Faster Hamiltonian Monte Carlo by Learning Leapfrog Scale

Changye Wu
Université Paris Dauphine, PSL Research University

Julien Stoehr
Université Paris Dauphine, PSL Research University

Christian P. Robert
Université Paris Dauphine, PSL Research University &
Department of Statistics, University of Warwick

Abstract

Hamiltonian Monte Carlo samplers have become standard algorithms for MCMC implementations, as opposed to more basic versions, but they still require some amount of tuning and calibration. Exploiting the U-turn criterion of the NUTS algorithm (Hoffman and Gelman, 2014), we propose a version of HMC that relies on the distribution of the integration time of the associated leapfrog integrator. Using in addition the primal-dual averaging method for tuning the step size of the integrator, we achieve an essentially calibration free version of HMC. When compared with the original NUTS on several benchmarks, this algorithm exhibits a significantly improved efficiency.

1 Introduction

Hamiltonian Monte Carlo (HMC, Duane et al., 1987; Neal et al., 2011) has emerged as an efficient Markov Chain Monte Carlo (MCMC) sampling method, which, in particular, is able to deal with high-dimensional target distribution. The method relies on a deterministic differential flow stemming from Hamiltonian mechanics to produce transitions across the parameter space of an augmented distribution, referred to as Hamiltonian. Such time-continuous dynamics leave the augmented distribution invariant but in practice the latter need to be discretised. The transitions are hence computed using a gradient-based symplectic integrator — the most popular one being the second order Störmer-Verlet or leapfrog integrator — and a Metropolis-Hastings acceptance ratio need to be added towards correcting the approximate numerical solution and hence preserving the proper target measure.

Whilst the algorithm theoretically benefits from a fast exploration of the parameter space by accepting large transitions with high probability, this is marred by its high sensitivity to hand-tuned parameters, namely the step size $\epsilon$ of the discretisation scheme, the number of steps $L$ of the integrator, and the covariance matrix of the auxiliary variables. Indeed, the discretisation error due
to a poorly tuned step size will lead to a low acceptance rate. Furthermore calibrating the number of steps of the integrator is paramount to avoid slow mixing chains or to save some computation cost. In other words, if $L$ is not large enough, HMC exhibits a random walk behaviour similar to standard Metropolis Hastings algorithms and may thus struggle to properly explore the support of the target. If $L$ is too large the associated dynamic retraces its steps back to a neighbourhood of the initial state (Betancourt et al., 2014) wasting computation efforts and diminishing mixing. Finally the choice of a well-suited covariance matrix for the auxiliary variable can enhance both the speed and the mixing of HMC.

Recent developments have addressed this tuning issue: the automatic tuning strategy of Wang et al. (2013), the Riemann manifold approach of Girolami and Calderhead (2011) that adapts the covariance matrix of the auxiliary variables to the curvature of the target distribution, just to name a few although these versions are not of direct interest. Among those, the No-U-Turn Sampler (NUTS, Hoffman and Gelman, 2014) is arguably the most popular, in particular because it automatically tunes both the step size and the number of leapfrogs. The algorithm is just as efficient, if not better than standard HMC, albeit this comes at an extra cost that may prove burdensome. The core idea behind NUTS is to pick the step size via primal-dual averaging (Nesterov, 2009) in a burn-in phase and to build at each iteration a proposal based on a locally longest path on a level set of the Hamiltonian. This is achieved by a recursive algorithm that, at each call to the leapfrog integrator, requires to evaluate both the gradient of the target distribution and the Hamiltonian itself. Roughly speaking an iteration of NUTS costs twice as much as HMC with the same number of calls to the integrator.

In this paper, we aim at reducing this extra cost and explore the opportunity to learn an empirical distribution of the longest leapfrog path — consistent with the target distribution — by exploiting the U-turn criterion of NUTS for the level set visited during a burn-in phase. The latter is then used to randomly pick $L$ at each iteration of an HMC scheme.

The paper begins with a brief description of HMC and NUTS in Section 2. We then introduce the learning strategy of the empirical distribution in Section 3. We illustrate the efficiency of the proposed algorithm compared to the original NUTS on several benchmarks in Section 4, and conclude in Section 5.

All examples in the paper can be reproduced using R and Rstan\(^1\) (Stan Development Team, 2018).

## 2 Hamiltonian Monte Carlo

Consider a probability measure $\pi$ on $\Theta \subset \mathbb{R}^d$ with density, also denoted $\pi$, with respect to the Lebesgue measure, $\pi(\theta) \propto \exp\{-U(\theta)\}$, where $U$ is a continuously differentiable function called the potential function. HMC allows to sample from $\pi$ by augmenting the target distribution with an auxiliary variable $v \in \mathbb{R}^d$, referred to as momentum variable (as opposed to $\theta$ called the position), distributed according to a $d$-dimensional Normal distribution, $\mathcal{N}(\cdot \mid 0, M)$, that is HMC samples from $\pi(\theta, v) = \pi(\theta)\mathcal{N}(v \mid 0, M)$, which marginal chain in $\theta$ is the distribution of interest. We refer the reader to Betancourt (2017) for a discussion about other momentum distributions and Girolami

\(^1\) https://github.com/wcythh/eHMC
Algorithm 1: Hamiltonian Monte Carlo

**Input:** Starting point $\theta_0$, step size $\epsilon$, number of leapfrog steps $L$, covariance matrix $M$, number of iterations $N$.

**Output:** sample $\{\theta_0, \ldots, \theta_N\}$ drawn from $\pi(\theta)$

for $n \leftarrow 1$ to $N$ do

| draw $v$ from $N(\cdot \mid 0, M)$
| compute $(\theta^*, v^*) = \text{Leapfrog}(\theta_{n-1}, v, \epsilon, L)$ compute

| $\rho = 1 \wedge \exp\{H(\theta_{n-1}, v) - H(\theta^*, -v^*)\}$
| set

| $(\theta_n, v_n) = \begin{cases} (\theta^*, -v^*), & \text{with probability } \rho \\ (\theta_{n-1}, v), & \text{otherwise.} \end{cases}$

end

return $(\theta_0, \ldots, \theta_N)$

**Function Leapfrog($\theta$, $v$, $\epsilon$, $L$)**

| compute $(\theta_0, v_0) = (\theta, v - \epsilon/2\nabla U(\theta))$
| for $\ell \leftarrow 1$ to $L$ do

| | compute $\theta_\ell = \theta_{\ell-1} + \epsilon M^{-1} v_{\ell-1}$
| | if $\ell < L$ then

| | | compute $v_\ell = v_{\ell-1} - \epsilon \nabla U(\theta_\ell)$
| end
| end

$v_L = v_{L-1} - \epsilon/2\nabla U(\theta_L)$

return $(\theta_L, v_L)$

and Calderhead (2011) for a $\theta$-dependent momentum distribution based on Riemann manifolds. Define the Hamiltonian as the unnormalised negative joint log-density

$$H(\theta, v) = U(\theta) + \frac{1}{2} v^T M^{-1} v.$$ 

HMC generates proposals for $\theta$ based on the Hamiltonian dynamics which write with respect to a fictitious time $t$

$$\frac{\partial H}{\partial v} = \frac{d\theta}{dt} = M^{-1} v \quad \text{and} \quad \frac{\partial H}{\partial \theta} = \frac{dv}{dt} = -\nabla U(\theta).$$ (1)

Such a mechanism aims at efficiently exploring the parameter space $\Theta \times \mathbb{R}^d$ as compared to standard random-walk Metropolis-Hastings proposals while preserving the measure $\pi(d\theta, dv)$ — the solution flow being reversible. In practice, the above differential equations cannot be solved analytically and HMC samplers resort to symplectic numerical integrators. The leapfrog integrator is commonly used for its trade-off between second order accuracy and computational cost. Given a discretisation time-step $\epsilon$, it yields a map $F_\epsilon : (\theta, v) \mapsto (\theta^*, v^*)$ defined by

$$\begin{cases} 
\theta^* = \theta + \epsilon M^{-1} r, \\
v^* = r - \epsilon/2\nabla U(\theta^*),
\end{cases} \quad \text{where} \quad r = v - \epsilon/2\nabla U(\theta).$$
It corresponds to a three stage procedure that alternatively updates \(v\) and \(\theta\) to approximate the solution at time \(\epsilon\), and to approximate solution at a time \(t\), one repeats the procedure \(L = \lceil t/\epsilon \rceil\) times. \(L\) is referred to as number of leapfrog steps. This discrete scheme does no longer leave the measure \(\pi(d\theta, dv)\) invariant. To account for the discretisation bias and preserve the targetted measure, an accept-reject step is introduced (see Algorithm 1). A transition from \((\theta, v)\) to a proposal \((\theta^*, -v^*)\) corresponding to the approximated solution for an integration time \(L\epsilon\) is accepted with probability

\[
\rho(\theta, v, \theta^*, v^*) = 1 \wedge \exp\{H(\theta, v) - H(\theta^*, -v^*)\}.
\] (2)

which implies that detailed balance is satisfied for the target \(\pi(d\theta, dv)\). The solution of (1) keeps the Hamiltonian constant, meaning the proposals are always accepted for the exact dynamic. After discretisation, the deviation to \(H(\theta, v)\) can be bounded (Leimkuhler and Reich, 2004),

\[
|H(\theta, v) - H(\theta^*, -v^*)| < C\epsilon^2.
\]

Hence, the acceptance rate in Algorithm 1 still tends to be high even for a proposal \((\theta^*, -v^*)\) quite far from \((\theta, v)\).

### 2.1 NUTS

In this section, we briefly introduce the NUTS algorithm, referring the reader to Hoffman and Gelman (2014) for more details.

The so-called no-U-Turn sampler (NUTS) is a version of HMC sampler that eliminates the need to specify the number \(L\) of HMC steps by adaptively choosing the locally largest value at each iteration of the algorithm. More precisely, given a leapfrog scale \(\epsilon\) and a current value \((\theta, v)\), NUTS first resamples the HMC momentum \(v\) from a Gaussian distribution \(N(0, M)\). Next, NUTS proceeds by doubling the leapfrog path, either forward or backward with equal probability, until the path begins to retrace towards the starting point. This means that the backward and forward end points of the path, \((\theta^-, v^-)\) and \((\theta^+, v^+)\), satisfy

\[
(\theta^+ - \theta^-) \cdot v^- < 0 \quad \text{or} \quad (\theta^+ - \theta^-) \cdot v^+ < 0.
\] (3)

Given the collection \(B\) of visited position-momentum pairs along the path, the final step of NUTS consists in selecting one point in \(B\) by a slice sampling move. This means generating a Uniform \(U(0, 1)\) and sampling uniformly in \(B\) one of the points being able to regenerate \(B\) and with Hamiltonian larger than \(\log(u) - H(\theta, v)\). This allows for detailed balance to hold and thus validates the NUTS algorithm.

In addition, the step size \(\epsilon\) in NUTS is tuned via the primal-dual averaging (Nesterov, 2009), by aiming at a targeted acceptance probability \(\delta_0 \in (0, 1)\).

Compared with the standard HMC sampler, which relies on a fixed length \(L\) across iterations, NUTS choose \(L\) adaptively at each iteration while it requires an evaluation of the Hamiltonian along its entire leapfrog path. This obviously doubles the computation cost, when evaluating \(U\) and its gradient require the same computation effort.

Even though the leapfrog path of NUTS is locally the longest possible in terms of Equation (3),
we note that the starting position-momentum pair is almost never one of the two endpoints of the generated leapfrog path. Therefore the distance between the position of the proposed value and the current one is smaller than it could be, which induces a waste of computation time.

3 Learning leapfrog scale

In this section, we explore the opportunity to use a U-turn condition similar to Equation (3) for choosing \( L \) in the HMC sampler based on the empirical distribution of the longest integration times. Regarding the step size \( \epsilon \), we also adopt the primal-dual averaging method implemented to NUTS.

3.1 Empirical distribution of leapfrog scale

Given a step size \( \epsilon \) and a starting point \((\theta, v)\), denote \((\theta_{\ell}, v_{\ell}) = \text{Leapfrog}(\theta, v, \epsilon, \ell)\), the value of the pair after \( \ell \) iterations of the leapfrog integrator, \( \ell \in \mathbb{N} \). We define the longest batch \( L_\epsilon(\theta, v) \) associated with \((\theta, v, \epsilon)\) as the first \( \ell \in \mathbb{N} \) such that \((\theta_{\ell} - \theta) \cdot v_{\ell} < 0\), referred to as U-turn condition in what follows. We can get an empirical distribution of the longest batches by running \( K \) iterations of HMC with the optimised step size and an initial number of leapfrog steps \( L_0 \) (see Algorithm 2). Specifically, each iteration of HMC is ran for \( L_0 \) leapfrog steps to generate the next state of the Markov chain. At the same time, we compute the longest batch for the current state of the chain, that is if \( L_\epsilon(\theta, v) \leq L_0 \) we store it on the go throughout the \( L_0 \) first steps, otherwise we keep simulating the dynamics till reaching the U-turn condition. Such an algorithm produces a sequence of longest batches

\[
\mathcal{L} = \{ L_\epsilon\left(\theta_0, v^{(1)}\right), \ldots, L_\epsilon\left(\theta_{K-1}, v^{(K)}\right) \}
\]

whose empirical measure is

\[
\hat{P}_\mathcal{L} = \frac{1}{K} \sum_{k=0}^{K-1} \delta_{L_\epsilon(\theta_k, v^{(k+1)})},
\]

where \( \delta_{L_\epsilon(\theta_k, v^{(k+1)})} \) denotes the Dirac measure at \( L_\epsilon(\theta_k, v^{(k+1)}) \), \( k = 0, \ldots, K - 1 \).

3.2 Convergence Analysis

Let \( Q_\epsilon(\cdot | \theta, v) \) be the distribution of the longest batch conditionally on the current state \((\theta, v)\) with step size \( \epsilon \) and \( Q_\epsilon \) its marginal distribution with respect to the augmented target \( \pi(d\theta, dv) \). The transition kernel of the HMC sampler can be written as the composition of two Markov kernels \( P_1 \) and \( P_2 \) over \( \Theta \times \mathbb{R}^d \):

\[
\begin{align*}
P_1((\theta, v), (d\theta, dv)) &= \delta_{\theta}(d\theta) \mathcal{N}(dv \mid 0, M) \\
P_2((\theta, v), (d\theta, dv)) &= \rho \delta_{(\theta^*, v^*)}(d\theta, dv) + (1 - \rho) \delta_{(\theta, v)}(d\theta, dv),
\end{align*}
\]

where \((\theta^*, v^*) = \text{Leapfrog}(\theta, v, \epsilon, L)\) and \( \rho \) is defined by Equation (2). Both kernels are reversible with respect to the augmented target \( \pi(d\theta, dv) \) and hence the composition \( P_2 \circ P_1 \) leaves the latter invariant. As a consequence, \( \hat{P}_\mathcal{L} \) produced by Algorithm 2 converges to \( Q_\epsilon \).
Algorithm 2: Longest batches empirical distribution

Input: Starting point \( \theta_0 \), step size \( \epsilon \), number of leapfrog steps \( L_0 \), covariance matrix \( M \), number of iterations \( K \).

Output: sequence \( \mathcal{L} = (\mathcal{L}_1, \ldots, \mathcal{L}_K) \) of longest batches

for \( k \leftarrow 1 \) to \( K \) do
  draw \( v^{(k)} \) from \( \mathcal{N}(\cdot | 0, M) \)
  /* Computing \( \mathcal{L}_k = L_k(\theta_{k-1}, v^{(k)}) \) */
  compute \( (\theta^*, v^*, \mathcal{L}_k) = \text{LongestBatch}(\theta_{k-1}, v^{(k)}, \epsilon, L_0) \)
  if \( \mathcal{L}_k < L_0 \) then
    compute \( (\theta^*, v^*) = \text{Leapfrog}(\theta^*, v^*, \epsilon, L_0 - \mathcal{L}_k) \)
  end
  compute \( \rho = 1 \wedge \exp \left\{ H(\theta_{k-1}, v^{(k)}) - H(\theta^*, -v^*) \right\} \)
  set \( (\theta_k, v_k) = \begin{cases} 
    (\theta^*, -v^*), \text{ with probability } \rho \\
    (\theta_{k-1}, v^{(k)}), \text{ otherwise.}
  \end{cases} \)
end
return \( (\mathcal{L}_1, \ldots, \mathcal{L}_K) \)

Function LongestBatch(\( \theta, v, \epsilon, L \))

set \( \ell = 0 \); \( (\theta^+, v^+) = (\theta, v) \); \( (\theta^*, v^*) = (\theta, v) \)
while \( (\theta^+ - \theta) \cdot v^+ \geq 0 \) do
  set \( \ell = \ell + 1 \)
  compute \( (\theta^+, v^+) = \text{Leapfrog}(\theta^+, v^+, \epsilon, 1) \)
  if \( \ell == L \) then
    set \( (\theta^*, v^*) = (\theta^+, v^+) \)
  end
end
return \( (\theta^*, v^*, \ell) \)

3.3 Empirical Hamiltonian Monte Carlo

We introduce a version of HMC, called empirical HMC (eHMC) that makes use of the empirical distribution \( \hat{P}_L \) constructed in Algorithm 2.

NUTS derives at each iteration a locally adapted scale for \( L \) used in a manner compatible with the stationary distribution. Indeed, running the longest batch at each iteration, albeit interesting in increasing the jumping distance between the current and the proposed states, creates a bias in the resulting stationary distribution. NUTS hence requires a slice auxiliary variable to keep the reversibility of the Markov chain. Here we propose an orthogonal direction by considering a global distribution on the batch sizes consistent with the target distribution.
Algorithm 3: Empirical Hamiltonian Monte Carlo (eHMC)

**Input:** Starting point $\theta_0$, step size $\epsilon$, covariance matrix $M$, number of iterations $N$, empirical distribution of longest batches $\hat{P}_L$ (generated by Algorithm 2).

**Output:** sample $\{\theta_0, \ldots, \theta_N\}$ drawn from $\pi(\theta)$

for $n \leftarrow 1$ to $N$ do
  draw $v$ from $\mathcal{N}(\cdot | 0, M)$
  draw $L$ from $\hat{P}_L$
  compute $(\theta^*, v^*) = \text{Leapfrog}(\theta_{n-1}, v, \epsilon, L)$
  compute
  \[
  \rho = 1 \wedge \exp\{H(\theta_{n-1}, v) - H(\theta^*, -v^*)\}
  \]
  set
  \[
  (\theta_n, v_n) = \begin{cases} 
  (\theta^*, -v^*), & \text{with probability } \rho \\
  (\theta_{n-1}, v), & \text{otherwise.}
  \end{cases}
  \]
end

return $(\theta_0, \ldots, \theta_N)$

The core idea of eHMC is to randomly pick a number of leapfrog steps according to the empirical distribution $\hat{P}_L$ at each iteration (see Algorithm 3). The advocated algorithm is valid since the choice of $L$ is independent from the current state of the chain. Thus the resulting transition kernel can be seen as a composition of multiple Markov kernels attached to the same stationary distribution $\pi(d\theta, dv)$ (Tierney, 1994).

### 3.4 Two Variants

In this section, we propose two further HMC-based samplers by leveraging $\hat{P}_L$ in two different ways. The first sampler, eHMCq, chooses an upper bound on the number of steps, $L^*$, based on the quantiles of $\hat{P}_L$ and the longest batch size in the HMC sampler is simulated at each iteration as $L \sim \mathcal{U}\{1, \ldots, L^*\}$. In our method, $L^* = \lceil q^{0.95}(L) \rceil$, the 0.95 quantile of $\hat{P}_L$ with $\lceil \cdot \rceil$ is the integer part by excess. The motivation for this version of uniformly distributed steps is that, when compared with standard HMC, a random number of steps helps the resulting HMC sampler to overcome the reducibility problem, which is caused by a (near-)periodicity. Hence randomness is beneficial for the mixing behaviour of the generated Markov chain. The underlying motivation for choosing a 0.95 quantile of $L$ is as follows. On the one hand, $L^*$ should be large enough. Since the number of steps at each iteration is distributed uniformly over $\{1, 2, \ldots, L^*\}$, the expected number of steps integrator is just $(1+L^*)/2$. As a result, we should choose $L^*$ to be something like the 0.95 quantile rather than the mean or the median of $L$. On the other hand, in order to prevent the choice of extremely large $L^*$’s, which will considerably waste computation efforts without meaningful improvement of the HMC sampler, we set $L$ as a quantile of $L$, instead of the maximum of $L$.

Inspired by the same appeal in adopting random steps, the second sampler, called eHMCu, runs the leapfrog integrator $L_n$ times in an HMC sampler for the $n$-th iteration, where $L_n \sim \mathcal{U}\{1, 2, \cdots, L^*_n\}$, $L^*_n \sim P_L$. 
4 Numerical Experiment

This section produces empirical comparisons of the performance of the NUTS and eHMC samplers, evaluated in terms of effective sample size (ESS) over several models with increasing complexity. We recall that the standard effective sample size associated with a Markov chain is defined as

\[ \text{ESS} = \frac{N}{1 + 2 \sum_{k>0} \rho_k}, \]

where \( N \) is the sample size and \( \rho_k \) is the auto-correlation of lag \( k \) of the Markov chain. Informally, the ESS of an MCMC outputs is understood as the equivalent number of independent simulations from the target distribution, where equivalent means with equivalent variance. The following examples resort to the `ess` function of the R package `mcmcse` (Flegal et al., 2016) to produce estimates of the ESS for each component of the parameter. Hence, the more efficient a sampler is in its approximation to \( i.i.d. \) sampling from the target, the higher the associated ESS should be. In order to differentiate between the computing requirements of the compared samplers, it seems fairer to evaluate samples generated under the same computation budget. As a result, the ESS is calibrated by the evaluation cost of the logarithm of target density function and of its gradient. This choice is based on the assumption that the largest portion of the computation budget is dedicated to compute both \( U \) and \( \nabla U \). The evaluations below report the minimum of ESS per evaluation over all components, which identifies the least effective part of the sampler.

Furthermore, considering that the ESS criterion only reflects on the marginal efficiency of a sampler, we report in addition the now traditional expected squared jump distance per evaluation of \( U \) and \( \nabla U \). While depending on the measure of the jump, this quantity appears as a global mixing assessment that measures another aspect of the efficiency of a sampler. We recall that, given a set of generated samples \( \{\theta_1, \ldots, \theta_N\} \), its estimated ESJD is defined as

\[ \text{EJSD} = \frac{1}{N-1} \sum_{n=1}^{N-1} \|\theta_{n+1} - \theta_n\|^2. \]

In each of the following experiments, NUTS is implemented in `Rstan` (Stan Development Team, 2018) and based on 25,000 iterations, with the first 5,000 iterations used to tune the step size \( \epsilon \) for each targeted accept probability \( \delta \) and the last 20,000 iterations used as sample draws. For each tuned \( \epsilon \), we run Algorithm 2 over 2,000 iterations to construct the set \( \mathcal{L} \), which is then exploited by eHMC. Each experiment is repeated 40 times. Besides, in our experiments, the mass matrix, \( M \), is set to the identity, for both NUTS and eHMC sampler.

4.1 Multivariate Normal Distribution

This toy example sets the target as a multivariate Normal distribution with zero mean and covariance matrix \( A \),

\[ \pi(\theta) \propto \exp \left\{ -\theta^T A^{-1} \theta / 2 \right\} \]

The dimension of the vector is chosen to be 100, with

\[ A_{i,j} = 0.99^{|i-j|}, \quad i, j = 1, \ldots, 100 \]
4.1 Numerical Experiment

Fig. 1: Comparison amongst NUTS, eHMC, eHMCq and eHMCu samplers for a multivariate Normal distribution: the x-axis corresponds to the targeted accept probability, $\delta$, associated with the primal-dual averaging step, and the y-axis in the two plots are the minimum of ESS across the parameter coordinates and ESJD per evaluation of $U$ and $\nabla U$ respectively. Each black dot shows the performance for a single experiment and the red curve is the median of the 40 dots’ y-values for a particular $\delta$.

The 15 targeted values for the ideal acceptance probability, $\delta$, in the primal-dual averaging step are spaced evenly between 0.25 and 0.95. Figure 1 displays the minimum ESS across the parameter components and ESJD per evaluation for each sampler. As is clear from the plots, the gain brought by using eHMC and its variants is important on most of the range of $\delta$’s, without ever exhibiting a significant loss of efficiency.

4.2 Bayesian Logistic Posterior

This example takes its target as the posterior distribution of a Bayesian logistic regression under a flat prior $\pi_0(\theta) \propto 1$,

$$\pi(\theta) \propto \prod_{i=1}^{N} \frac{\exp(y_i x_i^T \theta)}{1 + \exp(x_i^T \theta)}$$

The inference is based on a German credit dataset obtained from UCI repository (Frank and Asuncion, 2010), which contains 1,000 observations and 24 covariates. As described by Hoffman and Gelman (2014), all covariates are normalized towards zero mean and unit variance. Once more, the targeted values of the acceptance probability in primal-dual averaging algorithm are evenly spaced...
between 0.25 and 0.95. Figure 2 displays the minimum of ESS across all dimensions and ESJD per evaluation when $\delta$ varies. In this high dimensional case, the improvement brought by eHMC and its variants is stronger, with improvement in ESS up to one order of magnitude.

![Graphs showing ESS and ESJD per evaluation for NUTS, eHMC, eHMCq, and eHMCu.]  

**Fig. 2:** Comparison amongst NUTS, eHMC, eHMCq and eHMCu for a Bayesian logistic model: the x-axis corresponds to the targeted accept probability, $\delta$, associated with the primal-dual averaging step, and the y-axis in the plots are the minimum of ESS across the parameter coordinates and ESJD per evaluation of $U$ and $\nabla U$.

### 4.3 Stochastic Volatility Model

The following example aims at a posterior distribution associated with a stochastic volatility model and $T$ artificial observations. The stochastic volatility model is based on the state-space equations:

$$x_t \sim \mathcal{N} \left( 0, \frac{\sigma^2}{1 - \varphi^2} \right),$$

for $t = 1, 2, \cdots, T$,

$$y_t = \epsilon_t \kappa \exp(0.5x_t),$$

$$\epsilon_t \sim \mathcal{N}(0, 1),$$
and for \( t = 2, \cdots, T \)
\[
x_t = \varphi x_{t-1} + \eta_t,
\]
\[
\eta_t \sim \mathcal{N}(0, \sigma^2).
\]
where only the \( y_t \)'s are observed. The prior is chosen to be \( p(\kappa) \propto 1/\kappa, 0.5(1 + \varphi) \sim \text{Beta}(20, 1.5), \)
and \( \sigma^{-2} \sim \chi^2(10, 0.05) \). In order to avoid overflow problems, we reparametrize the three parameters \( \varphi, \kappa \) and \( \sigma^2 \) as \( \alpha = \log\left(1 + \frac{\varphi}{1 - \varphi}\right), \beta = \log(\kappa) \) and \( \gamma = \log(\sigma^2) \). In this example, also used by Girolami and Calderhead (2011), we generate \( T = 1,000 \) observations with parameters chosen as \( \varphi_0 = 0.98, \kappa_0 = 0.65 \) and \( \sigma_0 = 0.15 \). The dimension of the target is thus \( T + 3 = 1,003 \), with \( 1,000 \) latent variables \( \{x_t\}_{t=1}^T \). The associated potential is thus
\[
U(\alpha, \beta, \gamma, x|y) = T\beta + \sum_{t=1}^T \frac{x_t^2}{2} + \sum_{t=1}^T \frac{y_t^2}{2\exp(2\beta)\exp(x_t)} - 20.5\alpha
\]
\[
+ 22.5\log(e^\alpha + 1) + \left(\frac{T}{2} + 5\right)\gamma + \frac{2x_1^2e^\alpha}{(e^\alpha + 1)^2e^\gamma}
\]
\[
+ \frac{1}{2}\sum_{t=2}^T \left\{ e^{-\gamma}(x_t - \frac{e^\alpha - 1}{e^\alpha + 1}x_{t-1})^2 \right\} + \frac{1}{4e^\gamma}.
\]
We split the parameter into two groups: \( \{x_t\}_{t=1}^T \) and \( (\varphi, \kappa, \sigma) \) according to the corresponding scales. Figure 3 compares the minimum ESS per evaluation of \( U \) and \( \nabla U \) of each parameter group and Figure 4 shows the ESJD on \( \{x_t\}_{t=1}^T \) and \( (\varphi, \kappa, \sigma) \) per evaluation of \( U \) and \( \nabla U \) for each sampler over 9 evenly spaced accept probability, \( \delta \), between 0.55 and 0.95, with 40 repetitions for each \( \delta \). The gain produced by eHMC and its variants is between two- and three-fold.

4.4 Logistic Item Response Theory Model

This example considers a hierarchical item response theory (IRT) model (Hambleton et al., 1991), written as
\[
\text{logit}(\mathbb{P}(y_{i,j} = 1|\eta, a, b)) = a_i(\eta_j - b_i)
\]
with
\[
\eta_j \sim \mathcal{N}(0, \sigma^2_\eta), \quad j = 1, 2, \cdots, J
\]
\[
a_i \sim \mathcal{L}\mathcal{N}(0, \sigma^2_a), \quad i = 1, 2, \cdots, I
\]
\[
b_i \sim \mathcal{L}\mathcal{N}(\mu_b, \sigma^2_b), \quad i = 1, 2, \cdots, I
\]
where \( y_{i,j} \) is the response for person \( j \) to item \( i \), \( a_i \) and \( b_i \) are called the discrimination and difficulty parameters, respectively, and \( \eta_j \) is called the ability parameter. The priors for the hyperparameters are \( \sigma_\eta \sim \text{Cauchy}(0, 2), \sigma_a \sim \text{Cauchy}(0, 2), \mu_b \sim \mathcal{N}(0, 25), \) and \( \sigma_b \sim \text{Cauchy}(0, 2) \) under the constraints \( \sigma_\eta > 0, \sigma_a > 0, \sigma_b > 0 \) and \( a_i > 0 \). These constraints are handled in HMC by looking at the logarithm transforms with the appropriate Jacobian adjustment. We use a benchmark dataset
Tab. 1: Comparison between NUTS and eHMC for a two parameter logistic item response theory model: each entry corresponds to the minimum ESS per evaluation of $U$ and $\nabla U$ over a group of parameters, maximised over the ten possible values of $\delta$.

| Sampler       | ESS ($\times 1e3$) per evaluation (mean ± sd) |
|---------------|-----------------------------------------------|
|               | {\eta_j}^{100}_{j=1} | {a_i}^{20}_{i=1} | {b_i}^{20}_{i=1} |
| NUTS          | 4.7 ± 1.1            | 3.9 ± 0.9        | 2.6 ± 0.5        |
| eHMC          | 11.7 ± 1.8           | 8.0 ± 1.9        | 8.0 ± 0.9        |
| eHMCq         | 11.8 ± 1.9           | 9.1 ± 2.4        | 6.9 ± 1.0        |
| eHMCu         | 10.7 ± 2.3           | 8.5 ± 2.2        | 5.8 ± 1.0        |

from STAN repository\(^2\), in which $I = 20, J = 100$. We examine 10 evenly spaced values between 0.5 and 0.95 as the targeted accept probability, for which a primal-dual averaging algorithm returns the associated $\epsilon$. As shown in Table 1, the ESS is two to three times larger for eHMC, depending on the quantity of interest. Figure 5, 6 and 7 show the detailed comparison in terms of ESS and ESJD for those $\delta$’s.

### 4.5 Susceptible-Infected-Recovered Model

Susceptible-infected-recovered (SIR) models are used to represent disease transmission, for epidemics like cholera, within a population. The model in this example is

\[
\eta_k \sim \text{Poisson}(y_{t-1,k,1} - y_{t,k,1}), \quad k = 1, \cdots, N_t,
\]

\[
\hat{B}_k \sim \mathcal{L}\mathcal{N}(y_{t,k,4}, 0.15^2), \quad k = 1, \cdots, N_t.
\]

The dynamic of $y_t \in \mathbb{R}^4$ is

\[
\frac{dy_{t,1}}{dt} = \frac{\beta y_{t,4}}{y_{t,4} + \kappa_0} y_{t,1},
\]

\[
\frac{dy_{t,2}}{dt} = \frac{\beta y_{t,4}}{y_{t,4} + \kappa_0} y_{t,1} - \gamma y_{t,2},
\]

\[
\frac{dy_{t,3}}{dt} = \gamma y_{t,3},
\]

\[
\frac{dy_{t,4}}{dt} = \xi y_{t,2} - \phi y_{t,4},
\]

\(^2\) https://github.com/stan-dev/stat_comp_benchmarks/tree/master/benchmarks/irt_2pl
Tab. 2: Comparison between NUTS and eHMC for a SIR model: each entry corresponds to the minimum ESS per evaluation of $U$ and $\nabla U$ over a group of parameters, maximised over the ten possible values of $\delta$.

| Sampler   | ESS ($\times 1e3$) per evaluation (mean $\pm$ sd) | $\beta$ | $\gamma$ | $\xi$ | $\phi$ |
|-----------|-------------------------------------------------|--------|--------|------|------|
| NUTS      |                                                 | 4.58  | 4.59   | 4.21 | 4.26 |
|           |                                                 | $\pm$ 0.92 | $\pm$ 0.96 | $\pm$ 0.66 | $\pm$ 0.76 |
| eHMC      |                                                 | 19.73 | 19.33  | 19.65 | 18.09 |
|           |                                                 | $\pm$ 2.77 | $\pm$ 3.05 | $\pm$ 3.09 | $\pm$ 2.46 |
| eHMCq     |                                                 | 20.20 | 19.76  | 20.15 | 20.22 |
|           |                                                 | $\pm$ 2.96 | $\pm$ 2.87 | $\pm$ 3.08 | $\pm$ 3.83 |
| eHMCu     |                                                 | 12.02 | 11.96  | 11.69 | 11.36 |
|           |                                                 | $\pm$ 1.62 | $\pm$ 1.60 | $\pm$ 1.40 | $\pm$ 1.38 |

where $y_{t,1}, y_{t,2}, y_{t,3}$ represent the number of susceptible, infected, and recovered persons, respectively, within the community, and $y_{t,4}$ represents the concentration of the virus in the water reservoir used by this population (Grad et al., 2012). In this model, the size of the population $y_{t,1} + y_{t,2} + y_{t,3}$ is assumed to be constant, which means that there is no death because of the disease or other reasons and no birth. The parameter $\eta_k$ represents the size of the population that becomes infected from being susceptible during the time interval $[t_{k-1}, t_k]$. This example uses $N_t = 20$ observations $\{\eta_k, \hat{B}_k\}_{k=1}^{N_t}$ over the time steps $t_k = 7k$, obtained from STAN repository\(^3\) and the priors over the parameters are $\beta \sim \mathcal{C}(0, 2.5)$, $\gamma \sim \mathcal{C}(0, 1)$, $\xi \sim \mathcal{C}(0, 25)$ and $\phi \sim \mathcal{C}(0, 1)$. Towards bypassing the constraints $\beta > 0$, $\gamma > 0$, $\xi > 0$ and $\phi > 0$, we once more use a reparametrisation into logarithms. Ten targeted accept probabilities are used for primal-dual tuning of the step size, evenly spaced from 0.5 to 0.95. Figure 8 shows the detailed comparison amongst NUTS, eHMC, eHMCq and eHMCu in terms of ESS and ESJD per evaluation of $U$ and $\nabla U$. Table 2 reports the best performance of each sampler across the 10 values of $\delta$. These experiments show once more that eHMC and its variants, when based upon $\hat{P}_\mathcal{L}$, exhibit a higher efficiency than NUTS in terms of ESS and ESJD.

## 5 Conclusion and Prospective

The eHMC algorithm is an alternative to NUTS that relies on an empirical version, $\hat{P}_\mathcal{L}$, of the distribution of the longest batch sizes in the leapfrog integrator, for a given step size $\epsilon$. Its motivation is to reduce wasted simulations created by NUTS, due to its stationarity constraint and the induced

\(^3\) [https://github.com/stan-dev/stat_comp_benchmarks/tree/master/benchmarks/sir](https://github.com/stan-dev/stat_comp_benchmarks/tree/master/benchmarks/sir)
backtracking. Even though the length of the path is *de facto* reduced, we have shown through a collection of Monte Carlo experiments, the proposed eHMC leads to an improved efficiency over the standard NUTS, when evaluated by ESS or by effective jumping distance per potential evaluation. While we do not aim here at optimising the length $L$ of the HMC step in terms of one of these criteria, the automated random choice of $L$ at each iteration shows clear promises.

The comparisons produced in this paper seem to contradict those of Hoffman and Gelman (2014). There are two reasons for this opposition. First, Hoffman and Gelman (2014) compared NUTS with the standard HMC sampler, which the number of steps $L$ is fixed at each and every iteration, instead of an HMC with a random number of steps. It has already been observed that resorting to a random integration time in an HMC sampler should improve performances. Second, the number of evaluations of both $U$ and $\nabla U$, rather than solely $\nabla U$ as in Hoffman and Gelman (2014), is adopted as an surrogate for the computation cost.

The improvement of eHMC over NUTS proceeds from two features. First, eHMC chooses a globally appropriate value of $L$ for an HMC sampler. Second, NUTS wastes computation effort to some extent. In fact, even though NUTS only generates longest batches to prevent from retracing at each iteration, it is impossible to make sure that the current position is close to an end-point of the generated leapfrog path. Furthermore, the NUTS proposal is uniformly distributed over the candidate set, instead of being one of the end-points. Both limitations restrict the distance between the current position and the proposal.

Obviously, $\hat{P}_L$ contains valuable information about the number of steps in the leapfrog integrator for HMC samplers and the related distribution deserves further investigation. Besides, we can also insert Algorithm 2 into a primal-dual averaging scheme to learn a rough version of $\mathcal{L}$ and hence save computation cost.

However, we stress that the usage of $\mathcal{P}_L$ need not be restricted to one of the special forms of eHMC, like the eHMCq and eHMCu samplers. For instance, instead of setting $L^* = \lceil q^{0.95}(\mathcal{L}) \rceil$ in eHMCq, choosing $L^*$ from $\lceil q^{\tau}(\mathcal{L}) \rceil$, for $\tau = 0.05k$, $k = 1, \cdots, 20$, towards maximizing ESJD is also an interesting direction to investigate, even though it requires more computation effort during warmup stage.

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5 Conclusion and Prospective

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Fig. 3: Comparison amongst NUTS, eHMC, eHMCq and eHMCu samplers for the stochastic volatility model: the x-axis is the targeted accept probability fed into primal-dual averaging, the y-axis is ESS of $\{x_t\}_{t=1}^T$ per evaluation of $U$ and $\nabla U$ for each parameter group.
Fig. 4: Comparison amongst NUTS, eHMC, eHMCq and eHMCu for the stochastic volatility model: the x-axis is the targeted accept probability fed into primal-dual averaging, the y-axis are ESJD of $\{x_t\}_{t=1}^T$ and ESJD of $\theta = (\phi, \kappa, \sigma)$ per evaluation of $U$ and $\nabla U$ respectively. Each black dot shows the performance for a single experiment and the red curve is the median of the 40 dots’ y-values for a particular $\delta$. 
Fig. 5: Comparison amongst NUTS, eHMC, eHMCq and eHMCu for the IRT model: the x-axis is the targeted accept probability fed into primal-dual averaging, the y-axis is the minimum ESS across the parameter coordinates per evaluation of $U$ and $\nabla U$ for each parameter group.
Fig. 6: Comparison amongst NUTS, eHMC, eHMCq and eHMCu for the IRT model: the x-axis is the targeted accept probability fed into primal-dual averaging, the y-axis is ESS of each hyperparameter per evaluation of $U$ and $\nabla U$. 
Fig. 7: Comparison amongst NUTS, eHMC, eHMCq and eHMCu for the IRT model: the x-axis is the targeted accept probability fed into primal-dual averaging, the y-axis is ESJD of each parameter group per evaluation of $U$ and $\nabla U$. 
Fig. 8: Comparison amongst NUTS, eHMC, eHMCq and eHMCu for the SIR model: the x-axis is the targeted accept probability fed into primal-dual averaging, the y-axis in the first four rows is ESS of each parameter per evaluation of $U$ and $\nabla U$ and the y-axis in the lowermost plots is ESJD of $\theta = (\beta, \gamma, \xi, \phi)$ per evaluation of $U$ and $\nabla U$. 

5 Conclusion and Prospective