

# Markov Chain Monte Carlo: Metropolis-Hastings & Hamiltonian Monte Carlo

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# 1 Introduction

All the code for this project (including code to generate the report and its graphs) can be found at <https://github.com/bollu/sampleraytracer>.

## 1.1 MCMC sampling: the fundamental algorithm

markov-chain-monte-carlo methods are a class of algorithms which blend together two or three properties; these properties blend together in subtle ways, and permit us to solve very different-looking-problems using the same toolkit, by leveraging different portions of the algorithm's power. Broadly, they all solve the following problem:

Given an **arbitrary** function  $\mathfrak{P} : X \rightarrow \mathbb{R}$ , **create a sampler** for the **normalized** probability distributed from  $\mathfrak{P}$ ,  $\mathfrak{P}(x) \equiv \frac{\mathfrak{P}(x)}{\int \mathfrak{P}(x)dx}$ . Furthermore, allow the sampling process to be **guided by** a proposal distribution:  $\text{Prop} : X \rightarrow (X \rightarrow [0, 1])$ . This proposal, for each location  $x_0 \in X$ , permits the specification of a '**likely direction** of higher likelihood',  $\text{Prop}(x_0) : X \rightarrow \mathbb{R}$ .

## 1.2 Sampling use case 1. Simulation And Sampling

Often, we do really want samples from a particular distribution. For example, we might often want to apply Bayes' rule and sample from the posterior distribution. Assume that we have a computational procedure to compute  $P(X = x_0|Y = y_0)$ . We now want to  $P(Y|X = x_0)$ .

$$P(Y|X = x_0) = \frac{P(X = x_0|Y)P(Y)}{\sum_y P(X = x_0|Y = y)}$$

There are two problems in sampling the above distribution:

- 1 The expression  $P(Y = y|X = x)$  has no a-priori structure. Hence, we will need an algorithm that can sample from an arbitrary distribution.
- 2 The denominator term, which is a normalization factor can be extremely expensive to compute due to the summation involved

Hence, we need to use MCMC to sample from  $P(Y|X = x_0)$ , and we can expedite this by sampling from  $\mathfrak{P}(Y|X = x_0) = P(X = x_0|Y)P(Y) \propto P(Y|X = x_0)$

## 1.3 Sampling use case 2. Gradient Free Optimisation

We want to maximize a function  $f : X \rightarrow \mathbb{R}$ . However, we lack gradients for  $f$ , hence we cannot use techniques such as gradient descent, or other techniques from convex optimisation. In such a case, we can consider  $f$  as some sort of unnormalized probability distribution, and use MCMC to sample from  $f$ .

That is, we set  $\mathfrak{P} \equiv f$ . Now, samples from  $\mathfrak{P}$  will be 'more likely' to come from those regions where  $f$  is large, since a sampler will be more likely to sample from regions of high probability.

### 1.4 Sampling use case 3. Numerical Integration

We wish to calculate  $\int_l^u f(x)dx$  where  $f$  is some complicated function with no closed form for the definite integral of  $f$ . In this case, we know that the average value of a function, denoted by  $\mathbb{E}[f]$ , can be computed as:

$$\mathbb{E}[f] \equiv \frac{1}{|u-l|} \int_l^u f(x)dx$$

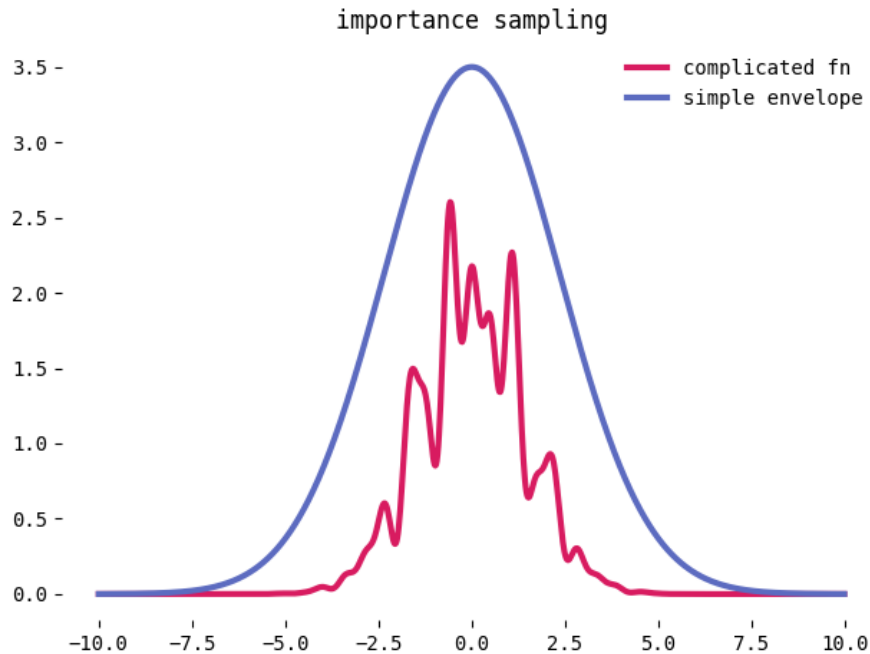
On rearrangement, we get:

$$\int_l^u f(x)dx = |u-l|\mathbb{E}[f]$$

Hence, if we have a good approximation of  $\mathbb{E}[f]$ , we have a good approximation for the integration. The naive approximation of  $\mathbb{E}[f]$  can be found by using:

$$\mathbb{E}[f] \simeq \frac{1}{n} \sum_{i=1}^n f(x_i)$$

However, we often know *something* about  $f$ , just not its *precise* shape:



In this case, we can *guide* the sampling process, by setting the proposal **Prop** as the envelope of the function  $f$ . That way, we will be more likely to pick up *useful samples*, which rapidly sample from the region of space that has mass for the integration.

## 2 Where it all begins: The Metropolis Hastings sampler

### 2.1 The big idea

We wish to sample from a distribution  $\mathfrak{P}$ , but we do not know how to do so. The idea is that we build a markov chain  $M[\mathfrak{P}, \text{Prop}]$  where  $\mathfrak{P}, \text{Prop}$  are supplied by the user. We will show that the *stationary distribution* of  $M[\mathfrak{P}, \text{Prop}]$  is going to be  $\mathfrak{P}$ . This will ensure that if we interpret *states of*  $M$  as samples, these samples will be distributed according to  $\mathfrak{P}$ .

### 2.2 detailed balance: A tool for proofs

We will first require a condition that will enable to rapidly establish that some distribution  $\mathfrak{P} : X \rightarrow \mathbb{R}$  is the stationary distribution of a markov chain  $M$ . If the transition kernel  $K : X \times X \rightarrow \mathbb{R}$  of  $M \equiv (X, K)$  is such that:

$$\forall x, x' \in X, \mathfrak{P}(x)K(x, x') = \mathfrak{P}(x')K(x', x)$$

Then  $\mathfrak{P}$  is said to be **detailed balanced** with respect to  $M$ .

**Theorem 1** *If  $\mathfrak{P}$  is detailed balanced to  $M \equiv (X, K : X \rightarrow (X \rightarrow [0, 1]))$ , then  $\mathfrak{P}$  is the stationary distribution of  $M$ .*

**Proof 1.1** *Let  $\mathfrak{P}$  be detailed balanced to  $M$ . This means that:*

$$\forall x, x' \in X, \mathfrak{P}(x)K(x)(x') = \mathfrak{P}(x')K(x')(x)$$

*Let us say that we are in state  $\mathfrak{P}$ . We wish to find the probability distribution after one step of transition. The probability of being in some state  $x'_0$  is going to be:*

$$P_{\text{next}}(x'_0) \equiv \sum_x \mathfrak{P}(x)K(x)(x'_0)$$

*since we have  $\mathfrak{P}(x)$  probability to be at a given  $x$ , and  $K(x, x'_0)$  probability to go from  $x$  to  $x'_0$ . If we add over all possible  $x \in X$ , we get the probability of all states to enter in  $x'_0$ . Manipulating  $P_{\text{next}}$ , we get:*

$$\begin{aligned}
Pnext(x'_0) &\equiv \sum_x \mathfrak{P}(x)K(x)(x'_0) \\
&= \sum_x \mathfrak{P}(x'_0)K(x'_0)(x) \quad (\text{by detailed balance}) \\
&= \mathfrak{P}(x'_0) \sum_x K(x'_0)(x) \quad (P(x_0) \text{ is constant}) \\
&= \mathfrak{P}(x'_0) \cdot 1 \quad (K(x'_0) \text{ is a distribution which is being summed over}) \\
&= \mathfrak{P}(x'_0) \quad (\text{eliminate multiplication with 1})
\end{aligned}$$

Hence,  $Pnext(n'_0) = \mathfrak{P}(x'_0)$  if  $\mathfrak{P}$  is the current state, and  $\mathfrak{P}$  is in detailed balance with the kernel  $K$ . This means that  $\mathfrak{P}$  is the stationary distribution of  $M$ .  $\triangle$

## 2.3 Metropolis Hastings

There are three key players in the metropolis hastig sampler:

- 1  $\mathfrak{P} : X \rightarrow \mathbb{R}$ : the probability distribution we wish to sample from.
- 2 **Prop** :  $X \rightarrow (X \rightarrow \mathbb{R})$ . For each  $x_0 \in X$ , provide a distribution **Prop**( $x$ ) :  $X \rightarrow \mathbb{R}$  that is used to sample points around  $x_0$ . **Prop** for *proposal*.
- 3  $M[\mathfrak{P}, \mathbf{Prop}] \equiv (X, K[\mathfrak{P}, \mathbf{Prop}] : X \rightarrow \mathbb{R})$ : The Metropolis Markov chain we will sample from, whose stationary distribution is  $\mathfrak{P}$  —  $M$  for *Markov*.

We want the stationary distribution of  $M[\mathfrak{P}, \mathbf{Prop}]$  to be  $\mathfrak{P}$ . We also wish for  $K[\mathfrak{P}, \mathbf{Prop}](x_0) \sim \mathbf{Prop}(x_0)$ : That is, at a point  $x_0$ , we want to choose new points in a way that is 'controlled' by the proposal distribution  $\mathbf{Prop}(x_0)$ , since this will allow us to 'guide' the markov chain towards regions where  $\mathfrak{P}$  is high. If we had a gradient, then we could use  $\mathfrak{P}'$  to 'move' from the current point  $x_0$  to a new point. Since we lack a gradient, we will provide a custom  $\mathbf{Prop}(x_0)$  for each  $x_0$  that will tell us how to pick a new  $x'$ , in a way that will improve  $\mathfrak{P}$ . So, we tentatively define

$$K[\mathfrak{P}, \mathbf{Prop}](x)(x') \stackrel{?}{=} \mathbf{Prop}(x)(x').$$

Recall that for  $\mathfrak{P}$  to be a stationary distribution of  $K$ , it is sufficient for  $\mathfrak{P}$  to be in detailed balance for  $K$ . So, we write:

$$\begin{aligned}
\mathfrak{P}(x)K(x, x') &\stackrel{?}{=} \mathfrak{P}(x')K(x', x) \quad (\text{going forward equally likely as coming back}) \\
\mathfrak{P}(x)\mathbf{Prop}(x)(x') &\stackrel{?}{=} \mathfrak{P}(x')\mathbf{Prop}(x')(x) \quad (\text{this is a hard condition to satisfy})
\end{aligned}$$

This is far too complicated a condition to impose on  $\mathbf{Prop}$  and  $\mathfrak{P}$ , and there is no reason for this condition to be satisfied in general. Hence, we add a custom

"fudge factor"  $\alpha \in X \rightarrow (X \rightarrow \mathbb{R})$  that tells us how often to transition from  $x$  to  $x'$ . We redefine the kernel as:

$$K[\mathfrak{P}, \text{Prop}](x)(x') \equiv \text{Prop}(x)(x')\alpha(x)(x')$$

Redoing detailed balance with this new  $K$ , we get:

$$\begin{aligned} \mathfrak{P}(x)K(x, x') &\stackrel{?}{=} \mathfrak{P}(x')K(x', x) \quad (\text{going forward equally likely as coming back}) \\ \mathfrak{P}(x)\text{Prop}(x)(x')\alpha(x)(x') &= \mathfrak{P}(x')\text{Prop}(x')(x)\alpha(x')(x) \quad (\text{Fudge a hard condition with } \alpha) \\ \frac{\alpha(x)(x')}{\alpha(x')(x)} &= \frac{\mathfrak{P}(x')\text{Prop}(x)(x')}{\mathfrak{P}(x)\text{Prop}(x')(x)} \quad (\text{Find conditions for } \alpha) \end{aligned}$$

What we have above is a *constraint* for  $\alpha$ . We now need to *pick* an  $\alpha$  that satisfies this. A reasonable choice is:

$$\alpha(x)(x') \equiv \min \left( 1, \frac{\mathfrak{P}(x')\text{Prop}(x')(x)}{\mathfrak{P}(x)\text{Prop}(x)(x')} \right)$$

since  $K$  is a transition kernel, we cannot have its entries be greater than 1. Hence, we choose to clamp it with a  $\min(1, \cdot)$ . This finally gives us the kernel as:

$$\begin{aligned} K[\mathfrak{P}, \text{Prop}](x)(x') &\equiv \text{Prop}(x)(x')\alpha(x)(x') \\ K[\mathfrak{P}, \text{Prop}](x)(x') &= \text{Prop}(x)(x') \min \left( 1, \frac{\mathfrak{P}(x')\text{Prop}(x')(x)}{\mathfrak{P}(x)\text{Prop}(x)(x')} \right) \\ K[\mathfrak{P}, \text{Prop}](x)(x') &= \min \left( \text{Prop}(x)(x'), \frac{\mathfrak{P}(x')\text{Prop}(x')(x)}{\mathfrak{P}(x)} \right) \end{aligned}$$

We can make sure that detailed balance is satisfied:

$$\begin{aligned} \mathfrak{P}(x)K[\mathfrak{P}, \text{Prop}](x)(x') &= \mathfrak{P}(x) \min \left( \text{Prop}(x)(x'), \frac{\mathfrak{P}(x')\text{Prop}(x')(x)}{\mathfrak{P}(x)} \right) \\ &= \min \left( \mathfrak{P}(x)\text{Prop}(x)(x'), \mathfrak{P}(x) \frac{\mathfrak{P}(x')\text{Prop}(x')(x)}{\mathfrak{P}(x)} \right) \\ &= \min (\mathfrak{P}(x)\text{Prop}(x)(x'), \mathfrak{P}(x')\text{Prop}(x')(x)) \end{aligned}$$

Note that the above right-hand-side is symmetric in  $x$  and  $x'$ , and hence we can state that:

$$\mathfrak{P}(x)K[\mathfrak{P}, \text{Prop}](x)(x') = \min (\mathfrak{P}(x)\text{Prop}(x)(x'), \mathfrak{P}(x')\text{Prop}(x')(x)) = \mathfrak{P}(x')K[\mathfrak{P}, \text{Prop}](x')(x)$$

Hence, we can wrap up, stating that our design of  $K$  does indeed give us a markov chain whose stationary distribution is  $\mathfrak{P}$ , since  $\mathfrak{P}$  is detailed balanced with  $K[\mathfrak{P}, \text{Prop}]$ . As an upshot, we also gained a level of control with  $\text{Prop}$ , where we are able to provide "good" samples for a given point.

## 2.4 Simplification when proposal is symmetric

If our function  $\text{Prop}$  is symmetric:  $\forall x, x' \text{Prop}(x)(x') = \text{Prop}(x')(x)$ , then a lot of the above derivation becomes much simpler. We will perform those simplifications here for pedagogy.

When we have  $\text{Prop}(x)(x') = \text{Prop}(x')(x)$ , we can simply  $\alpha$ :

$$\begin{aligned}\alpha(x)(x') &\equiv \min \left( 1, \frac{\mathfrak{P}(x')\text{Prop}(x')(x)}{\mathfrak{P}(x)\text{Prop}(x)(x')} \right) \\ \alpha(x)(x') &= \min \left( 1, \frac{\mathfrak{P}(x')}{\mathfrak{P}(x)} \right) \quad [\text{cancelling: } \text{Prop}(x)(x') = \text{Prop}(x')(x)]\end{aligned}$$

This also makes the kernel look a lot more pleasing:

$$\begin{aligned}K[\mathfrak{P}, \text{Prop}](x)(x') &\equiv \text{Prop}(x)(x')\alpha(x)(x') \\ K[\mathfrak{P}, \text{Prop}](x)(x') &= \text{Prop}(x)(x') \min \left( 1, \frac{\mathfrak{P}(x')}{\mathfrak{P}(x)} \right)\end{aligned}$$

```

# prob is the distribution to sample from;
# symproposal is the *symmetric* proposal function
# symproposal: X -> X; produces a new 'X' from a
#             given 'X' with some distribution.
# prob: X -> |R: gives probability of point 'xi'.
# N: number of markov chain walks before returning a new sample.
def metropolis_hastings(prob, symproposal, x0, N):
    x = x0
    while True:
        for i in range(N):
            # xnext chosen with Prop(x)(x') prob.
            xnext = symproposal(x); px = prob(x); pxnext = prob(xnext);
            # x' chosen with Prop(x)(x') * alpha prob.
            r = uniform01(); alpha = min(1, pxnext / px); if r < alpha: x = xnext
        yield x

```

## 2.5 Implementing MH: Devil in the detailed balance

### 2.5.1 Naive implementation

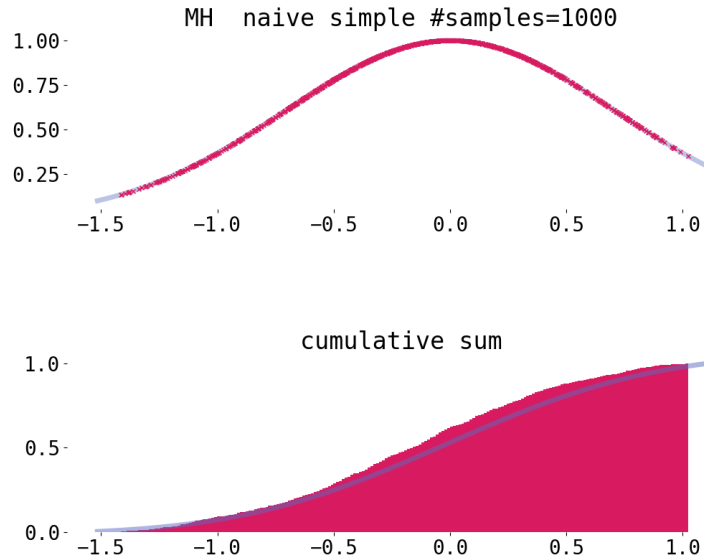
Let us try to transcribe the equations we have derived for symmetric proposal into code, and see what happens. Let us choose  $\mathfrak{P}(x) \equiv \text{normal}(0, 1) = e^{-x*x}$  and the proposal function to be  $P(x_0)(x) = \text{normal}(x_0, 1e-2)$  is, a Gaussian centered around  $x_0$  with standard deviation  $1e-2$ . This gives us the code:

```

# mcmc1d.py
def mhsimple(x0, prob, prop):
    yield x0; x = x0;
    while true:
        xnext = prop(x); p = prob(x); pnext = prob(xnext)
        r = np.random.uniform() + 1e-5;
        if r < pnext/p: x = xnext
        yield xnext
    ...
def exp(x): return np.exp(-x*x)
def expprop(x): return np.random.normal(loc=x, scale=1e-1)
...
nsamples = 1000
xs = list(itertools.islice(mhsimple(0, exp, expprop), nsamples))

```



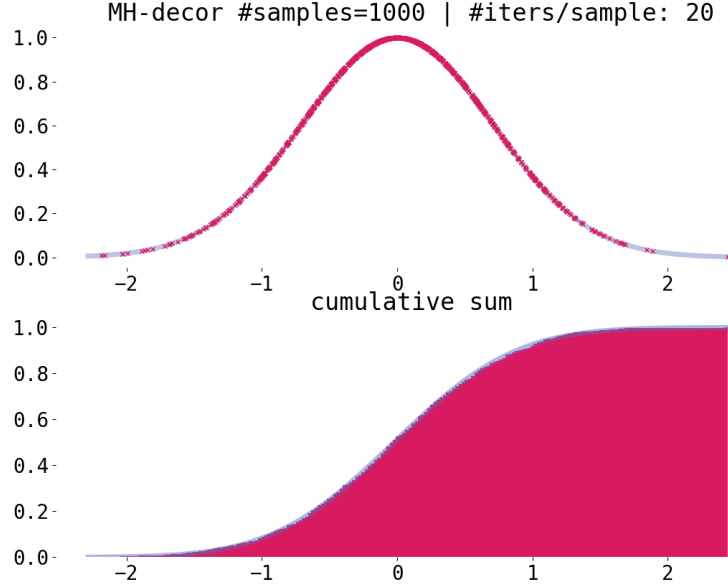


We can see from the plots of the raw samples and the cumulative distribution that we wind up overshooting. This is because the markov chain, by definition, has correlations between samples; However, we are supposed to be drawing *independent* samples from  $\mathfrak{P}$  for plotting/downstream use.

## 2.5.2 Sampling per `iters_per_sample` steps

The solution is to take samples that are *spaced out* — that is, we do not consider each step from the markov chain as a sample. Rather, we consider the state we are in after some `iters_per_sample` steps to be a sample. In code, this is now:

```
# mcmc1d.py
def mh_uncorr(x0, prob, prop, iters_per_sample):
    yield x0; x = x0;
    while True:
        for i in range(iters_per_sample):
            xnext = prop(x); p = prob(x); pnext = prob(xnext)
            r = np.random.uniform() + 1e-5;
            if r < min(1, pnext/p): x = xnext
        yield xnext
...
def exp(x): return np.exp(-x*x)
def expprop(x): return np.random.normal(loc=x, scale=1e-1)
...
NSAMPLES = 1000; ITERS_PER_SAMPLE = 20
xs = list(itertools.islice(mhsimple(0, exp, expprop, ITERS_PER_SAMPLE), NSAMPLES))
```



### 3 Hamiltonian Monte Carlo

If our target probability density  $\mathfrak{P} : X \rightarrow [0, 1]$  is *differentiable*, then we can use the derivative of  $\mathfrak{P}(x)$  to provide better proposals. The idea is as follows:

- Interpret the probability landscape as a potential, with points of high probability being "valleys" and points of low probability being "peaks" (ie, invert the probability density with a transform such as  $U[\mathfrak{P}](x) = -\log \mathfrak{P}(x)$ . This way, a ball rolling on this terrain will try to move towards the valleys — which are the locations of high probability  $\mathfrak{P}$ .
- For a proposal at a position  $x_0 \in X$ , keep a ball at  $x_0$ , *randomly choose its velocity*, simulate the ball according to classical mechanics (Newton's laws of motion) for a fixed duration  $D \in \mathbb{R}$  and propose the final position as the final position of the ball. This is reversible and detailed balanced because *classical mechanics is reversible and detailed balanced*.

We wish to sample from a new distribution  $P_H$ , which is defined as:

$$\begin{aligned}
P_H[\mathfrak{P}](\mathbf{p}, \mathbf{q}) &\equiv \exp(-H[\mathfrak{P}](\mathbf{p}, \mathbf{q})) && \text{(Sample states with low energy: Boltzmann/Ising model)} \\
&= \exp(-(U[\mathfrak{P}](\mathbf{q}) + K(\mathbf{p}))) && \text{(by defn. of hamiltonian, } H[\mathfrak{P}] = U[\mathfrak{P}] + K) \\
&= \exp(-(-\log \mathfrak{P}(\mathbf{q}) + \mathbf{p}^T \mathbf{p}/2)) && \text{(by choice of } U \text{ as NLL, } K \text{ as classical KE)} \\
&= \exp(\log \mathfrak{P}(\mathbf{q}) - \mathbf{p}^T \mathbf{p}/2) \\
&= \exp(\log \mathfrak{P}(\mathbf{q})) \cdot \exp(-\mathbf{p}^T \mathbf{p}/2) \\
&= \mathfrak{P}(\mathbf{q}) \cdot \exp(-\mathbf{p}^T \mathbf{p}/2)
\end{aligned}$$

Note that the probability distribution for  $P_H[\mathfrak{P}]$  has split into two independent distributions:  $\mathfrak{P}(\mathbf{q})$ , and  $\exp(-\mathbf{p}^T \mathbf{p}/2)$ . Hence, sampling  $(\mathbf{p}, \mathbf{q}) \sim P_H[\mathfrak{P}]$  correctly is *equivalent* to sampling  $\mathbf{q} \sim \mathfrak{P}$ , and  $\mathbf{p} \sim \exp(-\mathbf{p}^T \mathbf{p}/2)$ . Therefore, if we can sample from  $P_H$  effectively, taking only  $(\mathbf{q}, -) \sim P_H[\mathfrak{P}]$  will correctly give us the samples we are looking for.

We will show that using MCMC to sample from the  $P_H[\mathfrak{P}]$  above, with a particular proposal function  $\text{Prop}_H$  that we shall define momentarily will provide us with samples  $(\mathbf{p}, \mathbf{q})$  such that the  $\mathbf{q}$  is sampled from  $\mathfrak{P}$ . This begs the question: "why do we need  $\mathbf{p}$  anyway?" We will show how introducing this  $\mathbf{p}$  allows for rapid exploration of the space of possible  $\mathbf{q}$ s.

### 3.1 The proposal function for HMC

In classical mechanics, once we have a hamiltonian  $H(\mathbf{q}, \mathbf{p})$ , the dynamics of the system are simulated according to the equations (called Hamilton's equations):

$$\frac{\partial \mathbf{q}}{\partial t} = \frac{\partial H[\mathfrak{P}]}{\partial \mathbf{p}} \quad \frac{\partial \mathbf{p}}{\partial t} = -\frac{\partial H[\mathfrak{P}]}{\partial \mathbf{q}}$$

These equations, specialized to our situation become:

$$\begin{aligned}
\frac{\partial \mathbf{q}}{\partial t} &= \frac{\partial H[\mathfrak{P}]}{\partial \mathbf{p}} = \frac{\partial (U[\mathfrak{P}](\mathbf{q}) + K(\mathbf{p}))}{\partial \mathbf{p}} = \frac{\partial K(\mathbf{p})}{\partial \mathbf{p}} = \frac{\partial (\mathbf{p}^T \mathbf{p})}{\partial \mathbf{p}} = 2\mathbf{p} \\
\frac{\partial \mathbf{p}}{\partial t} &= -\frac{\partial H[\mathfrak{P}]}{\partial \mathbf{q}} = -\frac{\partial (U[\mathfrak{P}](\mathbf{q}) + K(\mathbf{p}))}{\partial \mathbf{q}} = -\frac{\partial U[\mathfrak{P}](\mathbf{q})}{\partial \mathbf{q}} = \frac{-\partial -\log \mathfrak{P}(\mathbf{q})}{\partial \mathbf{q}} = \frac{\partial \log \mathfrak{P}(\mathbf{q})}{\partial \mathbf{q}}
\end{aligned}$$

We will denote a solution to the above system of equations as  $(\mathbf{q}_{final}, \mathbf{p}_{final}) \equiv X_H[\mathfrak{P}](\mathbf{q}_0, \mathbf{p}_0, T_0)$ . That is, starting from the position  $(\mathbf{p}_0, \mathbf{q}_0)$ , simulate the system for  $T_0 \in \mathbb{R}$  time, according to Hamilton's equations. The final (position, momentum) is  $(\mathbf{q}_{final}, \mathbf{p}_{final})$ .

Now, our proposal function will be:

$$\text{Prop}(\mathbf{q}_0, -) \equiv \text{let } \mathbf{p}_0 \sim \text{normal}(0, 1) \text{ in } X_H[\mathfrak{P}](\mathbf{q}_0, \mathbf{p}_0, T_0)$$

That is, we will propose the new point as one obtained from time evolution of the solutions to the hamiltonian; (a) we start from the point  $\mathbf{q}_0$ ; (b) pick a *random velocity*  $\mathbf{p}_0$ ; (c) simulate the system for  $T_0$  time using hamilton's equations; (d) return the final (position, momentum) as our proposal.

### 3.2 Simulating the above equations to sample $\mathfrak{P} \equiv \exp(-x^2)$

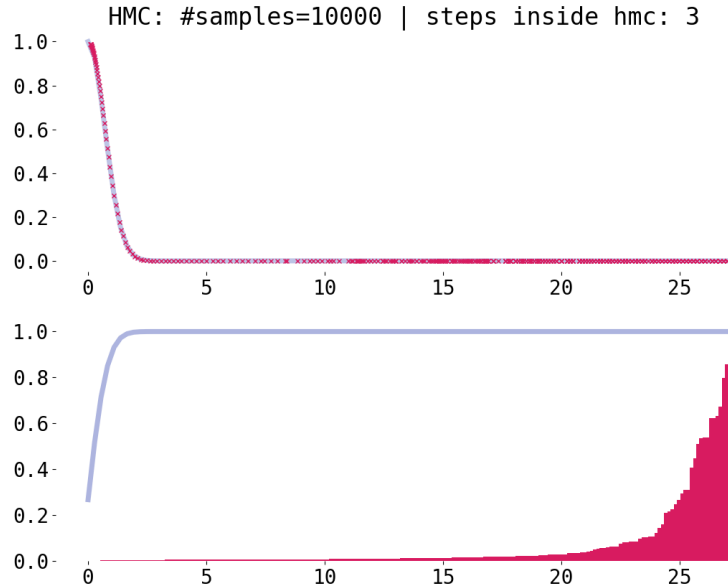
```
def euler(dhdp, dhq, q, p, dt): % f(x + dx) = f(x) + f'(x) * dx
    pnew = p + -dhdp(q, p) * dt; qnew = q + dhq(q, p) * dt
    return (qnew, pnew)

def hmc(q0, U, dU, nsteps, dt):
    # hamiltonian definition
    def h(q, p): return U(q) + 0.5*p*p
    def hdp(q, p): return p
    def hdq(q, p): return dU(q)
    def nextsample(q, p): # run `euler` for n steps
        for _ in range(nsteps):
            (q, p) = euler(hdq, hdp, q, p, dt)
        return (q, p)

    yield q0; q = q0
    while True:
        p = np.random.normal(0, 1) # (a) pick random momentum
        (qnext, pnext) = nextsample(q, p) # (b) simulate next sample
        pnext = -p # (c) reverse momentum so our process is reversible
        r = np.random.uniform(); # (d) if accept according to MH, accept.
        if np.log(r) < h(q, p) - h(qnext, pnext): q = qnext
        yield q # return point
```

Let's quickly explain the code;

- (a) We start by picking a random momentum for the proposal, which is sampled from a uniform normal distribution. This is `p = np.random.normal(0, 1)`.
- (b) We now find the point `(qnext, pnext)` which is the value  $(\mathbf{q}_{next}, \mathbf{p}_{next}) = X_H[\mathfrak{P}](\mathbf{q}, \mathbf{p}, dt)$ . Unfortunately, we do not have a closed form for  $X_H$ . So, we solve Hamilton's equations using *numerical integration*. We use the Euler integrator, which uses the taylor expansion:  $f(x + \Delta x) \simeq f(x) + f'(x)\Delta x$ . In the code, this is performed by the function `euler`.
- (c) We compute the acceptance probability  $\alpha$  as  $\mathfrak{P}_H(\mathbf{q}_{next}, \mathbf{p}_{next})/P_H(\mathbf{q}, \mathbf{p}) = \exp(H(\mathbf{q}_{next}, \mathbf{p}_{next}) - H(\mathbf{q}, \mathbf{p}))$ . Rather than computing the acceptance as  $r < \alpha$ , we compute  $\log r < \log \alpha$  for better numerical accuracy. This leads to the code being `if np.log(r) < h(q, p) - h(qnext, pnext)`.



This has sampled disastrously: what is going wrong?

### 3.3 Simulation: Euler integration

Unfortunately, it turns out that running this simulation is in fact numerically unstable on using a naive integrator such as Euler. We shall explore this by trying to integrate the orbits of a planet under gravitational force. We are using a bog-standard Hamiltonian with  $K(\mathbf{p}) = \mathbf{p}^T \mathbf{p}$ ,  $U(\mathbf{q}) = \sqrt{\mathbf{q}^T \mathbf{q}}$ ,  $H(\mathbf{q}, \mathbf{p}) = U(\mathbf{q}) + K(\mathbf{p})$ . We will integrate Hamilton's equations using the `euler` integrator and look at the orbits. Ideally, we want the orbits to be **time-reversible**, since our **proposal should be symmetric!**

Let us say that we wish to simulate the orbit of a planet. Recall that we want the proposal to be symmetric: so, if we simulate the trajectory of the planet for  $N$  timesteps, each timestep of time  $\delta t$ , and then *reverse* the momentum of the planet, run the next phase of the simulation for  $N$  timesteps with timestep  $\Delta t$ , we should begin where we started. However, if we try to use the euler integration equations, here is what we see:

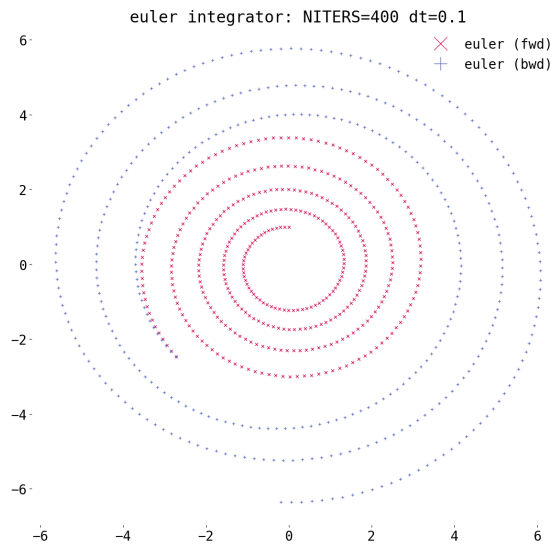
```
def euler(dhdp, dhdq, q, p, dt):
    pnew = p + -dhdp(q, p) * dt
    qnew = q + dhdp(q, p) * dt
    return (qnew, pnew)
...
def planet(q, p, integrator, n, dt):
```

```

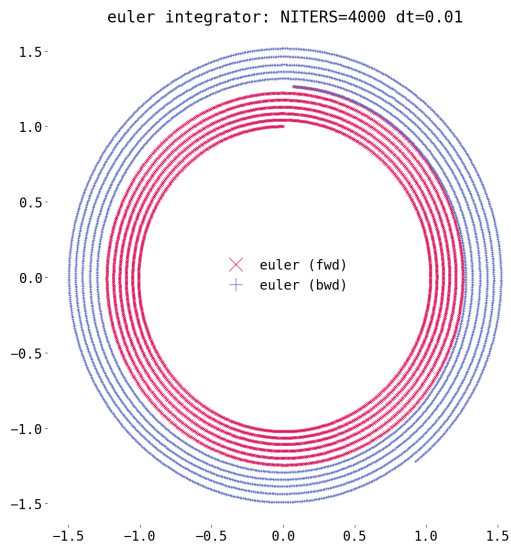
STRENGTH = 0.5
# minimise potential  $V(q)$ :  $q$ ,  $K(p, q)$   $p^2$ 
#  $H = \text{STRENGTH} * |q|$  (potential) +  $p^2/2$  (kinetic)
def H(qcur, pcur): return STRENGTH * np.linalg.norm(q) + np.dot(p, p) / 2
def dhdp(qcur, pcur): return p
def dhdq(qcur, pcur): return STRENGTH * 2 * q / np.linalg.norm(q)

for i in range(n): (q, p) = integrator(dhdp, dhdq, q, p, dt) ...
return np.asarray(qs), np.asarray(ps)

```



We can clearly see the forward trajectory (in pink) spiralling out, and the backward trajectory (in blue), spiralling out even more. We can attempt to fix this by making  $\Delta t$  smaller:

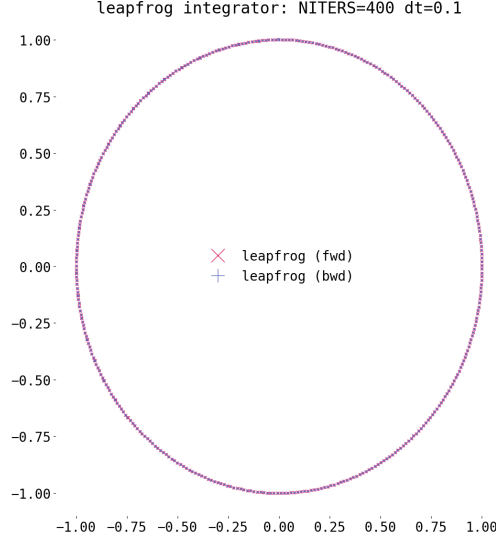


to no avail. Indeed, this is a **fundamental limitation of euler integration**. Hence, we will need to explore more refined integration schemes.

### 3.4 Simulation: Symplectic integrator

The type of integrators that will allow us to get 'reasonable orbits' that do not decay with time are known as *symplectic integrators*. (An aside: the word *symplectic* comes from Weyl, who substituted the latin root in the word *complex* by the corresponding greek root. It is a branch of differential geometry which formalizes the constructs needed to carry out hamiltonian mechanics on spaces that are more complicated than Euclidian  $\mathbb{R}^n$ ).

```
## dq/dt = dH/dp|_{p0, q0}, dp/dt = -dH/dq|_{p0, q0}
def leapfrog(dhdp, dhdq, q0, p0, dt):
    p0 += -dhdq(q0, p0) * 0.5 * dt # kick: half step momentum
    q0 += dhdp(q0, p0) * dt # drift: full step position
    p0 += -dhdq(q0, p0) * 0.5 * dt # kick: half step momentum
    return (q0, p0)
```



It is clear from the plots that the leapfrog integrator is stable: orbits stay as orbits, and running-in-reverse works as expected. We provide a formal proof of time reversibility below. We also prove that this type of integrator preserves energy. In total, these two properties ensure that the **proposals we make will be symmetric**.

### 3.5 Proof that leapfrog is time-reversible

We will assume that  $H(\mathbf{q}, \mathbf{p}) \equiv U(\mathbf{q}) + K(\mathbf{p})$ . That is, the kinetic energy depends only on momentum, and the potential energy depends only on position. This allows us to write the derivatives as  $\frac{\partial H}{\partial \mathbf{q}} \equiv U'(\mathbf{q})$ ,  $\frac{\partial H}{\partial \mathbf{p}} \equiv K'(\mathbf{p})$ . This also modifies Hamilton's equations into:

$$\frac{\partial \mathbf{q}}{\partial t} = \frac{\partial H(\mathbf{q}, \mathbf{p})}{\partial \mathbf{p}} = K'(\mathbf{p}) \quad \frac{\partial \mathbf{p}}{\partial t} = -\frac{\partial H(\mathbf{q}, \mathbf{p})}{\partial \mathbf{q}} = -U'(\mathbf{q})$$

We will also assume that  $K'(-\mathbf{p}) = -K'(\mathbf{p})$ . This is true of our usual choice of kinetic energy being  $K(\mathbf{p}) \equiv \mathbf{p}^T \mathbf{p}$ . We will write down the forward simulation according to the leapfrog equations, and then the backward steps. This will show us that the final state of the backward equations  $(\mathbf{q}'_1, \mathbf{p}'_2)$  will be equal to the reversed initial state  $(\mathbf{q}_0, -\mathbf{p}_0)$ .

```
fwd 1  [q0, p0]
fwd 2  [q0, p1 ≡ p0 - 0.5U'(q0)dt]
fwd 3  [q1 ≡ q0 + K'(p1)dt, p1]
fwd 4  [q1, p2 ≡ p1 - 0.5U'(q1)dt]
```



bwd 1  $[\mathbf{q}'_0 \equiv \mathbf{q}_1 = \mathbf{q}_0 + K'(\mathbf{p}_1)dt, \mathbf{p}'_0 \equiv -\mathbf{p}_2 = \mathbf{p}_1 - 0.5U'(\mathbf{q}_1)dt]$   
 bwd 2  $[\mathbf{q}'_0, \mathbf{p}'_1 \equiv \mathbf{p}'_0 - 0.5U'(\mathbf{q}'_0)dt = -(\mathbf{p}_1 - 0.5U'(\mathbf{q}_1)dt) - 0.5U'(\mathbf{q}_1)dt = -\mathbf{p}_1]$   
 bwd 3  $[\mathbf{q}'_1 \equiv \mathbf{q}'_0 + K'(\mathbf{p}'_1)dt = (\mathbf{q}_0 + K'(\mathbf{p}_1)dt) + K'(-\mathbf{p}_1)dt = (\mathbf{q}_0 + K'(\mathbf{p}_1)dt) - K'(\mathbf{p}_1)dt = \mathbf{q}_0, \mathbf{p}'_1]$   
 bwd 4  $[\mathbf{q}'_1 \equiv \mathbf{q}_0, \mathbf{p}'_2 \equiv \mathbf{p}'_1 - 0.5U'(\mathbf{q}'_1)dt = -\mathbf{p}_1 - 0.5U'(\mathbf{q}_0)dt = -(\mathbf{p}_0 - 0.5U'(\mathbf{q}_0)) - 0.5U'(\mathbf{q}_0)dt = -\mathbf{p}_0]$

n	fwd $\mathbf{q}$	fwd $\mathbf{p}$
1	$\mathbf{q}_0$	$\mathbf{p}_0$
2	$\mathbf{q}_0$	$\mathbf{p}_1 = \mathbf{p}_0 - 0.5U'(\mathbf{q}_0)dt$
3	$\mathbf{q}_1 = \mathbf{q}_0 + K'(\mathbf{p}_1)dt$	$\mathbf{p}_1$
4	$\mathbf{q}_1$	$\mathbf{p}_2 = \mathbf{p}_1 - 0.5U'(\mathbf{q}_1)dt$
n	bwd $\mathbf{q}$	bwd $\mathbf{p}$
1	$\mathbf{q}'_0 = \mathbf{q}_1$	$\mathbf{p}'_0 = -\mathbf{p}_2$
2	$\mathbf{q}'_0 = \mathbf{q}_1$	$\mathbf{p}'_1 = -\mathbf{p}_1$
3	$\mathbf{q}'_1 = \mathbf{q}_0$	$\mathbf{p}'_1 = -\mathbf{p}_1$
4	$\mathbf{q}'_1 = \mathbf{q}_0$	$\mathbf{p}'_2 = -\mathbf{p}_0$

Indeed, we see that the backward equations where we set  $(\mathbf{q} \mapsto \mathbf{q}, \mathbf{p} \mapsto -\mathbf{p})$  retraces our dynamics, just running backward. Hence, **the leapfrog equations are reversible**, and therefore act as a **symmetric proposal**.

### 3.6 Using HMC on the 1D gaussian

Now that we have the math to setup a symmetric proposal distribution using leapfrog, let's code up HMC on a 1D gaussian:

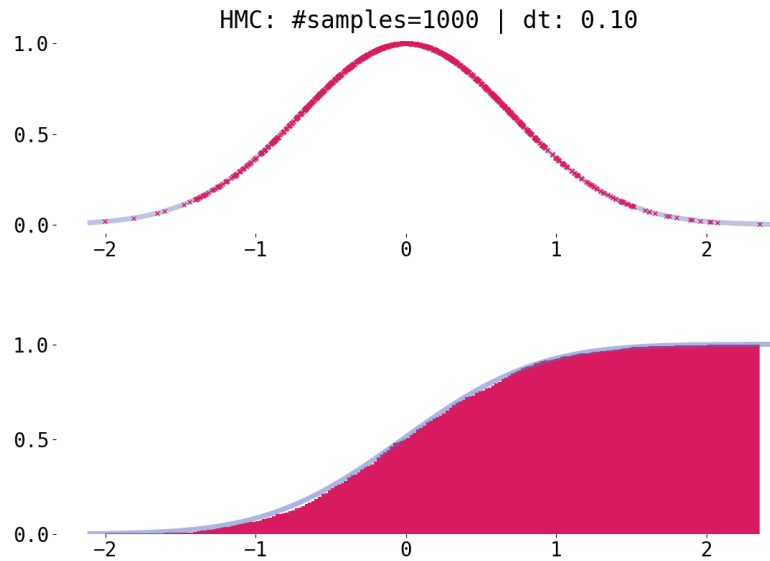
```

def leapfrog(dhdq, dhdp, q0, p0, dt):
    p0 += -dhdq(q0, p0) * 0.5 * dt # kick: half step momentum
    q0 += dhdp(q0, p0) * dt # drift: full step position
    p0 += -dhdq(q0, p0) * 0.5 * dt # kick: half step momentum
    return (q0, p0)

def hmc(q0, U, dU, nsteps, dt):
    def h(q, p): return U(q) + 0.5 * p*p
    def nextsample(q, p):
        for _ in range(nsteps):
            def hdp(q, p): return p
            def hdq(q, p): return dU(q)
            (q, p) = leapfrog(hdq, hdp, q, p, dt)
        return (q, p)

    yield q0; q = q0
    while True:
        p = np.random.normal(0, 1)
        (qnext, pnext) = nextsample(q, p)
        pnext = -p # reverse momentum so our process is reversible
        r = np.random.uniform();
        if np.log(r) < h(q, p) - h(qnext, pnext): q = qnext
        yield q
    ...
def neglogexp(x): return -1 * logexp(x)
def neglogexpgrad(x): return -1 * logexpgrad(x)
xs = list(take_every_nth(DECORRELATE_STEPS,
    itertools.islice(hmc(1, neglogexp, neglogexpgrad, NSTEPS, DT), NSAMPLES*DECORRELATE_STEPS)))

```

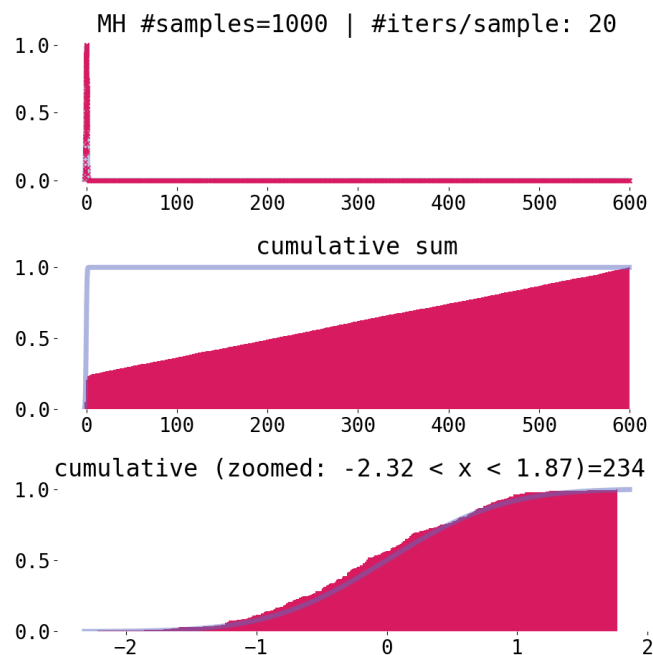


This looks far worse than the results we got from vanilla metropolis hastings: why would anybody use this technique?

### 3.7 HMC v/s MH when the proposal is atypical

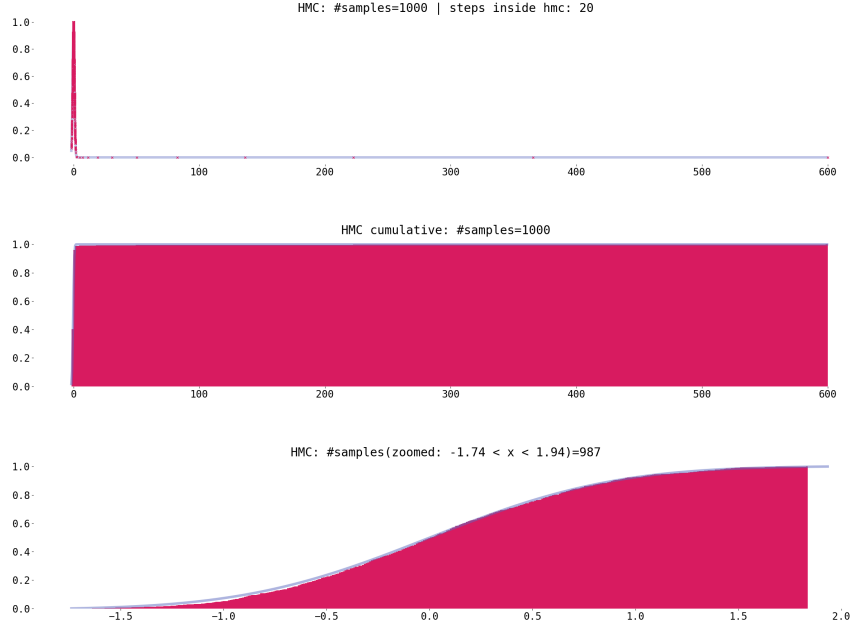
So far, I've hidden one thing under the rug: the *initialization* of the distribution. We've been starting at  $x = 1$  — let's now change that, and start at  $x = 600$ . Note that this is very far from the "region of interest" in the case of a standard normal distribution: 99% of the probability mass is in  $[-3, 3]$  (the  $3\sigma$  rule).

### 3.7.1 MH starting at $x = 600$



Note that out of the 1000 samples we started from, only 234 are present in the region of  $-2 \leq x \leq 2$ . We have wasted around 80% of the samples we have *moving through the space* to get to the typical set.

### 3.7.2 HMC starting at $x = 600$



Note that out of the 1000 samples we started from, only 987 are present in the region of  $-2 \leq x \leq 2$ . Notice the distribution of samples (pink crosses) in the hamiltonian monte-carlo case: most samples clustered around the gaussian; our initial samples that are far away are powered by a strong potential energy to move towards the center.

This is in stark contrast to the MH case, where the entire  $x$ -axis is pink, due to the 'current point' having to move, proposal-by-proposal (which allows at most a movement of distance 1), from 600 to 0.

## References

- [1] Michael Betancourt. A conceptual introduction to hamiltonian monte carlo. *arXiv preprint arXiv:1701.02434*, 2017.
- [2] Steve Brooks, Andrew Gelman, Galin Jones, and Xiao-Li Meng. *Handbook of markov chain monte carlo*. CRC press, 2011.
- [3] Marin Kobilarov, Keenan Crane, and Mathieu Desbrun. Lie group integrators for animation and control of vehicles. *ACM transactions on Graphics (TOG)*, 28(2):1–14, 2009.