### Hamiltonian Monte Carlo Inference for a First Order Probabilistic Programming Language

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### Abstract

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### 1 Introduction

Monte Carlo Markov Chain (MCMC) methods are a set of powerful inference algorithms (Berg and Billoire, 2008) that enable us to evaluate, model and analyze complicated probabilistic models. These include, but are not limited to, areas in machine learning, such as Bayesian inference and learning, optimisation for finding the optimal hyper-parameters (Andrieu et al., 2003) and in natural systems, such as those found in Biology (Sorensen and Gianola, 2007) and Physics (Duane et al., 1987). However, as the dimensionality of the problem grows many MCMC methods, such as Metropolis-Hastings (Hastings, 1970), rejection and importance sampling, become ineffective at being able to generate samples effectively. This can be overcome in some instances by tuning particular parameters, or generating a better proposal distribution, but in practice this cannot always be done. One MCMC method that is able to circumvent this problem is Hamiltonian Monte Carlo (HMC) (Neal et al., 2011)(Duane et al., 1987), which takes inspiration from the physical world and uses a dynamical model to generate new proposals. This in turn enables us to explore larger spaces more effectively globally, rather than getting trapped in local regions.

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Choosing the right inference algorithm is critical for probabilistic programming languages (Tolpin et al., 2015) such as Anglican (Wood et al., 2014) and others, where we rely upon accurate inference and sampling procedures to evaluate our programs. Although, in practice there is no one inference or sampling algorithm to rule them all. Thus we rely on a combination of techniques to deal with discretem, finite continuous and infinite parameter spaces (non-parametric models). To analyze more effectively a subset of the problems that Anglican can, such as finite graphs, FOPPL, a first order probabilistic programming language was constructed so that we could take advantage of fast inference algorithms, such as HMC.

In this work we make two contributions, we introduce a FOPPL compiler that transforms a FOPPL output, a finite graph, into python code that takes advantage of the Automatic differentiation package within Pytorch (PyTorch, 2017) and an HMC that correctly deals with conditional statements and finite continuous parameters. In section 2 we talk about FOPPL, its syntax and primary use, in section 3 we introduce HMC, in section 4 we give examples of FOPPL programs and the results generated through HMC inference. In section 6 we provide details of HMC implementation and some examples of the compiled FOPPL output.

### 2 FOPPL

In this section include some stuff about FOPPL, what is it, the syntax etc. The length of the loops are deterministic and finite, whereas in higher order probabilistic programming languages enable a loop to be unrolled an infinite number of times.

### 3 Hamiltonian Monte Carlo

In a top level view HMC is a two step process. In step one we define a Hamiltonian function in terms of the probability distribution of the model that we aim to perform inference on and in step two, HMC proposes new states generated via Hamiltonian dynamics

for which we apply Metropolis updates. As the proposals are being generated via a physical process, we are able to comprehensively explore our model space (Neal et al., 2011). This is in part due to certain physical properties of the Hamiltonian itself, that make HMC a very powerful, multi-purpose inference algorithm. Adopting the notations from the machine learning literature, we use  $\mathbf{x} \in \mathbb{R}^{n \times d}$  to represent the parameters of interest, our latent variables, rather than the typical  $\theta$  and  $\mathbf{q}$  in the HMC literature. Where n represents the number of parameters of interest and d is the dimension of the system.

The Hamiltonian of a physical system is defined completely in terms of the sets of points  $(\mathbf{x}, \mathbf{p})$ , the position and momentum variables respectively. These points span what is called the phase space, which formally is defined as the cotangent bundle  $T^*\mathcal{M}$  of the configuration space  $\mathcal{M}$ . Simply put, we can imagine the phase space as manifold that shows us both how our model evolves, with respect to  $\mathbf{x}$  and  $\mathbf{p}$  and how it is constrained in regards to the total energy within the system. Where the total energy of the system is given by the Hamiltonian,  $H(\mathbf{x}, \mathbf{p})$ . The Hamiltonian is the Legendre transform of the Lagrangian and is formally defined as  $H(\mathbf{x}, \mathbf{p}) = K(\mathbf{p}) + U(\mathbf{x})$  where  $K(\mathbf{p})$ represents our kinetic energy and  $U(\mathbf{x})$  is the potential energy and the Legendre transform is given by  $H(\mathbf{x}, \mathbf{p}) = \sum_{i=1}^{d} \dot{x}_i p_i - L(\mathbf{x}, \dot{\mathbf{x}}(\mathbf{x}, \mathbf{p}))^{1}$ . Thus, for simplicity, if we set d = 1, we can derive Hamiltonian equations:

$$\frac{\partial H}{\partial p} = \dot{x} + p \frac{\partial \dot{x}}{\partial p} - \frac{\partial L}{\partial \dot{x}} \frac{\partial \dot{x}}{\partial p} = \dot{x} \tag{1}$$

and

$$\frac{\partial H}{\partial x} = p \frac{\partial \dot{x}}{\partial x} - \frac{\partial L}{\partial x} - \frac{\partial L}{\partial \dot{x}} \frac{\partial \dot{x}}{\partial x} = -\frac{\partial L}{\partial x} = -\dot{p} \qquad (2)$$

from which we can vectorize for higher dimensions. It should be noted that the derivatives for the Lagrangian L, come from the Euler-Lagrange equations  $\frac{d}{dt}\left(\frac{\partial L}{d\dot{x}}\right)=\frac{\partial L}{dx}$  and the Lagrangian itself, is just a reformulation of Newtonian mechanics.

Within the HMC framework the positions,  $\mathbf{x}$ , are the variables of interest, but in order to simulate Hamiltonian dynamics properly, for each  $\mathbf{x}$  we must introduce an auxillary momentum variable  $\mathbf{p}$ . But what form should  $\mathbf{p}$  take? Typically,  $\mathbf{p}$  is sampled from a normal distribution  $\mathbf{p} \sim \mathcal{N}(\mathbf{0}, \mathbf{1})$ , although this need not be the case. In HMC, the potential energy  $U(\mathbf{x})$  represents the negative of the log joint distribution of the model and is a key component within the algorithm. The kinetic energy  $K(\mathbf{p})$ , is typically taken to

be the mean field approximation, which corresponds directly to the log of a centered Gaussian distribution  $K(\mathbf{p}) = \frac{\mathbf{p}^T \mathbf{M}^{-1} \mathbf{p}}{2}$ , where  $\mathbf{M}$ , the mass matrix, is a symmetric, positive definite and typically diagonal matrix. Although, again we need not choose this form of kinetic energy and in some cases, such as those when we are dealing with discrete parameters, it is actually more beneficial to use a different kinetic function(Nishimura et al., 2017). Thus, if we are to use the standard kinetic energy, which we do for all our current models, then Hamilton's equations take the form  $\dot{\mathbf{x}} = \frac{d\mathbf{x}}{dt} = [\mathbf{M}^{-1}\mathbf{p}]$  and  $\dot{\mathbf{p}} = \frac{d\mathbf{p}}{dt} = -\frac{\partial U}{\partial \mathbf{x}}$ . To understand why the potential energy represents

To understand why the potential energy represents the joint, we take inspiration from the canonical distribution found in statistical mechanics  $P(\mathbf{x}, \mathbf{p}) = \frac{1}{Z} \exp\left(\frac{-E(\mathbf{x}, \mathbf{p})\kappa_b}{T}\right)$ , where Z is a normalization constant  $^2$ , E represents the total energy of the system, our Hamiltonian, and  $\kappa_b = T = 1$  are constants that we define to be unit. Substituting the Hamiltonian H into the canonical distribution gives us the joint density of the system, not our model:

$$P(\mathbf{x}, \mathbf{p}) = \frac{1}{Z} \exp(-U(\mathbf{x})) \exp(-K(\mathbf{p}))$$
 (3)

It should be noted, that it is not always the case that Hamiltonian is separable, for example see Riemannian HMC (Girolami and Calderhead, 2011). As this expression is exponentiated and there are no implicit dependencies between the parameters, we can marginalize out the distribution of axillary momentum, leaving us with just the target distribution, the joint,  $P(\mathbf{x}) = \exp(-U(\mathbf{x}))$ , from which can take the ln to get:

$$U(\mathbf{x}) = -\ln P(\mathbf{x}) \tag{4}$$

and so the potential is entirely dependent on the choice of the joint distribution. However, the expression  $P(\mathbf{x})$  factorizes further via the product rule, into the product of a prior  $p(\mathbf{x})$  for the parameters of interest and a likelihood  $p(\mathbf{x}|\mathbf{y})$  given the observations  $\mathbf{y}$ :

$$U(\mathbf{x}) = -\log[p(\mathbf{x})p(\mathbf{x}|\mathbf{y})] \tag{5}$$

### 3.1 The Integrator

In order to implement HMC correctly we require an integrator that will enable us to solve the Hamilton's equations, equations 1 - 2. For an integrator to do this it must be both time reversible and volume preserving, as the flow of the phase space is fixed. The time reversibility is due to the fact that no physical system should have a preferred direction of time, if

 $<sup>^1{\</sup>rm The}~\dot{x}$  represents that the variable is being differentiated with respect to time.

<sup>&</sup>lt;sup>2</sup>This is actually the partition function, which to those familiar with neural nets, will know this as the *softmax* function.

I start at my initial conditions, I should eventually arrive back at those initial conditions. In order to ensure that our integrator is volume preserving, we require our integrator to be symplectic. This means that given a transformation  $\mathbf{Q} \in Sp(2d, \mathbb{R})$  such that  $\mathbf{Q}(\mathbf{p}_0, \mathbf{x}_0) \mapsto (\mathbf{x}, \mathbf{p})$ , which maps an initial state to some evolved state, in order for that transformation to preserve Hamilton's equations it must be canonical. But, this can be only true if given some matrix  $J = \begin{pmatrix} \mathbf{0} & \mathbb{I} \\ -\mathbb{I} & \mathbf{0} \end{pmatrix}$  the relation  $\mathbf{Q}^T J \mathbf{Q} = J$  is satisfied, which can only be done if  $\mathbf{Q}$  is symplectic. This can be proved as follows. If we have a transformation  $R = R(\mathbf{x})$ , then  $\dot{R} = \mathbf{Q}^T J \mathbf{Q} \frac{\partial H}{\partial \mathbf{Q}} = J \frac{\partial H}{\partial \mathbf{Q}}^3$ , which is true if and only if  $\mathbf{Q}^T J \mathbf{Q} = J$  and thus the transformation is sympletic.

A popular choice within the HMC literature is the Leapfrog method, equations 6-8. Not only does it satisfy the physical constraints of the model, but it has very small local  $\mathcal{O}(\epsilon^2)$  and global errors  $\mathcal{O}(\epsilon^3)$  with fast convergence (Neal et al., 2011). We shall be using the Leapfrog integrator throughout our current work, however, this to can take alternative forms, see for example (Girolami and Calderhead, 2011) (Nishimura et al., 2017) and (Blanes and Iserles, 2012). The Leapfrog method enables us to generate new proposals given some initial state, that is, if start with a state at t=0and then evaluate at a subsequent time  $t+\epsilon, \ldots, t+N\epsilon$ , where  $\epsilon$  is the step in which we increase and N is the number of time steps, we will generate a new state  $(\mathbf{x}(t+N\epsilon),\mathbf{p}(t+N\epsilon))$  which will act as our new proposal.

$$\mathbf{p}(t + \frac{\epsilon}{2}) = \mathbf{p}(t) - \left(\frac{\epsilon}{2}\right) \nabla_{\mathbf{x}} U(\mathbf{x}(t)) \tag{6}$$

$$\mathbf{x}(t+\epsilon) = \mathbf{x}(t) + \epsilon \nabla_{\mathbf{p}} K(\mathbf{p}(t+\frac{\epsilon}{2}))$$
 (7)

$$\mathbf{p}(t+\epsilon) = \mathbf{p}(t+\frac{\epsilon}{2}) - \left(\frac{\epsilon}{2}\right) \nabla_{\mathbf{x}} U(\mathbf{x}(t+\epsilon))$$
 (8)

### 3.2 The Algorithm

Before we provide the algorithm we shall briefly discuss how the second stage of HMC works, that is the Metropolis step. Starting with the current state  $(\mathbf{x}, \mathbf{p})$ , Hamiltonian dynamics is simulated for L steps using the Leapfrog integrator, with a step size of  $\epsilon$ . After, L steps we generate a new proposed state and in order to decide whether we should accept or reject this

proposal (Duane et al., 1987) introduced the following:

$$\min[1, \exp(-H(\mathbf{x}^*, \mathbf{p}^*) + H(\mathbf{x}, \mathbf{p})] = \min[1, \exp(-U(\mathbf{x}^*) + U(\mathbf{x}) - K(\mathbf{p}^*) + K(\mathbf{p}))] \quad (9)$$

where  $(\mathbf{x}^*, \mathbf{p}^*)$  is the proposed state and  $(\mathbf{x}, \mathbf{p})$  is the current state. The authors issue a note of caution, as the potential is the negative of the joint, we have the above. However, many implementations of HMC do not take this into account and so the proposal is in some instances defined as above, but the potential is defined to be the positive of the joint. In our implementation, when the Hamiltonians are being computed we are dealing with the negative of the joint, but during the leapfrog step we are dealing with the positive of the joint, hence the sign changes in algorithm 1. If the proposed state is rejected, then the next state

## Algorithm 1 Continuous Hamiltonian Monte Carlo MCMC

```
1: procedure HMC(x_0, \epsilon, L,U, M)
                 for m = 1 to M do
  2:
                        p^0 \sim \mathcal{N}(0, 1)
  3:
                        (\mathbf{x}_0, \mathbf{p}_0) \leftarrow (\mathbf{x}^{(t)}, \mathbf{p}^{(t)})
  4:
                        \mathbf{p}_0 \leftarrow \mathbf{p}_0 + \frac{\epsilon}{2} \nabla_{\mathbf{x}} U(\mathbf{x}_0)
  5:
                        for i = 1 to L do
  6:
  7:
                                (\hat{\mathbf{x}}, \hat{\mathbf{p}}) \leftarrow \text{Leapfrog}(\mathbf{x}_0, \mathbf{p}_0, \epsilon)
  8:
                        end for
  9:
                        \mathbf{p}_L \leftarrow \mathbf{p}_L - \frac{\epsilon}{2} \nabla_{\mathbf{x}} U(\mathbf{x}_L)
                        \alpha = \min \left\{ 1, \exp \left\{ H(\mathbf{x}^{(t)}, \mathbf{p}^{(t)}) - H(\hat{\mathbf{x}}, \hat{\mathbf{p}}) \right\} \right\}
10:
                        u \sim Uniform(0,1)
11:
12:
                        if u < \alpha then
                                \mathbf{return}\ \mathbf{x}^{(t+1)} \leftarrow \hat{\mathbf{x}}
                                                                                                      ▶ Accept
13:
                        else
14:
                                \mathbf{return}\ \mathbf{x}^{(t+1)} \leftarrow \mathbf{x}^t
                                                                                                        ▶ Reject
15:
                        end if
16:
17:
                 end for
                 Leapfrog(\mathbf{x}, \mathbf{p}, \epsilon)
18:
                 \mathbf{x}_i \leftarrow \mathbf{x}_i + \epsilon \nabla_{\mathbf{p}} K(\mathbf{p}_i)
19:
                \mathbf{p}_i \leftarrow \mathbf{p}_{i-1} + \frac{\epsilon}{2} \nabla_{\mathbf{x}} U(\mathbf{x}_{i-1})
20:
                 return x , p
21:
22: end procedure
```

is the same as the current state and is counted again when calculating the expected value of some function. The negation of the momentum variables at the end of the trajectory makes the Metropolis proposal symmetrical, as needed for the acceptance probability above to be valid. This negation need not be done in practice, since K(p) = K(-p) for the Gaussian momentum, and the momentum will be replaced before it is used again in the first step of the next iteration. A function that implements a single iteration of the HMC algorithm is given in algorithm 1. There are three additional functions within this iteration: U, which returns the

<sup>&</sup>lt;sup>3</sup>We can write  $\mathbf{z} = (\mathbf{x}, \mathbf{p})$  and taking the vectorized form of equations 1 - 2, in terms of Laplacians, we can succinctly write Hamilton's equations as  $\dot{\mathbf{z}} = J\nabla_{\mathbf{z}}H(\mathbf{z})$ .

potential energy given a value for x,  $\nabla U$ , which returns the vector of partial derivatives of U given x and  $\nabla K$ , which returns the vector of partial derivatives of K given p. Other arguments are the stepsize,  $\epsilon$ , the number of Leapfrog steps to perform in each trajectory, L. It should be noted, that L and  $\epsilon$  are parameters that need to be tuned. Likewise, if the form of the kinetic is taken to be the log of a Gaussian, M becomes another parameter that needs to be tuned. Although, one could use Riemannian HMC (Girolami and Calderhead, 2011) to generate a mass matrix on the fly, which is based on the properties of the model that you are sampling from.

# 4 Example Programs and Experiments

### 4.1 Programs

We now present a few simple FOPPL programs and discuss both their statistical forms and the results generated via HMC inference. In all the graphical model plots, shaded circles represent observed parameters, un-shaded circles represent the latent variables, our parameters of interest and diamonds represent a deterministic statement. To generate our graphical plots, all models were run for 1000 iterations, with no burn in.

### 4.1.1 Conjugate Gaussian

The conjugate Gaussian is a model in which we can analytically calculate the true posterior  $p(x|y) \propto p(x,y)$ , as the product of two Gaussians is also a Gaussian. For our particular model we sample  $x \sim \mathcal{N}(0,1)$  and we observe y=7, with likelihood  $p(y|x)=\mathcal{N}(y|x,1)$  and we aim to infer the mean of the posterior. In FOPPL we have the following program:

```
;;; conjugate_gaussian
(def src0
  (foppl-query
    (let [x (sample (normal 0.0 1.0))]
        (observe (normal x 1.0) 7.0)
        x)))
```

This model has the following joint  $p(x,y) \propto p(x|y) = p(x)p(y|x) = \mathcal{N}(\bar{\mu},\bar{\sigma}^2)$ , where  $\bar{\mu} = \left(\frac{\mu_0\sigma^2 + \sigma_0^2\sum_{i=1}^ny_i}{\sigma^2\sigma_0^2}\right)\bar{\sigma}^2$  and  $\bar{\sigma}^2 = \left(\frac{1}{\sigma_0^2} + \frac{n}{\sigma^2}\right)^{-1}$ . Where in this model n is the total number of observed datum  $y, \mu_0 = 0$  and  $\sigma_0^2 = 1$  are the prior mean and variance and  $\sigma^2 = 1.0$  is the likelihood variance. Thus, the true mean that our model should infer is  $\bar{\mu} = 5$ . This is indeed the value that we get as can be seen via figures 4a-4c.



Figure 1: The FOPPL code for the conditional Gaussian

### 4.1.2 Conditional If

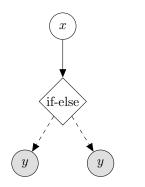


Figure 2: Conditional if graphical model

The if statement is typically challenging to implement for gradient based methods, due to the branching effects that occur at the condition. For trace based samplers, such as importance sampling, this is not a problem as multiple traces are recorded for each path taken. However, in higher dimensions these types of samplers are heavily impaired, which is why we need additional MCMC methods. In this model, we have a joint distribution of the form  $p(x,y) \propto p(x|y) = \mathcal{N}(0,1)\mathcal{N}(y=0)$  $1|1,1)^{\mathbb{I}(x>0)}\mathcal{N}(y=1|-1,1)^{\mathbb{I}(x<0)}, \text{ where } \mathbb{I}(\cdot) \text{ repre-}$ sents the indicator function. The empirical mean that we generate for this model is 0.58 and if you plot the unnormalized joint, the shape is the same, but the density values are different, see figures 4d-4f. This implies that we can be confident in the results generated by the HMC.

### 4.1.3 Linear Regression

```
;;; linear regression
(def lr-src
```

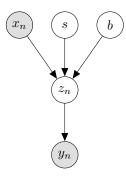


Figure 3: Linear regression model as a graph.

In this problem we have a set of points (x,y) and we wish to infer equation of a line in a Bayesian manner, that goes through all of those points. To do this, we must infer the slope and the bias of the line, which is done by placing priors on our parameters of interest and observations. In this model for both the slope and bias, we sample from  $\mathcal{N}(0, 10.0)$  and we state that likelihood of the model is of the form of a conditional Gaussian  $\mathcal{N}(y_n|z_n, 1.0)$ with a mean dependent on our sampled line. Therefore, we can construct the joint for this model as follows:  $p(x_n, s, b, z_n, y_n) \propto p(s, b, z_n | x_n, y_n) =$  $p(s)p(b)p(y|z_n,1) = \mathcal{N}(0,5^2)\mathcal{N}(y_n|z_n,1.0)$ . We can analytically calculate the equation of a straight line by using the formula  $\left(\frac{y-y_*}{x-x_*}\right)=m$ , which leads to y=mx+b. From this we find that the true slope m = 1.6 and the bias b = 0.5. We again see from figures 4g-4i, that the HMC correctly calculates the true values of the parameters.

### 4.2 Experimental Results

### 5 Discussion

### 6 Supplementary Material

In the supplementary material we show some examples of the compiler output for the linear regression and conjugate Gaussian models. We also discuss the implementation of the HMC algorithm itself in pytorch and state how we have intertwined both the inference and FOPPL. As the FOPPL program produces an actual directed graph as output, like the ones seen in section 4, we must take that structure and map the edges, vertices and nodes accordingly into the right model output. This means that we must take care to ensure that the structure of language specific statements such as observe, sample, let, defn, if and language grammar such as variable, constant, procedure.

c24039= Variable(torch.Tensor([1.0]))

```
c24040= Variable(torch.Tensor([2.0]))
x24041 = Normal(c24039, c24040)
x22542 = Variable(torch.Tensor([0.0]),\
  requires_grad = True)
# x22542.detach()
\# x22542 = x24041.sample()
                              #sample
p24042 = x24041.logpdf(x22542)
c24043= Variable(torch.Tensor([3.0]))
x24044 = Normal(x22542, c24043)
c24045= Variable(torch.Tensor([7.0]))
y22543 = c24045
p24046 = x24044.logpdf(y22543)
p24047 = Variable.add(p24042, p24046)
return p24047, x22542
# FOPPL compiler output
c23582= torch.Tensor([0.0])
c23583= torch.Tensor([10.0])
x23584 = Normal(c23582, c23583)
#sample
x23474 =
          x23584.sample()
#prior
p23585 = x23584.logpdf(x23474)
c23586= torch.Tensor([0.0])
c23587= torch.Tensor([10.0])
x23588 = Normal(c23586, c23587)
#sample
x23471 = x23588.sample()
#prior
p23589 = x23588.logpdf(x23471)
c23590= torch.Tensor([1.0])
x23591 = torch.mul(x23471.data, c23590)
x23592 = torch.add(x23591,x23474.data)
```

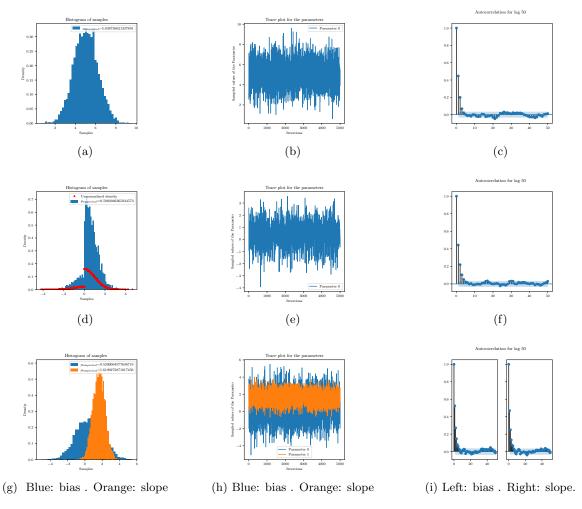


Figure 4: Each row corresponds to the inference output of each model and provides a histogram of the samples, the trace of the samples for each parameter of interest in the model and the autocorrelation between the samples for a lag l = 50. The top row represents the conjugate Gaussian model, the middle row represents the conditional if model and the bottom row represents the linear regression model with parameter 0, in blue, representing the bias and parameter 1, in orange, represents the slope of the line.

```
c23593= torch.Tensor([1.0])
                                                 c23604= torch.Tensor([3.0])
x23594 = Normal(x23592, c23593)
                                                 x23605 = torch.mul(x23471, c23604)
#obs, log likelihood
                                                 x23606 = torch.add(x23605, x23474)
c23595= torch.Tensor([2.1])
                                                 c23607= torch.Tensor([1.0])
y23481 = c23595
                                                 x23608 = Normal(x23606, c23607)
p23596 = x23594.logpdf(y23481)
                                                 #obs, log likelihood
                                                 c23609= torch.Tensor([5.3])
c23597= torch.Tensor([2.0])
                                                 v23527 = c23609
x23598 = torch.mul(x23471, c23597)
                                                 p23610 = x23608.log_pdf(y23527)
x23599 = torch.add(x23598, x23474)
                                                 p23611 = torch.add([p23585,p23589,/
                                                                 p23596,p23603,p23610])
c23600= torch.Tensor([1.0])
x23601 = Normal(x23599, c23600)
                                                 # return E from the model
#obs, log likelihood
                                                 x23612 = [x23471, x23474]
c23602= torch.Tensor([3.9])
y23502 = c23602
                                                 return p23611, x23612
p23603 = x23601.logpdf(y23502)
```

```
import torch
import numpy as np
                                                       return samples_reduced, samples, mean
import importlib
from torch.autograd import Variable
                                                   c24039= Variable(torch.Tensor([1.0]))
from Utils.kinetic import Kinetic
                                                   c24040= Variable(torch.Tensor([2.0]))
from Utils.integrator import Integrator
                                                   x24041 = Normal(c24039, c24040)
from Utils.metropolis_step import Metropolis
                                                   x22542 = Variable(torch.Tensor([0.0]),\
                                                     requires_grad = True)
class HMCsampler():
                                                   # x22542.detach()
                                                   \# x22542 = x24041.sample()
                                                                                  #sample
  def __init__(self, burn_in= 100, \
                                                   p24042 = x24041.logpdf(x22542)
        n_samples= 1000, model = 'conjgauss',\
                                                   c24043= Variable(torch.Tensor([3.0]))
        M= None, min_step= None,\
                                                   x24044 = Normal(x22542, c24043)
        max_step= None, min_traj= None,\
                                                   c24045= Variable(torch.Tensor([7.0]))
        max_traj= None):
                                                   y22543 = c24045
    self.burn_in
                     = burn_in
                                                   p24046 = x24044.logpdf(y22543)
    self.n_samples = n_samples
                                                   p24047 = Variable.add(p24042, p24046)
    self.M
                     = M
    self.model
                     = model
                                                   return p24047, x22542
    # External dependencies
    program
                                                   Acknowledgements
    getattr(importlib.\
                                                   Use unnumbered third level headings for the acknowl-
     import_module('Utils.program'), model)
                                                   edgements. All acknowledgements go at the end of the
    self.potential = program()
                                                   paper.
    self.integrator= Integrator(\
            self.potential,min_step,\
             max_step, min_traj, max_traj)
                                                   References
                                                   Andrieu, C., De Freitas, N., Doucet, A., and Jordan,
                                                     M. I. (2003). An introduction to mcmc for machine
  def run_sampler(self):
                                                     learning. Machine learning.
    print(' The sampler is now running')
                                                   Berg, B. A. and Billoire, A. (2008). Markov chain
    logjoint_init, values_init, grad_init,\
                                                     monte carlo simulations. Wiley Online Library.
     dim = self.potential.generate()
    metropolis = Metropolis(\
                                                   Blanes, S. and Iserles, A. (2012). Explicit adaptive
     self.potential,self.integrator, self.M)
                                                     symplectic integrators for solving hamiltonian sys-
                                                     tems. Celestial Mechanics and Dynamical Astron-
    temp,count = metropolis.acceptance(\
     values_init,logjoint_init, grad_init)
                                                     omy.
    samples = \
                                                   Duane, S., Kennedy, A. D., Pendleton, B. J., and
     Variable(torch.zeros(self.n_samples,dim))
                                                     Roweth, D. (1987). Hybrid monte carlo. Physics
    samples[0] = temp.data.t()
                                                     letters B.
                                                   Girolami, M. and Calderhead, B. (2011). Riemann
                                                     manifold langevin and hamiltonian monte carlo
    # Then run for loop from 2:n_samples
                                                     methods. Journal of the Royal Statistical Society:
    for i in range(self.n_samples-1):
                                                     Series B (Statistical Methodology).
      logjoint_init, grad_init = \
      self.potential.eval(temp,grad_loop= True) Hastings, W. K. (1970). Monte carlo sampling meth-
                                                    ods using markov chains and their applications.
      temp, count = metropolis.acceptance(temp,\)
                                                     Biometrika.
       logjoint_init,grad_init)
      samples[i + 1, :] = temp.data.t()
                                                   Neal, R. M. et al. (2011). Mcmc using hamiltonian
                                                     dynamics. Handbook of Markov Chain Monte Carlo.
    # Basic summary statistics
    target_acceptance = count / (self.n_samples) Nishimura, A., Dunson, D., and Lu, J. (2017). Discon-
                                                     tinuous hamiltonian monte carlo for sampling dis-
    samples_reduced = samples[self.burn_in:, :]
                                                     crete parameters. arXiv preprint arXiv:1705.08510.
    mean = torch.mean(samples_reduced,dim=0,\)
```

keepdim= True)

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package. https://github.com/pytorch/pytorch.

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