [Pin75].

**Definition 5.1.** Let $(\mathcal{X}, \langle \cdot, \cdot \rangle)$ be a Riemannian manifold, and let $\pi$ be a probability distribution on $\mathcal{X}$. Let $V$ be the potential energy function associated to $\pi$ by (4.2). For $h \in \mathbb{R}$, we define the Jacobi metric to be

$$g_h(\cdot, \cdot) = 2(h - V)\langle \cdot, \cdot \rangle.$$  

**Remark 5.2.** $(\mathcal{X}, g_h)$ is not necessarily a Riemannian manifold, since $g_h$ will not be positive definite if $h - V$ is ever nonpositive. We could remedy this situation by restricting to the subset of $\mathcal{X}$ on which $h - V > 0$. In fact, this restriction will happen automatically, as we will always select values of $h$ for which $h - V > 0$; indeed, $h$ will be $V + K$, and if $d \geq 2$, $K$ will always be positive almost surely.

The point of the Jacobi metric is the following result of Jacobi, following Maupertuis:

**Theorem 5.3** (Jacobi-Maupertuis Principle, [Jac09]). Trajectories $q(t)$ of the Hamiltonian equations 4.1 with total energy $h$ are geodesics of $\mathcal{X}$ with the Jacobi metric $g_h$.

This theorem provides a link between a probability distribution $\pi$ and the Hamiltonian system from HMC. The Riemannian manifold equipped with the Jacobi metric encodes both the behavior of HMC and the target distribution $\pi$. This allows us to reduce the analysis of HMC to a geometric problem by studying the geodesics of this Riemannian manifold through the usual geometric tools such as curvature. In the spirit of comparison theorems in classical Riemannian geometry where complicated geometries are compared to the three main types of spaces — the negatively curved spaces, where geodesics starting at the same point spread out; flat spaces, where geodesics correspond to straight lines; and positively curved spaces, where geodesics starting at the same point meet again — we will show that the manifolds associated to HMC are close to spheres in high dimensions, and that a HMC random walk reduces to a geodesic random walk on a sphere (with geodesics corresponding to great circles on the sphere).

The most convenient way for us to think about the Jacobi metric on $\mathcal{X}$ is as distorting the space to suit the probability measure. In order to do this, we make regions of high density larger, and we make regions of low density smaller. However, the Jacobi metric does not completely override the old notion of distance and scale; the Jacobi metric provides a *compromise* between physical distance and density of the probability measure.

Another, essentially equivalent, way to think about the Jacobi metric is as a distortion of time. This is particularly natural since Hamiltonians describe how states of a system evolve over time. In this analogy, the Jacobi metric slows down time in regions of high probability and speeds it up in regions of low probability. As a result it takes a long time to move from high to low probability regions, but less time to move in the opposite direction.
As the Hamiltonian Monte Carlo progresses $h$ changes at every step, the metric structure varies as we run the chain moving between different Riemannian manifolds. In practice, however, we prefer to think of the chain as running on a single manifold, with a changing structure.

Another important notion for us is that of the exponential map. Given a Riemannian manifold $\mathcal{X}$ and a point $x \in \mathcal{X}$, there is a canonical map $\exp : T_x \mathcal{X} \to \mathcal{X}$. If $v \in T_x \mathcal{X}$, then $\exp(v)$ is obtained by following the unique geodesic in the direction of $v$ whose distance is $\|v\|$ measured in Riemannian metric; $\exp(v)$ is then the endpoint of this geodesic.

Instead of defining formally the notions of curvature, we provide some facts that give an intuition about sectional curvature as needed.

The **sectional curvature** in the plane spanned by two linearly independent tangent vectors $u, v \in T_x \mathcal{X}$ is defined for $\mathcal{X}$ a $d$-dimensional Riemannian manifold. $x, y \in \mathcal{X}$ are two distinct points, $v \in T_x \mathcal{X}, v' \in T_y \mathcal{X}$ are two tangent vectors at $x$ and $y$ that are related to each other by parallel transport along the geodesic in the direction of $u$. Let $\delta$ be the length of the geodesic between $x$ and $y$, and $\varepsilon$ the length of $v$ (same as $v'$). The sectional curvature $\text{Sec}_x(u, v)$ at point $x$ is defined in terms of the geodesic distance $\rho$ between the two endpoints $\exp_x(\varepsilon v)$ and $\exp_y(\varepsilon v')$ as the quantity that fulfills the equation:

$$\rho(\exp_x(\varepsilon v), \exp_y(\varepsilon v')) = \delta \left( 1 - \frac{\varepsilon^2}{2} \text{Sec}_x(u, v) + O(\varepsilon^3 + \varepsilon^2 \delta) \right)$$

as $(\varepsilon, \delta) \to 0$.

Figure 3 depicts the sectional curvature on a sphere, where the endpoints of the two red curves starting at $x$ and $y$ correspond to the endpoints $\exp_x(\varepsilon v)$ and $\exp_y(\varepsilon v')$. The dashed lines indicate geodesics going from $x$ to $y$, and from $\exp_x(\varepsilon v)$ to $\exp_y(\varepsilon v')$. As we get closer to the north pole, endpoints get closer together. Sectional curvature describes this convergence of endpoints: higher curvature means faster convergence. See also Proposition 6 in [Oll09].

We let $\text{Inf Sec}$ denote the infimum of $\text{Sec}_x(u, v)$, where $x$ runs over $\mathcal{X}$ and $u, v$ run over all pairs of linearly independent tangent vectors at $x$. 
Remark 5.4. In practice, it may not be easy to compute Inf Sec precisely. As a result, we can approximate it by running a suitable Markov chain on the collection of pairs of linearly independent tangent vectors of $X$; say we reach states $(x_1, u_1, v_1), (x_2, u_2, v_2), \ldots, (x_t, u_t, v_t)$. Then we can approximate Inf Sec by the empirical infimum of the sectional curvatures $\inf_{1 \leq i \leq t} \text{Sec}_{x_i}(u_i, v_i)$. This approach has computational benefits, but also theoretical benefits: it allows us to ignore low sectional curvatures that are unlikely to arise in practice.

Note that Sec depends on the metric. There is a formula, due to Pin [Pin75], connecting the sectional curvature of a Riemannian manifold equipped with some reference metric, with that of the Jacobi metric. We write down an expression for the sectional curvature in the special case where $X$ is a Euclidean space and $u$ and $v$ are orthonormal tangent vectors at a point $x \in X$:

\[
\text{Sec}(u, v) = -\frac{1}{8(h - V)^2} \left( 2(h - V) \left[ \langle (\text{Hess} V) u, u \rangle + \langle (\text{Hess} V) v, v \rangle \right] + 3 \left[ \| \text{grad} V \|^2 \cos^2(\theta) + \| \text{grad} V \|^2 \cos^2(\beta) \right] - \| \text{grad} V \|^2 \right).
\]

Here, $\theta$ is defined as the angle between $\text{grad} V$ and $u$, and $\beta$ as the angle between $\text{grad} V$ and $v$, in the standard Euclidean metric. We will not use the standard Ricci curvature on Riemannian manifolds, but a special notion of curvature, known as coarse Ricci curvature for Markov chains. We will use the distance between measures to be the standard Wasserstein metric.

Definition 5.5. Let $X$ be a metric measure space with metric $\rho$, and let $\mu$ and $\nu$ be two probability measures on $X$. Then the Wasserstein distance between them is defined as

\[
W_1(\mu, \nu) = \inf_{\xi \in \Pi(\mu, \nu)} \int \int_{X \times X} \rho(x, y) \xi(dx, dy).
\]

Here $\Pi$ is the set of measures on $X \times X$ whose marginals are $\mu$ and $\nu$.

If $P$ is the transition kernel for a Markov chain on a metric space $(X, \rho)$, let $P_x$ denote the transition probabilities starting from state $x$. We define the coarse Ricci curvature $\kappa(x, y)$ as the function that verifies:

\[
W_1(P_x, P_y) = (1 - \kappa(x, y))\rho(x, y).
\]

We write $\kappa$ for $\inf_{x, y \in X} \kappa(x, y)$.

We shall see in §7, in particular in Proposition 7.4, that there is a close connection between sectional curvature of a Riemannian manifold and coarse Ricci curvature of a Markov chain.

5.1. Positive Curvature. In order to produce error bounds for a distribution $\pi$, it is necessary for the HMC process associated to $\pi$ to have positive curvature. Thus, it is important to know, at an intuitive level, when to expect this to happen, and when to expect this to fail.

Roughly, coarse Ricci curvature for a Markov chain on a metric space $X$ can be interpreted as follows: Suppose $x, y \in X$ are two nearby points. Suppose we take a step starting from $x$ to a point $x'$, and we take the “corresponding” step from $y$ to $y'$, then, on average, the distance between $x'$ and $y'$ is smaller than the distance between $x$ and $y$. By contrast, if the curvature is 0, then the distance between $x'$ and $y'$ is on average equal to the distance between $x$ and $y$, whereas if
the curvature is negative, then the distance between $x'$ and $y'$ is on average greater than the distance between $x$ and $y$.

Based on this interpretation, we expect multimodal distributions $\pi$ to give us negative curvature. To see this, suppose $\pi$ is a symmetric bimodal distribution with modes $a$ and $b$, and let $x$ and $y$ be two nearby points between the two modes, with $x$ slightly closer to $a$ than $b$, and $y$ slightly closer to $b$ than $a$. Then, if we take a step from $x$, the resulting point $x'$ is likely to move toward $a$, whereas if we take a step from $y$, the resulting point $y'$ is likely to move toward $b$. Hence, we expect the distance between $x'$ and $y'$ to be larger than the distance between $x$ and $y$, giving us negative curvature; see Figure 4 for an illustration.

By contrast, unimodal distributions frequently have positive curvature, since points want to move closer to the mode, as we saw in Example 4.6.

6. Concentration Inequalities

Now that we have introduced all the necessary ingredients, we review the concentration results of Joulin and Ollivier and apply them to the setting of Hamiltonian Monte Carlo.

From [Oll09], we use the following definitions.

**Definition 6.1.** The Lipschitz norm of a function $f : (X, \rho) \to \mathbb{R}$ is

$$
\|f\|_{\text{Lip}} := \sup_{x, y \in \mathbb{R}^d} \frac{|f(x) - f(y)|}{\rho(x, y)}.
$$

If $\|f\|_{\text{Lip}} \leq C$, we say that $f$ is $C$-Lipschitz.

**Definition 6.2.** The coarse diffusion constant of a Markov chain on a metric space $(X, \rho)$ with kernel $P$ at a state $q \in X$ is the quantity

$$
\sigma(q)^2 := \frac{1}{2} \int_{X \times X} \rho(x, y)^2 P_q(dx) P_q(dy).
$$

The coarse diffusion constant controls the size of the steps at a point $q \in X$. 
Definition 6.3. The local dimension $n_q$ is
\[ n_q := \inf_{f: X \to \mathbb{R}} \frac{\int_{X \times X} \rho(x, y)^2 \, P_q(dx) \, P_q(dy)}{\int_{X \times X} \|f(x) - f(y)\|^2 \, P_q(dx) \, P_q(dy)}. \]

We record the values for these and other expressions that show up in the concentration inequalities in Table 1 on page 18, in the case of a multivariate Gaussian distribution.

Definition 6.4. The eccentricity $E(x)$ at a point $x \in X$ is defined to be
\[ E(x) = \int_X \rho(x, y) \, \pi(dy). \]

The eccentricity measures how far $x$ is from the bulk of the distribution of $\pi$. We set
\[ V^2(\kappa, T) = \frac{1}{\kappa T} \left( 1 + \frac{T_0}{T} \right) \sup_{q \in X} \frac{\sigma(q)^2}{n_q \kappa}. \]

We now state Joulin and Ollivier’s error bounds. We assume that the $x_i$’s are chosen by running a Markov chain (not necessarily HMC) with stationary distribution $\pi$ on a metric space $X$, and that the coarse Ricci curvature $\kappa$ is positive.

Theorem 6.5 ([JO10]). If $f: X \to \mathbb{R}$ is a Lipschitz function, then
\[ |E_x \hat{I} - I| \leq \frac{(1 - \kappa) T_0 + 1}{\kappa T} E(x) \|f\|_{\text{Lip}}. \]

Theorem 6.6 ([JO10]).
\[ \text{Var}_x(\hat{I}) \leq \frac{\|f\|_{\text{Lip}}^2}{\kappa T} \left( 1 + \frac{1}{\kappa T} \right) \sup_{x \in X} \frac{\sigma(x)^2}{n_x \kappa}. \]

Theorem 6.7 ([JO10]). Let
\[ V^2(\kappa, T) = \frac{1}{\kappa T} \left( 1 + \frac{T_0}{T} \right) \sup_{x \in X} \frac{\sigma(x)^2}{n_x \kappa}. \]

Then, assuming that the diameters of the $P_x$’s are unbounded, we have
\[ \mathbb{P}_x(|\hat{I} - E_x \hat{I}| \geq r \|f\|_{\text{Lip}}) \leq 2e^{-r^2/(16V^2(\kappa, T))}. \]

Remark 6.8. The appearance of $\kappa$ in these expressions has an elegant interpretation. As we run a Markov chain, the samples drawn are not independent. The curvature $\kappa$ can be thought of as a measure of the deviation from independence, so that $1/\kappa$ samples drawn from running the chain substitute for one independent sample.

In order to use these in the case of HMC, we must say something about the symbols that appear in the above expressions, and what they mean in our context. The only one that poses any serious difficulties is the Lipschitz norm, which ought to be computed in the Jacobi metric. However, we have a different Jacobi metric for each total energy $h$, and the only requirement on $h$ is that it be at least as large as $V$, which would suggest that we define the Lipschitz norm for HMC to be the supremum of the Lipschitz quotient over all pairs of points and $h \geq V$. However, this approach will not be successful, as it would require division by $h - V$, which can be made arbitrarily small.

Instead, we make use of high dimensionality, and recall that the momentum is distributed according to $N(0, I_d)$, and that $K = \frac{1}{2} \|p\|^2$, so that the distance $\rho_h(x, y)$
between two very close points \(x\) and \(y\) in the Jacobi metric \(g_h\) is \(\|p\|^2 \|x - y\| + O(\|x - y\|^2)\). Hence the Lipschitz quotient in the Jacobi metric between two nearby points is

\[
\frac{|f(x) - f(y)|}{\rho_h(x, y)} = \frac{|f(x) - f(y)|}{\|p\|^2 \|x - y\| + O(\|x - y\|^2)},
\]

or the standard Lipschitz norm divided by \(\|p\|^2\), up to higher order terms. Since \(\|p\|^{-2}\) is distributed according the inverse \(\chi^2\) distribution, which has mean \(\frac{1}{2} + O\left(\frac{1}{d^2}\right)\) and variance \(O\left(\frac{1}{d^{3/2}}\right)\), the Jacobi Lipschitz norm is the standard Lipschitz norm multiplied by \(\frac{1}{2} + O(d^{-3/2})\). We have taken an empirical approach to the computation of the Lipschitz norm; in the next section, we will continue in this spirit.

7. Examples

Here we show how curvature can quantify burn-in time \(T_0\) and running time \(T\) in three examples: the multivariate Gaussian distribution, the multivariate \(t\) distribution, and Bayesian image registration. We prove a positive lower bound on curvature in the Gaussian example, and show high concentration of positive (and nearly constant) curvature empirically in the other two examples. We give evidence that empirical curvature is an interesting diagnostic tool to assess the convergence of HMC in practice.
Figure 6. (Identity covariance structure) HMC after $T = 10^4$ steps for multivariate Gaussian $\pi$ with identity covariance in $d = 10, 100, 1000$ dimensions. At each step we compute the sectional curvature for $d$ uniformly sampled orthonormal 2-frames in $T_qX$ (see Remark 7.2).

7.1. Multivariate Gaussian Distribution. We apply Theorem 6.7 to the case of multivariate Gaussian distributions, running a HMC Markov chain to sample from $\pi = \mathcal{N}(0, \Sigma)$. We prove that, with high probability, the lower bound on sectional curvature is positive. Empirically, we can see in Figure 6 that the distribution of sectional curvatures approaches a Gaussian, which does imply that sectional curvatures are in fact positive. Furthermore, Figure 5 shows that the minimum and mean sectional curvatures during the HMC random walk tend closer with increasing dimensionality and meet visually at around 30 dimensions. More formally, we now state a Lemma that proves that sectional curvature is indeed positive with high probability in high dimensions; furthermore, the proof shows that, with high probability, the sectional curvature is very close to the mean. This lemma will
justify our use of the mean sectional curvature instead of the infimum (see Remark 7.3) in Proposition 7.4.

**Lemma 7.1.** Let $C$ be a universal constant and $\pi$ be the $d$-dimensional multivariate Gaussian $\mathcal{N}(0, \Sigma)$, where $\Sigma$ is a $(d \times d)$ covariance matrix, all of whose eigenvalues lie in the range $[1/C, C]$. We denote by $\Lambda = \Sigma^{-1}$ the precision matrix. Let $q$ be distributed according to $\pi$, and $p$ according to a Gaussian $\mathcal{N}(0, I_d)$. Further, $h = V(q) + K(q, p)$ is the sum of the potential and the kinetic energy. The Euclidean state space $\mathcal{X}$ is equipped with the Jacobi metric $g_h$. Pick two orthonormal tangent vectors $u, v$ in the tangent space $T_q \mathcal{X}$ at point $q$. Then the sectional curvature $Sec$ from expression (5.1) is a random variable bounded from below with probability

$$P(d^2 Sec \geq K_1) \geq 1 - K_2 e^{-K_3 \sqrt{q}}.$$

$K_1, K_2$, and $K_3$ are positive constants that depend on $C$.

**Remark 7.2.** To sample a 2-dimensional orthonormal frame in $\mathbb{R}^d$, we can sample from the Stiefel manifold of orthonormal 2-frames as follows: Fill a matrix $A \in \mathbb{R}^{d \times 2}$ with i.i.d. normals $\mathcal{N}(0, 1)$. Compute the QR factorization of $A$. Then, $Q$ of the QR factorization is a uniformly drawn sample from the Stiefel manifold.

**Proof of Lemma 7.1.** We recall the expression (5.1) for the sectional curvature from the previous section. We easily compute some of the expressions showing up in (5.1):

$$\text{Hess} V = \left( \frac{\partial^2 V}{\partial q_i \partial q_j} \right) = \Lambda, \quad \text{grad} V = \left( \frac{\partial V}{\partial q_1}, \ldots, \frac{\partial V}{\partial q_n} \right)^T = \Lambda q.$$

Note that $2K = \|p\|^2$. Let $\| \cdot \|$ be the Euclidean norm. Substituting these expressions into the expression (5.1) gives the full definition of the random variable

$$Sec = \frac{u^T \Lambda u}{\|p\|^4 \|x\|^2} + \frac{v^T \Lambda v}{\|p\|^4 \|y\|^2} + \frac{3 \|\Lambda q\|^2 \cos^2 \theta}{\|p\|^6} + \frac{3 \|\Lambda q\|^2 \cos^2 \beta}{\|p\|^6} - \frac{\|\Lambda q\|^2}{\|p\|^6}.$$

Note that $q$ may be written as $\Lambda^{1/2}z$ where $z$ is a standard Gaussian vector $z \sim \mathcal{N}(0, I_d)$. Therefore

$$\|\Lambda q\|^2 = z^T \Lambda z.$$

Next, note that $u$ and $v$ may be written as $u = x/\|x\|$ and $v = y/\|y\|$ where $x$ and $y$ are standard Gaussian vectors (but not independent of each other). The terms involving cosines can be left out since they are always positive and small. The other three terms can be written as three quadratic forms in standard Gaussian random vectors $x, y, z$ ($x$ and $y$ are not independent of each other), so that we have

$$Sec \geq \frac{x^T \Lambda x}{\|p\|^4 \|x\|^2} + \frac{y^T \Lambda y}{\|p\|^4 \|y\|^2} - \frac{z^T \Lambda z}{\|p\|^6}.$$

We now calculate tail inequalities for all these terms using Chernoff-type bounds. Let $\lambda_1, \ldots, \lambda_d$ be the eigenvalues of $\Lambda$, repeated by multiplicities. By assumption, they are bounded between $1/C$ and $C$, where $C \geq 1$. Let $w_1, \ldots, w_d$ be a corresponding set of orthonormal eigenvectors. Let $a_i = x^T w_i$, so that

$$x^T \Lambda x = \sum_{i=1}^d \lambda_i a_i^2.$$
Note that \(a_1, \ldots, a_d\) are i.i.d. \(N(0, 1)\) random variables. Therefore

\[
\mathbb{E}(x^T \Lambda x) = \sum_{i=1}^d \lambda_i = \text{Tr}(\Lambda).
\]

Let \(S = x^T \Lambda x - \mathbb{E}(x^T \Lambda x)\). Then for any \(\theta \in (-1/C, 1/C)\),

\[
\mathbb{E}(e^{\theta S}) = \prod_{i=1}^d \mathbb{E}(e^{\theta \lambda_i (a_i^2 - 1)}) = e^{-\frac{1}{2} \sum \lambda_i} \prod_{i=1}^d (1 - \theta \lambda_i)^{-1/2}.
\]

Now note that if \(b \in [0, 1/2]\), then \(\log(1 - b) \geq -b - b^2\). This shows that if we choose \(\theta = 2(\sum \lambda_i^2)^{-1/2}\), then

\[
\mathbb{E}(e^{\theta S}) = e^{\frac{1}{2}}.
\]

Thus, for any \(t \geq 0\), using Markov’s inequality and by assumption \(\lambda_i \leq C\),

\[
\mathbb{P}(S \geq t) \leq e^{-\frac{1}{2} \theta t} \mathbb{E}(e^{\theta S}) \leq e^{\frac{1}{2}} e^{-\frac{1}{2} t (\sum \lambda_i^2)^{-1/2}} \leq e^{\frac{1}{2}} e^{-\frac{\sqrt{C}}{2\sqrt{d}} t}.
\]

Similarly the same bound holds for the lower tail, as well as for \(y^T \Lambda y - \mathbb{E}(y^T \Lambda y)\) and \(z^T \Lambda z - \mathbb{E}(z^T \Lambda z)\), since these random variables have the same distribution as \(x^T \Lambda x - \mathbb{E}(x^T \Lambda x)\). By a similar calculation,

\[
\mathbb{P}(||x||^2 - \mathbb{E}||x||^2 \geq t) \leq 2e^{\frac{1}{2}} e^{-\frac{\sqrt{C}}{2\sqrt{d}} t},
\]

and the same bound holds for \(||p||^2\) and \(||y||^2\). Note that \(\mathbb{E}||x||^2 = d\). Let \(\mu := \sum \lambda_i / d\). Note that \(\mu \in [1/C, C]\). Take some \(t\) small enough and let \(E\) be the event that all of the following events happen: \(|x^T \Lambda x - \mu d| \leq t\), \(|y^T \Lambda y - \mu d| \leq t\), \(|z^T \Lambda z - \mu d| \leq t\), \(||x||^2 - d| \leq t\), \(||y||^2 - d| \leq t\) and \(||p||^2 - d| \leq t\). By the above calculations,

\[
\mathbb{P}(E) \geq 1 - 24e^{-\frac{1}{4\sqrt{C}} t}.
\]

If \(E\) happens, and \(t\) is small enough, then

\[
\text{Sec} \geq \frac{2(\mu d - t)}{(d + t)^3} - \frac{\mu d + t}{(d - t)^3}.
\]

Choose \(t = \varepsilon d\) for some sufficiently small constant \(\varepsilon\) (depending on \(C\)), the above inequalities show that

\[
\mathbb{P}(d^2 \text{Sec} \geq K_1) \geq 1 - K_2 e^{-K_3 \sqrt{d}},
\]

where \(K_1\), \(K_2\) and \(K_3\) are positive constants that depend only on \(C\).

**Remark 7.3.** We can easily see from the proof that the expectation of the sectional curvature is bounded from below by \(\mathbb{E}(	ext{Sec}) \geq \frac{\text{Tr}(\Lambda)}{d^3}\). Furthermore, note that

\[
K_1 = \frac{2(\mu - \varepsilon)}{\varepsilon + 1} - \frac{(\mu + \varepsilon)}{(1 - \varepsilon)^3} = \mu - O(\varepsilon),
\]

which yields \(\mathbb{P}(\text{Sec} \geq \frac{\text{Tr}(\Lambda)}{d^3} - O(\varepsilon)) \geq 1 - K_2 e^{-K_3 \sqrt{d}}\). Therefore, asymptotically, as \(d \to \infty\), the sectional curvature is very close to its expected value, as the probability of deviating from it decreases like \(K_2 e^{-K_3 \sqrt{d}}\). Since we are interested in truly high dimensional problems, we will work in this asymptotic regime and assume that \(\text{Sec} \geq \frac{\text{Tr}(\Lambda)}{d^3}\).
| Name                      | Symbol | Approximate value |
|---------------------------|--------|-------------------|
| Coarse Ricci curvature    | $\kappa$ | $\frac{\text{Tr}(\Lambda)}{6d^2}$ |
| Coarse diffusion constant | $\sigma(x)^2$ | $\frac{d}{d}$ |
| Local dimension           | $n_x$  | $d$               |
| Eccentricity at 0         | $E(0)$ | $\leq \sqrt{2d \frac{\Gamma((d+1)/2)}{\Gamma(d/2)}}$ |

Table 1. A table of some expressions that show up in the concentration inequality, together with their approximate values for an identity Gaussian kernel walk on $\mathbb{R}^d$ with $\pi$ a multivariate Gaussian distribution with precision matrix $\Lambda$.

**Proposition 7.4.** A HMC random walk on $\mathcal{X} = \mathbb{R}^d$ with Gaussian $\pi$ as in Theorem 6.7 has coarse Ricci curvature

$$\kappa \geq \frac{\text{Tr}(\Lambda)}{6d^2} + O\left(\frac{1}{d^2}\right)$$

as $d \to \infty$.

**Proof.** By Lemma 7.1, we know that $\text{Sec} \geq \frac{\text{Tr}(\Lambda)}{d^2}$ as $d \to \infty$ (see Remark 7.3). Spheres are manifolds with constant positive sectional curvatures, and so for our purposes we can consider $\mathcal{X}$ as behaving like a sphere with the sectional curvature $\frac{\text{Tr}(\Lambda)}{d^2}$ in the limit, and by the Rauch Comparison Theorem [Rau51], we may work with the sphere in the following. Recall that the coarse Ricci curvature $\kappa$ is defined by

$$W_1(P_x, P_y) = (1 - \kappa(x, y))\rho(x, y).$$

Here, we are assuming that $x$ and $y$ are points on the sphere, and that $\rho$ is the spherical distance. We compute the distance between geodesics originating from $x$ and $y$ using Jacobi fields, which measure the difference between a geodesic and a slightly perturbed one originating from the same point. This is well known for the sphere of sectional curvature $\text{Sec}$, namely

$$J_S(t) = \frac{\sin(\sqrt{\text{Sec}} t)}{\sqrt{\text{Sec}}},$$

and for Euclidean space, where we have

$$J_E(t) = t.$$  

We already know that the $W_1$ Wasserstein distance on Euclidean space is the distance between the two center points $\rho(x, y)$. So if we know the $W_1$ Wasserstein distance ratio from Euclidean space to the sphere, we know the distance on the sphere. The average ratio is given by the integral

$$\frac{W_1(P_x, P_y)}{\rho(x, y)} = \int_{\mathbb{R}^d} \frac{J_S}{J_E} \frac{1}{(2\pi)^{d/2}} \exp\left(-\frac{1}{2} \|x\|^2\right) \, dV$$

$$= \frac{1}{(2\pi)^{d/2}} \int_0^\infty e^{-x^2/2} x^{d-1} \sin(\sqrt{\text{Sec}} x) \frac{\sqrt{\text{Sec}} x}{\sqrt{\text{Sec}}} \, dx$$

$$= 1 - \text{Sec} \frac{d}{6} + O(\text{Sec}^2 d^2).$$
Letting $\text{Sec} \geq \frac{\text{Tr}(\Lambda)}{d^2}$, we obtain

$$\kappa \geq \frac{\text{Tr}(\Lambda)}{6d^2}$$

as $d \to \infty$. ■

**Proposition 7.5.** The coarse diffusion constant $\sigma(q)^2$ is $d$.

**Proof.** Since the transition kernel is insensitive to the starting point, we may assume that $q = 0$. We have

$$\sigma(q)^2 = \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{1}{(2\pi)^d} \exp\left(-\frac{1}{2}(\|x\|^2 + \|y\|^2)\right) \|x - y\|^2 dV(x) dV(y)$$

$$= \frac{1}{2(2\pi)^d} \int_{\mathbb{R}^d} \exp\left(-\frac{1}{2}(\|x\|^2 + \|y\|^2)\right) \sum_i (x_i^2 - 2x_iy_i + y_i^2) dV(x) dV(y)$$

$$= \frac{1}{2(2\pi)^d} \int_{\mathbb{R}^d} e^{-\|z\|^2/2} \|z\|^2 dV$$

$$= \frac{SA_{2d-1}}{2(2\pi)^d} \int_0^{\infty} e^{-r^2/2} r^{2d-1} dr$$

$$= d.$$ ■

Based on [Oll09], it follows that the local dimension $n_q$ is $d + O(1)$.

We show now how the coarse Ricci curvature, coarse diffusion constant, local dimension, and eccentricity from Table 7.1 can be used to calculate concentration inequalities for a specific example. We focus on the Gaussian distribution with weak dependencies between variables. But first we need to introduce two propositions.

**Proposition 7.6.** The eccentricity of a HMC random walk with Gaussian measure $\pi$ on $\mathbb{R}^d$ as in Theorem 6.7 with starting point $x = 0$ is approximately upper bounded by

$$E(0) \approx \sqrt{2d} \frac{\Gamma((d + 1)/2)}{\Gamma(d/2)}.$$

**Proof.** Starting with Definition 6.4

$$E(0) := \int_{X} \rho(0, y) \pi(dy) = \int_{\mathbb{R}^n} \sqrt{2K} \|y\| \pi(dy)$$

$$= \sqrt{2K} \int_{\mathbb{R}^n} \|y\| \pi(dy) = E(||p||) E(||y||)$$

The momentum $||p||$ follows a $\chi$ distribution with $d$ degrees of freedom. Its expectation and variance are given by

$$E(||p||) = \sqrt{2} \frac{\Gamma((d + 1)/2)}{\Gamma(d/2)}, \quad \text{Var}(||p||) = d - E(||p||)^2.$$

The position $y$ follows a zero mean Gaussian distribution with covariance $\Lambda^{-1}$. By the Cauchy-Schwarz inequality, we have

$$E(||y||) \leq E(||y||^2)^{1/2} = \text{Tr}(I_d)^{1/2} = \sqrt{d},$$

so we obtain an upper bound on the expectation of the length of $||y||$. Both variances are small in high dimensions. ■
Proposition 7.7. The Lipschitz norm of a coordinate function 

\[ f_i : q \rightarrow q_i \]

of a HMC random walk with Gaussian measure \( \pi \) on \( \mathbb{R}^d \) as in Theorem 6.7 is approximately given by

\[ \| f \|_{\text{Lip}} \approx \frac{\Gamma((d-1)/2)}{\sqrt{2} \Gamma(d/2)}. \]

Proof. Starting with Definition 6.1

\[ \| f \|_{\text{Lip}} := \sup_{x, y \in \mathcal{X}} \frac{|f(x) - f(y)|}{\rho(x, y)} = \frac{1}{\sqrt{2K}} = \| p \|^{-1} \approx \mathbb{E}(\| p \|^{-1}). \]

The inverse momentum \( \| p \|^{-1} \) follows an inverse \( \chi \) distribution with \( d \) degrees of freedom. Its expectation and variance are given by

\[ \mathbb{E}(\| p \|^{-1}) = \frac{\Gamma((d-1)/2)}{\sqrt{2} \Gamma(d/2)}, \quad \text{Var}(\| p \|^{-1}) = \frac{1}{d-2} - \mathbb{E}(\| p \|^{-1})^2. \]

The variance is small in high dimensions. \( \blacksquare \)

Now we are ready to go through an example. Our aim is to sample from an 100-dimensional multivariate Gaussian with Gaussian decay between the absolute distance squared of the variable indices

\[ \pi \sim \mathcal{N}(0, \exp(-|i-j|^2)) \]

and with the following HMC parameters, constants taken from Table 7.1 and from Propositions 7.6 and 7.7:

| Parameter                  | Value                        |
|----------------------------|------------------------------|
| Error bound                | \( r = 0.05 \)               |
| Starting point             | \( q_0 = 0 \)                |
| Markov chain kernel        | \( P \sim \mathcal{N}(0, I_{100}) \) |
| Coarse Ricci curvature     | \( \kappa = 0.0024 \)        |
| Coarse diffusion constant  | \( \sigma^2(q) = 100 \)      |
| Local dimension            | \( n_q = 100 \)              |
| Lipschitz norm             | \( \| f \|_{\text{Lip}} = 0.1 \) |
| Eccentricity               | \( E(0) = 99.75 \)           |

In our example, the observable function \( f \) is the first coordinate function

\[ I = \int_{\mathbb{R}^{100}} q_1 \pi(dq), \]

so the correct solution to this integral is \( I = 0 \). In Figure 7 on the left, we show 1000 simulations of this HMC chain and for each simulations we plot the sample mean approximation to the integral. The red lines indicated the requested error bound at \( r = 0.05 \). From these simulation results, we would expect the right burn-in and running time to be around \( T_0 = 0.05 \). In Figure 7 on the right, we see our theoretical concentration inequality as a function of burn-in and running time \( T + T_0 \) (in logarithmic scale). The probability of making an error above our defined error bound \( r = 0.05 \) is close to zero at burn-in time \( T_0 = 0 \) and running time \( T = e^{19} \). The discrepancy between the predicted theoretical results and the actual simulations suggest there might be hope for improvements in future work.
7.2. Multivariate \( t \) Distribution. In the previous section, we showed how to obtain concentration results for HMC Markov chains by using asymptotic sectional curvature estimates as \( d \to \infty \). This was possible since our target distribution was a multivariate Gaussian, for which we proved that the probability of deviating from \( \mathbb{E}(\text{Sec}) \) decreases like \( K_2 e^{-K_3 \sqrt{d}} \) as \( d \to \infty \). For most distributions of interest, e.g., posterior distributions in Bayesian statistics, such a proof is not feasible. In these cases, we propose to compute the empirical sectional curvature distribution and use the sample mean or sample infimum as a numerical approximation. Besides the practical benefits, as mentioned in Remark 5.4, computing empirical curvatures ignores unlikely curvatures that we never see in practice.

To illustrate this, we show how it can be done for the multivariate \( t \) distribution

\[
\pi(q) = \frac{\Gamma((\nu + d)/2)}{(\Gamma(\nu/2)\sqrt{\det(\Sigma)(\nu\pi)^d})} \left(1 + \frac{q^T \Sigma^{-1} q}{\nu}\right)^{-(\nu+d)/2}.
\]

Here \( d \) is the dimension of the space, and \( \nu \) is the degrees of freedom. Let \( \Sigma \) be the covariance matrix. Let us write \( \Sigma^{-1} = (a_{ij}) \). Write \( Q(q) \) for the quadratic form \( q^T \Sigma^{-1} q = \sum_{i,j} a_{ij} q_i q_j \). Hence, we can take the potential energy function \( V \) to be

\[
V(q) = \frac{\nu + d}{2} \log \left(1 + \frac{Q(q)}{\nu}\right).
\]

The gradient is a \( d \)-dimensional vector, whose \( i^{\text{th}} \) component is

\[
\frac{\partial V}{\partial q_i} = (\nu + d) a_{ij} \frac{Q(q) + \nu}{Q(q)}.
\]

The Hessian is a \( d \) by \( d \) matrix whose \( ij \) component is

\[
\frac{\partial^2 V}{\partial q_i \partial q_j} = (\nu + d) a_{ij} \left(\frac{Q(q) + \nu}{Q(q)}\right)^2 - 2 \left(\sum_i a_{ij} q_i\right) \left(\sum_m a_{jm} q_m\right)/(Q(q) + \nu)^2.
\]
Figure 8 shows empirical sectional curvature distribution for different values of \( \nu \) in dimension \( d = 100 \). With increasing degrees of freedom \( \nu \), we approach the curvature distribution of the Gaussian example; compare with Figure 6. This makes sense, as we know that as \( \nu \to \infty \), the multivariate \( t \) distribution converges to a multivariate Gaussian. For lower degrees of freedom, the curvature is more spread out. This can be explained by the larger tails of the \( t \) distribution and the sharper peak at its mode. Intuitively, larger tails means more equidensity regions of the space, and so we would expect curvature values closer to zero when we are far from the mode. Similarly, we get higher curvature around the mode of the distribution.

To transfer the sample curvature results into concentration inequalities, we can now pick either the sample mean or the sample infimum of the curvature sample distribution. For instance, in the case of \( \nu = 100 \), we would take the sectional...
curvature to be around $10^{-4}$, which would give us similar concentration inequality figures as in the previous section for the Gaussian case.

7.3. Bayesian Image Registration. In the previous section, we were able to compute empirical sectional curvatures from known closed-form gradients and Hessians of the potential function $V$. In applied problems, the analytical form of the Hessian is usually hard to derive and even harder to compute. A common way to approximate it is by first order Taylor expansion [GM78]; in numerical methods literature this is referred to as the Gauss-Newton approximation to the Hessian. We will come back to what kind of conditions are needed for this approximation to make sense in our application; see [AJS07a] for more details.

In this section, we use Gauss-Newton approximation to compute the Hessian of a real-world medical image problem and to compute empirical curvature similarly to what we did for the multivariate $t$ distribution. This allows us to obtain concentration inequalities for a Bayesian approach to medical image registration.

The goal in medical image registration is to find a deformation field that maps one image to another image. For instance, these deformations are then used for the statistical analysis of shape differences between groups of patients. After introducing a basic mathematical formulation of the registration problem, we show how our concentration results can be used as a diagnostic tool for HMC complementary to other tools like visual assessment via trace plots or statistical tests of Markov chains [GR92].

We explain the problem of medical image registration with a two-dimensional example. We extracted two frontal slices from computed tomography (CT) images; see Figure 9. The goal is to spatially deform the moving image (Figure 9, right) to the fixed image (Figure 9, left). The voxel coordinates $(x, y)$ are related by a global
affine transformation \( A \) and a local deformation field \( \varphi(x, y) \) of the form

\[
\begin{bmatrix}
x' \\
y' \\
1
\end{bmatrix} = A \begin{bmatrix}
x \\
y \\
1
\end{bmatrix} + \begin{bmatrix}
\varphi_x(x, y) \\
\varphi_y(x, y)
\end{bmatrix}.
\]

Here we will assume that \( A \) is known and that we are only estimating the local deformation \( \varphi(x, y) \). We choose to parametrize the deformations \( \varphi(x, y) \) using cubic B-splines and follow the presentation by Andersson, Jenkinson and Smith [AJS07b]. Let \( (q_{i,j})^{(x)} \) denote the spline weights in direction \( x \) at control points \((i, j)\), and similarly for \( y \). Then we reshape the two matrices into a column vector \( q = \begin{bmatrix} \text{Vec}((q_{i,j})^{(x)}) \\ \text{Vec}((q_{i,j})^{(y)}) \end{bmatrix} \), where \( \text{Vec} \) takes each row of the matrix and concatenates it into a column vector.

We can write any deformation as a linear combination of tensor products of one-dimensional cubic B-splines [RSH+99]:

\[
\varphi(x, y) = \sum_{\ell=0}^{3} \sum_{m=0}^{3} B_{\ell}(u)B_{m}(v)q_{i+\ell,j+m},
\]

where the sum goes over 16 neighboring control points with indices calculated as \( i = \lfloor x/n_x \rfloor - 1, j = \lfloor y/n_y \rfloor - 1, u = x/n_x - \lfloor x/n_x \rfloor, \) and \( v = y/n_y - \lfloor y/n_y \rfloor \), and the spline basis functions \( B_0(u), \ldots, B_3(u) \). Figure 10 shows the 12 \( \times \) 7 control points that we choose for our example. This choice defines a certain amount of regularity of the deformation: more control points allow for more local flexibility.

The parameters of interest are the weights \( q \) of the spline basis function at control points. In our case, we have 12 \( \times \) 7 control points in two dimensions, which gives a total of 168 parameters. In a Bayesian approach we estimate these parameters from data, which are the fixed and moving patient images, by first defining a prior probability

\[
\pi_1(q) = \mathcal{N}(0, (\lambda\Lambda)^{-1})
\]

and a likelihood

\[
\pi_2(F \mid M, q) = \frac{1}{Z} \exp \left(-\frac{\phi}{2} ||r||^2 \right),
\]

in terms of \( r \), the residual error vector with length equal to the number of voxels in \( M \) (or \( F \)), computed by

\[
r_i = F(x_i, y_i) - M(x'_i, y'_i) = F(x_i, y_i) - M(\varphi(x_i, y_i)).
\]

at a predefined coordinate grid \((x_i, y_i)\) over the entire image domain. The deformation field \( \varphi \) is a function of \( q \) (7.1). The deformed coordinates \((x'_i, y'_i)\) usually fall between grid points \((x_i, y_i)\) and need to be linearly interpolated.

We do not have a physical model that describes how to deform one spine to another. Such a model would only make sense when registering two images of the same patient, for instance taken before and after a surgical procedure. In that case, we could relate voxel intensities to tissue material following a mechanical law and perform mechanical simulations. The corresponding material laws from mechanics would then allow us to define a prior on the possible class of deformations. This is not possible in the absence of such a mechanical model when registering spine images from two different patients. Nevertheless, we can define a prior that is inspired
Figure 10. Left: Red control points overlaid on moving image and B-spline weight vectors. The small vector between control point are interpolated using B-splines. Middle: Difference image of deformed moving and fixed after 100 iterations. Bright pixels represent small and dark larger differences. Right: Sum of squared difference similarity metric $\sum_i (F(x_i,y_i) - M(x_i',y_i'))^2$, and mean sample sectional curvature for $d = 168$ uniformly sampled orthonormal $2$-frames in $\mathbb{R}^d$ (see Remark 7.2) at each iteration.

by mechanics, such as the membrane energy, $E_m = \lambda \sum_{i \in \Omega} \sum_{j=1}^{2} \sum_{k=1}^{2} \left| \frac{\partial \phi_j}{\partial x_k} \right|_i^2$, which measures the size of the first derivative of the deformation. To minimize $E_m$ we look for deformations with small local changes. For details on how to construct the precision matrix $\Lambda$ for our Gaussian prior from membrane energy $E_m$ see §3.5 in [AJS07b].

The posterior is not analytically tractable and we need to use a Markov chain to sample from it. Since it is high dimensional, HMC is a good candidate. Simpson and coauthors recently sampled from this posterior distribution for brain images using Variation Bayes [SSG+12]. Other recent related work in Bayesian approaches to image registration are [RSW10] using Metropolis-Hastings and [VL09, ZSF13] using HMC. For our example, we sample directly from the posterior distribution $\pi(q) = \frac{1}{Z} \pi_2(F \mid M, q) \pi_1(q)$ using HMC and in addition to provide concentration inequalities using our empirical curvature results. The integral of interest is

$$I = \int_{\mathbb{R}^{168}} q \pi(dq).$$

We call $J$ the Jacobi matrix that contains information about the image gradient and the spline coefficients and is of size (number of voxels) $\times$ (dimension of $q$). For details on how to construct this matrix see §3.1 in [AJS07b]. Then the gradient of
the potential energy $V$ is given by 

$$\text{grad } V = \phi J^T r + \lambda A q.$$ 

To avoid numerical problems we approximate the Hessian by Taylor expansion around the current $q$ and only keep the first order term

$$\text{Hess } V = \phi J^T J + \lambda A.$$ 

In contrast to the multivariate $t$ distribution, we not only need to empirically find the sectional curvature, but also approximate the Hessian of the potential. The error induced by this approximation is not considered here, but can be kept under control as long as the residual error $\|r\|$ is small relative to $\|J^T J\|$; see [GM78] and [AJS07a] for details.

Figure 10 shows sectional curvature numerically computed at different iterations steps $k$:

$$q^{(k)} = q^{(k-1)} - (\text{Hess } V)^{-1} \text{grad } V.$$ 

This corresponds to a Gauss-Newton minimization of the potential function $V$; see [GM78] for details. If we assume that the local minimum of the potential function $V$ is an interesting mode of the posterior probability distribution $\pi$, then the sectional curvature close to that minimum will tell us how a HMC Markov chain will perform within that mode. From Figure 10, we can see that the sectional curvature is fluctuating around $10^{-4}$ after only few iterations. This is roughly the same curvature obtained in the multivariate Gaussian example, and thus the concentration inequalities carry over.

A full analysis of HMC for an image registration application to compare the shape of spines of back pain and abdominal pain patients is in preparation; see [SRSH14b] for details.

8. Conclusions and Open Problems

The introduction of the Jacobi metric into the world of Markov chains promises to yield new links between geometry, statistics, and probability. It provides us with an intuitive connection between these fields by distorting the underlying space. We only scratch the surface here, and naturally we introduce some open problems:

- In this article, we have not focused on the numerical solving of the Hamilton equations (4.1), although our simulations were promising on this point. There are standard methods of solving differential equations numerically, such as the leapfrog method (see [Nea11]): how might we modify Joulin and Ollivier’s concentration inequality to include the parameters for the leapfrog algorithm or other algorithms?

- Girolami and Calderhead [GC11] introduced an elegant way to adapt the proposal distribution from which the momentum vector is drawn based on the underlying geometry of the distribution. Our framework can be applied also in this setting by using a non-standard reference metric. The difficulty here is to write down the expression for the sectional curvature.

- Our approach can be extended to the setting of an infinite-dimensional Hilbert space. Since our results improve in high dimensions, we expect everything to carry over to the infinite-dimensional setting, but we have not investigated this. Recently, there has been some work, for instance in
[BPSSS11], on HMC on a Hilbert space, suggesting that this topic is worthy of further study.

- It remains to be investigated whether we can still obtain error bounds in the case of some amount of negative curvature, perhaps in a small but essential region. Alternatively, is it possible to modify the algorithm so as to give positive curvature in cases where we currently have some negative curvature?

We are currently working on estimating sectional curvatures in large-scale medical image registration projects. We believe that geometric properties about the Markov chains in such high dimensional problems can be used to assess the convergence of the chain complementary to traditional visual assessment via trace plots or statistical tests. In the context of registration, this is important since computing one step of the chain can be computationally expensive. Therefore an estimate on the number of steps becomes essential.

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