Langevin MC,
or the curse of dimensionality

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1 Introduction

In Bayesian statistics, we are interested in performing inference on the posterior distribution of a parameter, θ. This is calculated using Bayes rule

$$\pi(\theta|x) = \frac{f(x|\theta)p(\theta)}{f(x)}$$

where $f(x|\theta)$ is the likelihood function of the data, and $p(\theta)$ is the prior distribution on the parameter. The term on the denominator, $f(x) = \int f(x)|\theta)p(\theta)d\theta$ is a normalising constant, such that π is a distribution. In general, this normalising constant is difficult to calculate, and so the posterior is usually only given up to proportionality.

$$\pi(\theta|x) \propto f(x|\theta)p(\theta)$$

In this report we consider the problem of sampling from a distribution of the form

$$\pi(x) \propto \exp(-U(x))$$

for some potential function U. In statistical mechanics, this distributions is called a Gibbs distribution, and is often used to model the positions and velocities of particles in a gas.

1.1 Markov Chain Monte Carlo

Monte Carlo methods are a class of algorithms that replace difficult or impossible analytical probability calculations with numerical approximations. Given a random variable X on a probability space $(\Omega, \mathcal{F}, \pi)$ with distribution given by π consider the problem of calculating

$$\mathbb{E}_\pi[g(X)] = \int_\Omega g(x)d\pi$$

If the distribution π does not take a well-known form, then analytically solving this expectation is very difficult. Instead, Monte Carlo integration uses the strong law of large numbers to approximate the integral. If X_n are a sequence of i.i.d. random variables distributed according to π, then

$$\frac{1}{N}\sum_{n=1}^{N} g(X_n) \to \mathbb{E}_\pi[g(X)] \quad \text{a.s. as } N \to \infty.$$

Hence we can approximate integrals by taking independent samples from the distribution π. However, for an arbitrary distribution, it is not necessarily possible to find sample independently in an efficient way. Markov chain Monte Carlo allows us to dispense with this assumption. Rather than sampling independently, we can instead construct a Markov chain with π as its invariant distribution. This chain can then be used to generate dependent samples, which can be used for Monte Carlo integration provided the chain is ergodic with respect to π.

Definition 1.1 (Ergodicity). Let $T : \Omega \to \Omega$ be a probability-preserving transformation on a probability space $(\Omega, \mathcal{F}, P)$. Then we say T is *ergodic* if for every $F \in \mathcal{F}$ with $T^{-1}(F) = F$, either $P(F) = 0$ or $P(F) = 1$.

Intuitively, this condition means that the process explores the whole space, without becoming stuck in a subregion. The ergodic theorem then provides the theoretical justification that permits the use of dependent samples for Monte Carlo integration.

Theorem 1.2 (Ergodic Theorem). *Let f be measurable, $\mathbb{E}_\pi(|f|) < \infty$, and T be an ergodic probability-preserving transformation. Then with probability 1:*

$$\frac{1}{N}\sum_{n=1}^{N} f(T^n(x)) \to \mathbb{E}_\pi[f] \quad \text{a.s. as } N \to \infty.$$

In other words, if T is ergodic, time averages converge to space averages. Hence, if we can construct a Markov chain which is ergodic with respect to a target measure π, it can be used to generate Monte Carlo samples. One method of constructing such a Markov chain is by using Langevin dynamics.

2 Langevin Monte Carlo Algorithms

The Langevin equation is a stochastic differential equation (SDE) originally developed to model the movement of a Brownian particle [4]. The form of interest here is the *overdamped* Langevin equation, in which the particle experiences no average acceleration. The equation is thus

$$\mathrm{d}X_t = -\nabla U(X_t)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t. \tag{1}$$

Here, W_t is a d-dimensional Wiener process (Brownian motion) and $U : \mathbb{R}^d \to \mathbb{R}$ is the potential function. The equation can be thought of as modelling a particle in a potential well with shape U. As each particle moves randomly, it is natural to ask what is the average position of many particles in such a well? It can be shown that in fact the position of a particle moving according to the above dynamics is exactly π +++Reference to earlier subsection/first mention of distribution+++. For a diffusion process this is called the *stationary distribution*[a] To show that π is indeed the stationary distribution the following lemma

Lemma. *For a one-dimensional Itô diffusion +++add conditions on diffusion/drift+++,*

$$\mathrm{d}X_t = \mu(X_t)\,\mathrm{d}t + \sigma^2(X_t)dW_t,$$

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[a]Another common term is *invariant measure* +++

the Fokker-Planck operator, $\mathcal{L}^*$, is

$$\mathcal{L}^* := -\partial_x(\mu(x)\cdot) + \frac{1}{2}\partial_x^2(\sigma^2(x)\cdot).$$

A measure π is invariant for the diffusion if and only if

$$\mathcal{L}^*\pi = 0$$

The proof of this is omitted however it can be seen by forming the Fokker-Planck equation for the probability density of the diffusion. The proof that π is the stationary measure of Equation (1) is given only in the one dimensional case, however it is extendable to higher dimensions. For the Langevin equation, the Fokker-Planck operator is

$$\mathcal{L}^* = \partial_x(U'(x)\cdot) + \partial_{xx}\cdot\,.$$

So it remains to calculate $\mathcal{L}^*\pi$.

$$\begin{aligned}
\mathcal{L}^*\pi &= \frac{\partial}{\partial x}\left[U'(x)\pi(x) + \frac{\partial}{\partial x}\pi(x)\right]\\
&= \frac{\partial}{\partial x}\left[U'(x)\mathcal{Z}e^{-U(x)} + \left(-U'(x)\mathcal{Z}e^{-U(x)}\right)\right]\\
&= \frac{\partial}{\partial x}[0]\\
&= 0
\end{aligned}$$

Hence π is indeed the invariant measure of (1). ∎

Although this shows that the Langevin equation has an invariant measure, the question of convergence to this measure remains unanswered. Roberts and Tweedie give the following restriction [7].

Theorem 2.1 (Theorem 2.1, [7]). *Let $P_X^t(x, A) = \mathbb{P}(X_t \in A | X_0 = x_0)$ and suppose that $\nabla U(x)$ is continuously differentiable and that, for some $N, a, b < \infty$,*

$$\nabla U(x) \cdot x \le a|x|^2 + b, \qquad |x| > N.$$

Then the measure π is invariant for the Langevin diffusion X. Moreover, for all $x \in \mathbb{R}^d$ and Borel sets A,

$$\|P_X^t(x, \cdot) - \pi\| = \frac{1}{2}\sup_A\left|P_X^t(x, A) - \pi(A)\right| \to 0$$

+++Should this norm be an integral? Add exponentially fast convergence/spectral gap inequality? Figure of $U = x^2/2$? 2d? +++

The problem of sampling from the high dimensional distribution has been reduced to being able to accurately simulate Langevin dynamics. However, this is not as simple as it sounds. To simulate the continuous process (1), it must first be discretised. However, doing so may not preserve the convergence to the invariant measure. The discretised process may not have the same stationary measure or it may not even exist. This means that the method used to discretise must be chosen carefully to ensure good convergence properties. The most natural way to discretise an SDE is to use the stochastic analogue of the (forward) Euler method used on ordinary differential equations, known as the Euler-Maruyama (EM) method. Doing so leads to the Unadjusted Langevin Algorithm (`ULA`).

2.1 The Unadjusted Langevin Algorithm

Applying the Euler-Maruyama method to Equation (1) gives the following iterative scheme.

$$X_{n+1} = X_n - h\nabla U(X_n) + \sqrt{2h}Z_{n+1}, \qquad X_0 = x_0$$

Here the Z_n are i.i.d. standard normal random variables and h is the step size. This is equivalent to $X_{n+1} \sim N(X_n - h\nabla U(X_n), 2hI_d)$.[b] A simple example shows that this discretisation does not converge to π. Let π be a standard Gaussian distribution, that is $U(x) = |x|^2/2$ and choose $h = 1$. Then the update is given by

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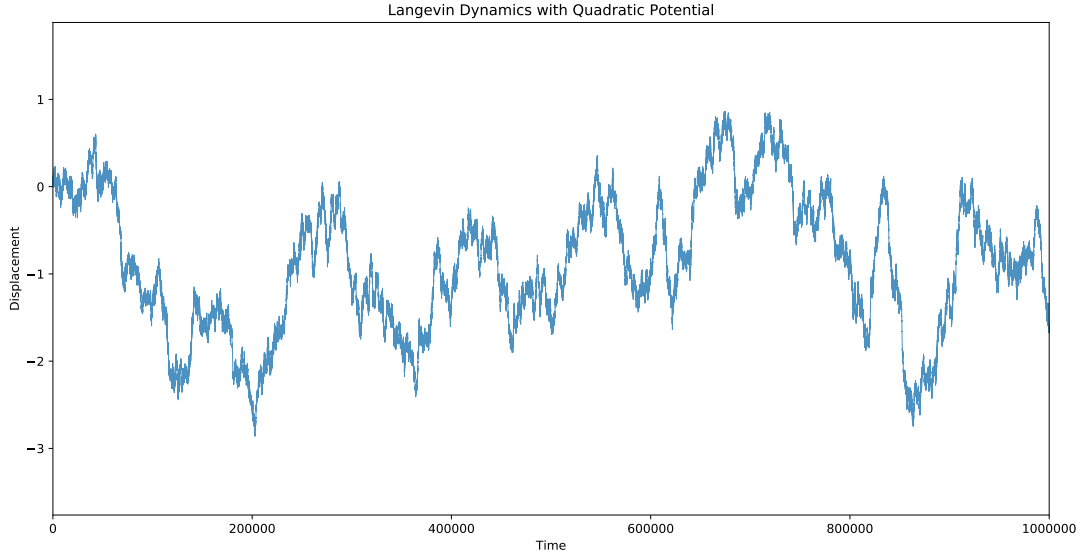[b]I_d denotes the $d \times d$ identity matrix.

Figure 1: Simulating Langevin dynamics in one dimension with a quadratic potential $U(x) = x^2/2$

$$X_{n+1} \sim N(X_n - \nabla U(X_n), 2)$$
$$\sim N(X_n - X_n, 2)$$
$$\sim N(0, 2) \not\sim \pi.$$

So the chain converges immediately, but to the wrong distribution. Let π_h^{ULA} denote the stationary distribution of `ULA` with a stepsize h. This is not the only issue that can occur. As well as not converging to the correct distribution, the discretised chain may not be ergodic, even when the continuous diffusion is exponentially ergodic [7]. In particular, the algorithm misbehaves when the gradient of the potential is superlinear. That is,

$$\liminf_{\|x\| \to \infty} \frac{\|\nabla U(x)\|}{\|x\|} = +\infty.$$

To mitigate these issues there are two main approaches: taming the gradient and Metropolisation. A further third method involves using a different discretisation scheme. Our main focus will be the former, although all three approaches will be discussed.

2.2 MALA

Before describing the Metropolis-adjusted Langevin algorithm `MALA`, it is pertinent at this point to recall the random walk Metropolis-Hastings algorithm `RWM` [3, 5]. This popular variant of the Metropolis-Hastings algorithm *proposes* values and then accepts/rejects them according to some probability α. So given X_n, propose a candidate Y_{n+1} as

$$Y_{n+1} = X_n + \sqrt{2h} Z_{n+1}.$$

Once again, h is the stepsize and Z is a normal random variable. Then, accept or reject this proposal using Metropolis rejection, that is with some probability

$$\alpha(X_n, Y_{n+1}) = 1 \wedge \frac{\pi(Y_{n+1})q(Y_{n+1}, X_n)}{\pi(X_n)q(X_n, Y_{n+1})}.^{\text{c}}$$

Here $q(x, y)$ is the transition probability, $\mathbb{P}(Y_{n+1} = y | X_n = x) \sim N(X_n, h^2)$. This rejection step is key in creating a kernel that is reversible and thus invariant for the measure π.

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[c] Here $t \wedge s = \min\{t, s\}$.

`MALA` can be seen as another variant of the Metropolis-Hastings algorithm, using Langevin dynamics to propose new states. It is perhaps better understood as `ULA` but with an added Metropolis rejection step [7]. Adding this rejection step means the algorithm always has the correct invariant distribution, although convergence is still not guaranteed as the following theorem shows.

Theorem 2.2 (Theroem 4.2, [7])**.** *If π is bounded, and*

$$\liminf_{\|x\|\to\infty} \frac{\|\nabla U(x)\|}{\|x\|} > \frac{4}{h}$$

then the `MALA` chain is not exponentially ergodic. +++define exp ergodic+++

So it can be seen that `MALA` is not without its issues, and does not solve all the problems of `ULA`. The concept of taming was introduced to try and reduce the magnitude of these problems.

2.3 Taming the Gradient

We have seen that both `ULA` and `MALA` run into issues when the gradient of the potential is superlinear. Given an SDE such as (1), taming adjusts the drift coefficient in such a way that preserves the invariant measure and improves speed of convergence [2, 7, 8]. To do this, a family of drift functions $(G_h)_{h>0}$, $G_h : \mathbb{R}^d \to \mathbb{R}^d$ are introduced. The SDE to be discretised is thus

$$\mathrm{d}X_t = -G_h(X_t)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t.$$

Applying the Euler-Maruyama method gives the following Markov chain

$$X_{k+1} = X_k - hG_h(X_k) + \sqrt{2h}Z_{k+1}, \qquad X_0 = x_0.$$

To preserve the invariant measure, some restrictions must be placed on $(G_h)_{h>0}$, namely that they are 'close' to ∇U (**A1**) while **A2** ensures ergodicity is preserved and improves stability [2].

A1 For all $h > 0, G_h$ is continuous. There exist $\alpha \geq 0, C_\alpha < +\infty$ such that for all $h > 0$ and $x \in \mathbb{R}^d$,

$$\|G_h(x) - \nabla U(x)\| \leq hC_\alpha(1 + \|x\|^\alpha).$$

A2 For all $h > 0$,

$$\liminf_{\|x\|\to\infty} \left[\left\langle \frac{x}{\|x\|}, G_h(x) \right\rangle - \frac{h}{2\|x\|}\|G_h(x)\|^2 \right] > 0$$

Here we consider two specific taming functions,

$$T_h(x) = \frac{\nabla U(x)}{1 + h\|\nabla U(x)\|}, \qquad\qquad T_h^{\mathrm{RT}} = \frac{\nabla U(x)}{1 \vee h\|\nabla U(x)\|}.$$

Brosse et al. introduced and studied T_h whilst Roberts & Tweedie suggested T_h^{RT}, later analysed by Bou-Rabee & Vanden-Eijnden [1, 2, 7]. Both taming functions retain the direction of the gradient, only reducing the magnitude of its effect. The latter is the usual `ULA` until the gradient gets large enough ($\|\nabla U(x)\| > 1/h$), at which point it begins normalising. In contrast, the first will always tame, regardless of size of the gradient. However for the scaling to have noticeable effect, the gradient must be $\mathcal{O}(h^{-1})$. When T_h is the taming function, the algorithm will be referred to as `tULA`, the tamed unadjusted Langevin algorithm. When the second is applied, it will be called `MALTA`, the Metropolis adjusted Langevin truncated algorithm after [7]. Any tamed algorithm using T_h will be prefixed with a lowercase `t`.

2.3.1 tULA/c

$$X_{n+1} = X_n - hT_h(X_n) + \sqrt{2h}Z_{n+1}, \qquad X_0 = x_0$$

where $T_h(x) = \frac{\nabla U(x)}{1+\|\nabla U(x)\|}$ or $T_h(x) = \left(\frac{\nabla U(x)}{1+|\partial_i U(x)|} \right)_{i=\{1,\dots,d\}}$

+++Show ill condition/stiff bad behaviour, how coordinatewise fixes+++

2.4 tMALA/c

Use the same taming T as in `tULA`. Is this sensible? Could compare with `MALTA`.

2.5 Discretise Differently

2.5.1 tHOLA

[**?**] Use an Itô-Taylor expansion

$$X_{n+1} - X_n + \mu_h(X_n)h + \sigma_h(X_n)\sqrt{h}Z_{n+1}$$

where

$$\mu_h(x) = -\nabla U_h(x) + \frac{h}{2}\left(\left(\nabla^2 U\nabla U\right)_h(x) - \vec{\Delta}(\nabla U)_h(x)\right),$$

and $\sigma_h(x) = \text{diag}\left(\left(\sigma_h^{(k)}(x)\right)_{k\in\{1,\dots,d\}}\right)$ with,

$$\sigma_h^{(k)}(x) = \sqrt{2 + \frac{2h^2}{3}\sum_{j=1}^d |\nabla^2 U_h^{(k,j)}(x)|^2 - 2h\nabla^2 U_h^{(k,k)}(x)}$$

ALSO need to define the h subscript, i.e. the tamed variables. Although fn depends on gamma it doesn't indicate that taming has occurred.

2.5.2 LM

[**?**] Non-Markovian scheme,

$$X_{n+1} = X_n + h\nabla U(X_n) + \sqrt{\frac{h}{2}}\left(Z_n + Z_{n+1}\right)$$

2.6 Other Methods

2.6.1 RWM

Popular variant of the Metropolis-Hastings algorithm (CITE) with a normal proposal.

$$U_{n+1} = X_n + \sqrt{2h}Z_{n+1}$$

Calculate acceptance probability

$$\alpha(X_n, U_{n+1}) = 1 \wedge \frac{\pi(U_{n+1})q(U_{n+1}, X_n)}{\pi(X_n)q(X_n, U_{n+1})}$$

Here $q(x,y)$ is the transition probability, $\mathbb{P}(X_{n+1} = y | X_n = x)$. If `rand`$\leq \alpha$,

$$X_{n+1} = U_{n+1}.$$

That is,

$$X_{n+1} = \mathbb{I}(u \leq \alpha)U_{n+1} + \mathbb{I}(u > \alpha)X_n$$

3 Beyond Moments

While first and second moments give us some idea of the performance of our sampling algorithms, we ideally would like a fuller picture. In this section we compare the performance of algorithms using the total variation distance, L^2-Wasserstein distance and Kullback–Leibler divergence. Using these measures, we can compare the performance to theoretical upper bounds for the `ULA`, `tULA` and `HOLA` algorithms.

3.1 Statistical Distances

Let $\mathcal{B}(\mathbb{R}^d)$ denote the Borel σ-algebra on $\mathbb{R}^d$. Let P and Q be probability measures on the space $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$. Then we define the total variation distance, Kullback–Leibler divergence and Wasserstein metric as follows:

Definition 3.1 (Total Variation)**.** The total variation distance between two probability measures P and Q on $(\Omega, \mathcal{F})$ is defined as

$$\|P - Q\|_{TV} = \sup_{A \in \mathcal{F}} |P(A) - Q(A)|.$$

Proposition 3.2. *If the set Ω is countable then this is equivalent to half the L^1 norm.*

$$\|P - Q\|_{TV} = \frac{1}{2} \|P - Q\|_1 = \frac{1}{2} \sum_{\omega \in \Omega} |P(\omega) - Q(\omega)|$$

Proof. Let $B = \{\omega : P(\omega) \geq Q(\omega)\}$ and let $A \in \mathcal{F}$ be any event. Then

$$P(A) - Q(A) \leq P(A \cap B) - Q(A \cap B) \leq P(B) - Q(B).$$

The first inequality holds since $P(\omega) - Q(\omega) < 0$ for any $\omega \in A \cap B^c$, and so the difference in probability cannot be greater if these elements are excluded. For the second inequality, we observe that including further elements of B cannot decrease the difference in probability. Similarly,

$$Q(A) - P(A) \leq Q(B^c) - P(B^c) = P(B) - Q(B)$$

Thus, setting $A = B$, we have that $|P(A) - Q(A)|$ is equal to the upper bound in the total variation distance. Hence,

$$\|P - Q\|_{TV} = \frac{1}{2} |P(B) - Q(B) + Q(B^c) - P(B^c)| = \frac{1}{2} \sum_{\omega \in \Omega} |P(x) - Q(x)|$$

$\blacksquare$

Definition 3.3 (Kullback–Leibler Divergence)**.** Let P and Q be two probability measures on $(\Omega, \mathcal{F})$. If $P \ll Q$, the Kullback–Leibler divergence of P with respect to Q is defined as

$$KL(P|Q) = \int_\Omega \frac{dP}{dQ} log\left(\frac{dP}{dQ}\right) dQ.$$

Finally we consider the Wasserstein distance. If P and Q are probability measures on $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$, we say that γ is a transport plan between two probability measures P and Q if it is a probability measure on $(\mathbb{R}^d \times \mathbb{R}^d, \mathcal{B}(\mathbb{R}^d \times \mathbb{R}^d))$ such that for any Borel set $A \subset \mathbb{R}^d$, $\gamma(A \times \mathbb{R}^d) = P(A)$ and $\gamma(\mathbb{R}^d \times A) = Q(A)$. We denote the set of all such transport plans by $\Pi(P, Q)$.

Definition 3.4 (Wasserstein distance)**.** For two probability measures, P and Q, the L^p-Wasserstein distance is given by

$$W_p(P, Q) = \left(\inf_{\gamma \in \Pi(P,Q)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \|x - y\|^p \, d\gamma(x, y)\right)^{1/p}.$$

We will restrict our attention here to the L^2-Wasserstein distance.

REMEMBER TO INCLUDE For 1D W_p^p is equivalent to $\int_0^1 |F^{-1}(t) - G^{-1}(t)|^p \, dt$ where F and G are the CDFs of P and Q respectively [6].

3.2 Theoretical Bounds

3.3 Implementation

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