Split Hamiltonian Monte Carlo
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Abstract
We show how the Hamiltonian Monte Carlo algorithm can sometimes be speeded up by “splitting” the Hamiltonian in a way that allows much of the movement around the state space to be done at low computational cost. One context where this is possible is when the log density of the distribution of interest (the potential energy function) can be written as the log of a Gaussian density, which is a quadratic function, plus a slowly varying function. Hamiltonian dynamics for quadratic energy functions can be analytically solved. With the splitting technique, only the slowly-varying part of the energy needs to be handled numerically, and this can be done with a larger stepsize (and hence fewer steps) than would be necessary with a direct simulation of the dynamics. Another context where splitting helps is when the most important terms of the potential energy function and its gradient can be evaluated quickly, with only a slowly-varying part requiring costly computations. With splitting, the quick portion can be handled with a small stepsize, while the costly portion uses a larger stepsize. We show that both of these splitting approaches can reduce the computational cost of sampling from the posterior distribution for a logistic regression model, using either a Gaussian approximation centered on the posterior mode, or a Hamiltonian split into a term that depends on only a small number of critical cases, and another term that involves the larger number of cases whose influence on the posterior distribution is small. Supplemental materials for this paper are available online.

Keywords: Markov chain Monte Carlo, Hamiltonian dynamics, Bayesian analysis

1 Introduction
The simple Metropolis algorithm (Metropolis et al. 1953) is often effective at exploring low-dimensional distributions, but it can be very inefficient for complex, high-dimensional distributions — successive states may exhibit high autocorrelation, due to the random walk nature of the movement. Faster exploration can be obtained using Hamiltonian Monte Carlo, which was first

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introduced by Duane et al. (1987), who called it “hybrid Monte Carlo”, and which has been recently reviewed by Neal (2010). Hamiltonian Monte Carlo (HMC) reduces the random walk behavior of Metropolis by proposing states that are distant from the current state, but nevertheless have a high probability of acceptance. These distant proposals are found by numerically simulating Hamiltonian dynamics for some specified amount of fictitious time.

For this simulation to be reasonably accurate (as required for a high acceptance probability), the stepsize used must be suitably small. This stepsize determines the number of steps needed to produce the proposed new state. Since each step of this simulation requires a costly evaluation of the gradient of the log density, the stepsize is the main determinant of computational cost.

In this paper, we show how the technique of “splitting” the Hamiltonian (Leimkuhler and Reich, 2004; Neal, 2010) can be used to reduce the computational cost of producing proposals for Hamiltonian Monte Carlo. In our approach, splitting separates the Hamiltonian, and consequently the simulation of the dynamics, into two parts. We discuss two contexts in which one of these parts can capture most of the rapid variation in the energy function, but is computationally cheap. Simulating the other, slowly-varying, part requires costly steps, but can use a large stepsize. The result is that fewer costly gradient evaluations are needed to produce a distant proposal. We illustrate these splitting methods using logistic regression models for classification problems. Computer programs for our methods are publicly available from http://www.ics.uci.edu/~babaks/Site/Codes.html.

Before discussing the splitting technique, we provide a brief overview of HMC. (See Neal, 2010, for an extended review of HMC.) To begin, we briefly discuss a physical interpretation of Hamiltonian dynamics. Consider a frictionless puck that slides on a surface of varying height. The state space of this dynamical system consists of its position, denoted by the vector $q$, and its momentum (mass, $m$, times velocity, $v$), denoted by a vector $p$. Based on $q$ and $p$, we define the potential energy, $U(q)$, and the kinetic energy, $K(p)$, of the puck. $U(q)$ is proportional to the height of the surface at position $q$. The kinetic energy is $m|v|^2/2$, so $K(p) = |p|^2/(2m)$. As the puck moves on an upward slope, its potential energy increases while its kinetic energy decreases, until it becomes zero. At that point, the puck slides back down, with its potential energy decreasing and its kinetic energy increasing.

The above dynamic system can be represented by a function of $q$ and $p$ known as the Hamilton-
tonian, which for HMC is usually defined as the sum of a potential energy, $U$, depending only on the position and a kinetic energy, $K$, depending only on the momentum:

$$H(q,p) = U(q) + K(p)$$

(1)

The partial derivatives of $H(q,p)$ determine how $q$ and $p$ change over time, according to Hamilton’s equations:

$$\frac{dq_j}{dt} = \frac{\partial H}{\partial p_j} = \frac{\partial U}{\partial p_j}$$

$$\frac{dp_j}{dt} = -\frac{\partial H}{\partial q_j} = -\frac{\partial K}{\partial q_j}$$

(2)

These equations define a mapping $T_s$ from the state at some time $t$ to the state at time $t + s$.

We can use Hamiltonian dynamics to sample from some distribution of interest by defining the potential energy function to be minus the log of the density function of this distribution (plus any constant). The position variables, $q$, then correspond to the variables of interest. We also introduce fictitious momentum variables, $p$, of the same dimension as $q$, which will have a distribution defined by the kinetic energy function. The joint density of $q$ and $p$ is defined by the Hamiltonian function as

$$P(q,p) = \frac{1}{Z} \exp\left(-H(q,p)\right)$$

When $H(q,p) = U(q) + K(p)$, as we assume in this paper, we have

$$P(q,p) = \frac{1}{Z} \exp\left(-U(q)\right) \exp\left(-K(p)\right)$$

so $q$ and $p$ are independent.

In applications to Bayesian statistics, $q$ consists of the model parameters (and perhaps latent variables), and our objective is to sample from the posterior distribution for $q$ given the observed data $D$. To this end, we set

$$U(q) = -\log(P(q)L(q|D))$$

where $P(q)$ is our prior and $L(q|D)$ is the likelihood function given data $D$.

Having defined a Hamiltonian function corresponding to the distribution of interest (e.g., a posterior distribution of model parameters), we could in theory use Hamilton’s equations, applied for some specified time period, to propose a new state in the Metropolis algorithm. Since
Hamiltonian dynamics leaves invariant the value of $H$ (and hence the probability density), and preserves volume, this proposal would always be accepted. (For a more detailed explanation, see Neal (2010).)

In practice, however, solving Hamiltonian’s equations exactly is too hard, so we need to approximate these equations by discretizing time, using some small step size $\epsilon$. For this purpose, the \textit{leapfrog} method is commonly used. It consists of iterating the following steps:

$$
\begin{align*}
p_j(t + \epsilon/2) &= p_j(t) - \left(\epsilon/2\right) \frac{\partial U}{\partial q_j}(q(t)) \\
q_j(t + \epsilon) &= q_j(t) + \epsilon \frac{\partial K}{\partial p_j}(p(t + \epsilon/2)) \\
p_j(t + \epsilon) &= p_j(t + \epsilon/2) - \left(\epsilon/2\right) \frac{\partial U}{\partial q_j}(q(t + \epsilon))
\end{align*}
$$

Typically, $K(p) = p^T M^{-1} p / 2$, with $M$ usually being a diagonal matrix with elements $m_1, \ldots, m_d$, so that $K(p) = \sum_i p_i^2 / 2m_i$. The $q_j$ are then independent and Gaussian with mean zero, with $p_j$ having variance $m_j$. The time derivative of $q_j$ is then $\frac{\partial K}{\partial p_j} = p_j / m_j$.

We can use some number, $L$, of these leapfrog steps, with some stepsize, $\epsilon$, to propose a new state in the Metropolis algorithm. We apply these steps starting at the current state $(q, p)$, with fictitious time set to $t = 0$. The final state, at time $t = L\epsilon$, is taken as the proposal, $(q^*, p^*)$. (To make the proposal symmetric, we would need to negate the momentum at the end of the trajectory, but this can be omitted when, as here, $K(p) = K(-p)$ and $p$ will be replaced (see below) before the next update.) This proposal is either accepted or rejected (with the state remaining unchanged), with the acceptance probability being

$$
\min[1, \exp(-H(q^*, p^*) + H(q, p))] = \min[1, \exp(-U(q^*) + U(q) - K(p^*) + K(p))]
$$

These Metropolis updates will leave $H$ approximately constant, and therefore do not explore the whole joint distribution of $q$ and $p$. The HMC method therefore alternates these Metropolis updates with updates in which the momentum is sampled from its distribution (which is independent of $q$). When $K(p) = \sum_i p_i^2 / 2m_i$, each $p_j$ is sampled independently from the Gaussian distribution with mean zero and variance $m_j$.

As an illustration, consider sampling from the following bivariate normal distribution

$$
q \sim N(\mu, \Sigma), \quad \text{with } \mu = \begin{pmatrix} 3 \\ 3 \end{pmatrix} \quad \text{and } \Sigma = \begin{pmatrix} 1 & 0.95 \\ 0.95 & 1 \end{pmatrix}
$$
For HMC, we set $L = 20$ and $\epsilon = 0.15$. The left plot in Figure 1 shows the first 30 states from an HMC run. The density contours of the bivariate normal distribution are shown as gray ellipses. The right plot shows every $20^{th}$ state from the first 600 iterations of a run of a simple random walk Metropolis (RWM) algorithm. (This takes time comparable to that for the HMC run.) The proposal distribution for RWM is a bivariate normal with the current state as the mean, and $0.15^2 I_2$ as the covariance matrix. (The standard deviation of this proposal is the same as the stepsize of HMC.) Figure 1 shows that HMC explores the distribution more efficiently, with successive samples being further from each other, and autocorrelations being smaller. For an extended review of HMC, its properties, and its advantages over the simple random walk Metropolis algorithm, see Neal (2010).

In this example, we have assumed that one leapfrog step for HMC (which requires evaluating the gradient of the log density) takes approximately the same computation time as one Metropolis update (which requires evaluating the log density), and that both move approximately the same
distance. The benefit of HMC comes from this movement being systematic, rather than in a random walk. We now propose a new approach called Split Hamiltonian Monte Carlo (Split HMC), which further improves the performance of HMC by modifying how steps are done, with the effect of reducing the time for one step or increasing the distance that one step moves.

2 Splitting the Hamiltonian

As discussed by Neal (2010), variations on HMC can be obtained by using discretizations of Hamiltonian dynamics derived by “splitting” the Hamiltonian, $H$, into several terms:

$$H(q, p) = H_1(q, p) + H_2(q, p) + \cdots + H_K(q, p)$$

We use $T_{i,t}$, for $i = 1, \ldots, k$ to denote the mapping defined by $H_i$ for time $t$. Assuming that we can implement Hamiltonian dynamics $H_k$ exactly, the composition $T_{1,\epsilon} \circ T_{2,\epsilon} \circ \cdots \circ T_{k,\epsilon}$ is a valid discretization of Hamiltonian dynamics based on $H$ if $H_i$ are twice differentiable (Leimkuhler and Reich, 2004). This discretization is symplectic and hence preserves volume. It will also be reversible if the sequence of $H_i$ are symmetric: $H_i(q, p) = H_{K-i+1}(q, p)$.

Indeed, the leapfrog method (3) can be regarded as a symmetric splitting of the Hamiltonian $H(q, p) = U(q) + K(p)$ as

$$H(q, p) = U(q)/2 + K(p) + U(q)/2$$

(4)

In this case, $H_1(q, p) = H_3(q, p) = U(q)/2$ and $H_2(q, p) = K(p)$. Hamiltonian dynamics for $H_1$ is

$$\frac{dq_j}{dt} = \frac{\partial H_1}{\partial p_j} = 0$$

$$\frac{dp_j}{dt} = -\frac{\partial H_1}{\partial q_j} = -\frac{1}{2} \frac{\partial U}{\partial q_j}$$

which for a duration of $\epsilon$ gives the first part of a leapfrog step. For $H_2$, the dynamics is

$$\frac{dq_j}{dt} = \frac{\partial H_2}{\partial p_j} = \frac{\partial K}{\partial p_j}$$

$$\frac{dp_j}{dt} = -\frac{\partial H_2}{\partial q_j} = 0$$

For time $\epsilon$, this gives the second part of the leapfrog step. Hamiltonian dynamics for $H_3$ is the same as that for $H_1$ since $H_1 = H_3$, giving the the third part of the leapfrog step.
2.1 Splitting the Hamiltonian when a partial analytic solution is available

Suppose the potential energy $U(q)$ can be written as $U_0(q) + U_1(q)$. Then, we can split $H$ as

$$H(q,p) = U_1(q)/2 + [U_0(q) + K(p)] + U_1(q)/2$$

Here, $H_1(q,p) = H_3(q,p) = U_1(q)/2$ and $H_2(q,p) = U_0(p) + K(p)$. The first and the last terms in this splitting are similar to Eq. (4), except that $U_1(q)$ replaces $U(q)$, so the first and the last part of a leapfrog step remain as before, except that we use $U_1(q)$ rather than $U(q)$ to update $p$. Now suppose that the middle part of the leapfrog, which is based on the Hamiltonian $U_0(q) + K(p)$, can be handled analytically; that is, we can compute the exact dynamics for any duration of time. We hope that since this part of the simulation introduces no error, we will be able to use a larger step size, and hence take fewer steps, reducing the computation time for the dynamical simulations.

We are mainly interested in situations where $U_0(q)$ provides a reasonable approximation to $U(q)$, and in particular on Bayesian applications, where we approximate $U$ by focusing on the the posterior mode, $\hat{q}$, and the second derivatives of $U$ at that point. We can obtain $\hat{q}$ using fast methods such as the Newton-Raphson, when analytical solutions are not available. We then approximate $U(q)$ with $U_0(q)$, the energy function for $N(\hat{q}, J^{-1}(\hat{q}))$, where $J(\hat{q})$ is the Hessian matrix of $U$ at $\hat{q}$. Finally, we set $U_1(q) = U(q) - U_0(q)$, the error in this approximation.

Beskos et al. (2011) have recently proposed a similar splitting strategy for HMC, in which a Gaussian component is handled analytically, in the context of high-dimensional approximations to a distribution on an infinite-dimensional Hilbert space. In such applications, the Gaussian distribution will typically be derived from the problem specification, rather than being found as a numerical approximation, as we do here.

Using a normal approximation in which $U_0(q) = \frac{1}{2}(q - \hat{q})^T J(\hat{q})(q - \hat{q})$, and letting $K(p) = \frac{1}{2}p^T p$ (the energy for the standard normal distribution), $H_2(q,p) = U_0(q) + K(p)$ in Eq. (5) will be quadratic, and Hamilton’s equations will be a system of first-order linear differential equations that can be handled analytically (Polyanin et al. 2002). Specifically, setting $q^* = q - \hat{q}$, the dynamical equations can be written as follows:

$$\frac{d}{dt} \begin{bmatrix} q^*(t) \\ p(t) \end{bmatrix} = \begin{bmatrix} 0 & I \\ -J(\hat{q}) & 0 \end{bmatrix} \begin{bmatrix} q^*(t) \\ p(t) \end{bmatrix}$$
where $I$ is the identity matrix. Defining $X = (q, p)$, this can be written as $\frac{d}{dt}X(t) = AX(t)$, where

$$A = \begin{bmatrix} 0 & I \\ -\mathcal{J}(\dot{q}) & 0 \end{bmatrix}$$

The solution of this system is $X(t) = e^{At}X_0$, where $X_0$ is the initial value at time $t = 0$. This can be simplified by diagonalizing the coefficient matrix $A$ as

$$A = \Gamma D \Gamma^{-1}$$

where $\Gamma$ is invertible and $D$ is a diagonal matrix. The system of equations can then be written as

$$\frac{d}{dt}X(t) = \Gamma D \Gamma^{-1}X(t)$$

Now, let $Y(t) = \Gamma^{-1}X(t)$. Then,

$$\frac{d}{dt}Y(t) = DY(t)$$

The solution for the above equation is $Y(t) = e^{Dt}Y_0$, where $Y_0 = \Gamma^{-1}X_0$. Therefore,

$$X(t) = \Gamma e^{Dt} \Gamma^{-1}X_0$$

and $e^{Dt}$ can be easily computed by simply exponentiating the diagonal elements of $D$ times $t$.

The above analytical solution is of course for the middle part (denoted as $H_2$) of Eq. (5) only. We still need to approximate the overall Hamiltonian dynamics based on $H$, using the leapfrog method. Algorithm 1 shows the corresponding leapfrog steps — after an initial step of size $\epsilon/2$ based on $U_1(q)$, we obtain the exact solution for a time step of $\epsilon$ based on $H_2(q, p) = U_0(q) + K(p)$, and finish by taking another step of size $\epsilon/2$ based on $U_1(q)$.

### 2.2 Splitting the Hamiltonian by splitting the data

The method discussed in the previous section requires that we be able to handle the Hamiltonian $H_2(q, p) = U_0(q) + K(p)$ analytically. If this is not so, splitting the Hamiltonian in this way may still be beneficial if the computational cost for $U_0(q)$ is substantially lower than for $U(q)$. In these situations, we can use the following split:

$$H(q, p) = \frac{U_1(q)}{2} + \sum_{m=1}^{M} \left[ \frac{U_0(p)}{2M} + \frac{K(p)}{M} + \frac{U_0(p)}{2M} \right] + \frac{U_1(q)}{2}$$ (6)
Algorithm 1: Leapfrog for split Hamiltonian Monte Carlo with a partial analytic solution.

\[ R \leftarrow \Gamma e^{D\epsilon} \Gamma^{-1} \]

Sample initial values for \( p \) from \( N(0, I) \)

for \( \ell = 1 \) to \( L \) do

\[ p \leftarrow p - (\epsilon/2) \frac{\partial U_1}{\partial q} \]

\[ q^* \leftarrow q - \hat{q} \]

\[ X_0 \leftarrow (q^*, p) \]

\[ (q^*, p) \leftarrow RX_0 \]

\[ q \leftarrow q^* + \hat{q} \]

\[ p \leftarrow p - (\epsilon/2) \frac{\partial U_1}{\partial q} \]

end for

Algorithm 2: Nested leapfrog for split Hamiltonian Monte Carlo with splitting of data.

Sample initial values for \( p \) from \( N(0, I) \)

for \( \ell = 1 \) to \( L \) do

\[ p \leftarrow p - (\epsilon/2) \frac{\partial U_1}{\partial q} \]

for \( m = 1 \) to \( M \) do

\[ p \leftarrow p - (\epsilon/2M) \frac{\partial U_0}{\partial q} \]

\[ q \leftarrow q + (\epsilon/M)p \]

\[ p \leftarrow p - (\epsilon/2M) \frac{\partial U_0}{\partial q} \]

end for

\[ p \leftarrow p - (\epsilon/2) \frac{\partial U_1}{\partial q} \]

end for

for some \( M > 1 \). The above discretization can be considered as a nested leapfrog, where the outer part takes half steps to update \( p \) based on \( U_1 \) alone, and the inner part involves \( M \) leapfrog steps of size \( \epsilon/M \) based on \( U_0 \). Algorithm 2 implements this nested leapfrog method.

For example, suppose our statistical analysis involves a large data set with many observations, but we believe that a small subset of data is sufficient to build a model that performs reasonably well (i.e., compared to the model that uses all the observations). In this case, we can construct \( U_0(q) \) based on a small part of the observed data, and use the remaining observations to construct \( U_1(q) \). That is, we divide the observed data, \( y \), into two subsets: \( R_0 \), which is used to construct \( U_0(q) \), and \( R_1 \), which is used to construct \( U_1(q) \):

\[
U(\theta) = U_0(\theta) + U_1(\theta)
\]

\[
U_0(\theta) = -\log[P(\theta)] - \sum_{i \in R_0} \log[P(y_i|\theta)] \tag{7}
\]

\[
U_1(\theta) = -\sum_{i' \in R_1} \log[P(y_{i'}|\theta)]
\]

Note that the prior appears in \( U_0(\theta) \) only.

[Neal (2010)] discusses a related strategy for splitting the Hamiltonian by splitting the observed data into multiple subsets. However, instead of randomly splitting data, as proposed there, here
Figure 2: An illustrative binary classification problem with $n = 100$ data points and two covariates, $x_1$ and $x_2$, with the two classes represented by white circles and black squares.

we split data by building an initial model based on the maximum a posterior (MAP) estimate, $\hat{q}$, and use this model to identify a small subset of data that captures most of the information in the full data set. We next illustrate this approach for logistic regression models.

3 Application of Split HMC to logistic regression models

We now look at how Split HMC can be applied to Bayesian logistic regression models for binary classification problems. We will illustrate this method using the simulated data set with $n = 100$ data points and $p = 2$ covariates that is shown in Figure 2.

The logistic regression model assigns probabilities to the two possible classes (denoted by 0
and 1) in case $i$ (for $i = 1, \ldots, n$) as follows:

$$P(y_i = 1 \mid x_i, \alpha, \beta) = \frac{\exp(\alpha + x_i^T \beta)}{1 + \exp(\alpha + x_i^T \beta)}$$

(8)

Here, $x_i$ is the vector of length $p$ with the observed values of the covariates in case $i$, $\alpha$ is the intercept, and $\beta$ is the vector of $p$ regression coefficients. We use $\theta$ to denote the vector of all $p + 1$ unknown parameters, $(\alpha, \beta)$.

Let $P(\theta)$ be the prior distribution for $\theta$. The posterior distribution of $\theta$ given $x$ and $y$ is proportional to $P(\theta) \prod_{i=1}^{n} P(y_i \mid x_i, \theta)$. The corresponding potential energy function is

$$U(\theta) = -\log[P(\theta)] - \sum_{i=1}^{n} \log[P(y_i \mid x_i, \theta)]$$

We assume the following (independent) priors for the model parameters:

$$\alpha \sim N(0, \sigma^2_{\alpha})$$

$$\beta_j \sim N(0, \sigma^2_{\beta}), \quad j = 1, \ldots, p$$

where $\sigma_{\alpha}$ and $\sigma_{\beta}$ are known constants.

The potential energy function for the above logistic regression model is therefore as follows:

$$U(\theta) = \frac{\alpha^2}{2\sigma^2_{\alpha}} + \sum_{j=1}^{p} \frac{\beta_j^2}{2\sigma^2_{\beta}} - \sum_{i=1}^{n} \left[ y_i(\alpha + x_i^T \beta) - \log(1 + \exp(\alpha + x_i^T \beta)) \right]$$

The partial derivatives of the energy function with respect to $\alpha$ and the $\beta_j$ are

$$\frac{\partial U}{\partial \alpha} = \frac{\alpha}{\sigma^2_{\alpha}} - \sum_{i=1}^{n} \left[ y_i - \frac{\exp(\alpha + x_i^T \beta)}{1 + \exp(\alpha + x_i^T \beta)} \right], \quad \frac{\partial U}{\partial \beta_j} = \frac{\beta_j}{\sigma^2_{\beta}} - \sum_{i=1}^{n} x_{ij} \left[ y_i - \frac{\exp(\alpha + x_i^T \beta)}{1 + \exp(\alpha + x_i^T \beta)} \right]$$

To apply Algorithm 1 for Split HMC to this problem, we approximate the potential energy function $U(\theta)$ for the logistic regression model with the potential energy function $U_0(\theta)$ of the normal distribution $N(\hat{\theta}, J^{-1}(\hat{\theta}))$, where $\hat{\theta}$ is the MAP estimate of model parameters. $U_0(\theta)$ usually provides a reasonable approximation to $U(\theta)$, as illustrated in Figure 3. In the plot on the left, the solid curve shows the value of the potential energy, $U$, as $\beta_1$ varies, with $\beta_2$ and $\alpha$ fixed to their MAP values, while the dashed curve shows $U_0$ for the approximating normal distribution. The right plot of Figure 3 compares the partial derivatives of $U$ and $U_0$ with respect to $\beta_1$, showing that $\partial U_0/\partial \beta_j$ provides a reasonable linear approximation to $\partial U/\partial \beta_j$. 

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Figure 3: Left plot: The potential energy, $U$, for the logistic regression model (solid curve) and its normal approximation, $U_0$ (dashed curve), as $\beta_1$ varies, with other parameters at their MAP values. Right plot: The partial derivatives of $U$ and $U_0$ with respect to $\beta_1$.

Since there is no error when solving Hamiltonian dynamics based on $U_0(\theta)$, we would expect that the total discretization error of the steps taken by Algorithm 1 will be less than for the standard leapfrog method, for a given stepsize, and that we will therefore be able to use a larger stepsize — and hence need fewer steps for a given trajectory length — while still maintaining a good acceptance rate. The stepsize will still be limited to the region of stability imposed by the discretization error from $U_1 = U - U_0$, but this limit will tend to be larger than for the standard leapfrog method.

To apply Algorithm 2 to this logistic regression model, we split the Hamiltonian by splitting the data into two subsets. Consider the illustrative example discussed above. In the left plot of Figure 4, the thick line represents the classification boundary using the MAP estimate, $\hat{\theta}$. For the points that fall on this boundary line, the estimated probabilities for the two groups are equal, both being 0.5. The probabilities of the two classes become less equal as the distance of the covariates from this line increases. We will define $U_0$ using the points within the region, $R_0$, within some
Figure 4: Left plot: A split of the data into two parts based on the MAP model, represented by the solid line; the energy function $U$ is then divided into $U_0$, based on the data points in $R_0$, and $U_1$, based on the data points in $R_1$. Right plot: The partial derivatives of $U$ and $U_0$ with respect to $\beta_1$, with other parameters at their MAP values.

distance of this line, and define $U_1$ using the points in the region, $R_1$, at a greater distance from this line. This split can also be viewed as putting in $R_0$ those points for which the prediction of the class based on the MAP parameter estimate has high entropy, with points where this entropy is lower going to $R_1$. (The entropy, which for a binary class with probabilities $P(0)$ and $P(1)$ is defined as $P(0) \log(1/P(0)) + P(1) \log(1/P(1))$, declines monotonically as the class probabilities move away from 0.5.)

The shaded area in Figure [4] shows the region, $R_0$, containing the 30% of the observations closest to the MAP line, or equivalently the 30% of observations with the highest entropy for the class prediction, or the 30% of observations for which the probability of class 1 is closest (in either direction) to 0.5. The unshaded region containing the remaining data points is denoted as $R_1$. Using these two subsets, we can split the energy function $U(\theta)$ into two terms: $U_0(\theta)$ based on the data points that fall within $R_0$, and $U_1$ based on the data points that fall within $R_1$ (see Eq. [7]).
Then, we use Eq. (6) to split the Hamiltonian dynamics.

Note that $U_0$ is not used to approximate the potential energy function, $U$, for the acceptance test at the end of the trajectory. Rather, $\partial U_0/\partial \beta_j$ is used to approximate $\partial U/\partial \beta_j$, which is the costly computation when we simulate Hamiltonian dynamics. Recall that

$$\frac{\partial U}{\partial \beta_j} = \frac{\beta_j}{\sigma^2} - \sum_{i=1}^{n} x_{ij} \left[ y_i - \frac{\exp(\alpha + x_i^T \beta)}{1 + \exp(\alpha + x_i^T \beta)} \right]$$

For a given $(\alpha, \beta)$, the term $\exp(\alpha + x_i^T \beta)/(1 + \exp(\alpha + x_i^T \beta))$ is in fact $P(y_i = 1|x_i, \alpha, \beta)$. For high entropy data points close to the boundary line defined based on $(\alpha, \beta)$, this estimated probability is close to 0.5, so $y_i - \exp(\alpha + x_i^T \beta)/(1 + \exp(\alpha + x_i^T \beta))$ tends to be large. (Note that $y_i$ is either zero or one.) This term is also large for misclassified cases. Such cases, however, are likely to be close to the boundary line too. Therefore, for a given $(\alpha, \beta)$, the value of $\partial U/\partial \beta_j$ is mainly dominated by high entropy data points (at least when $\theta$ is close to $\hat{\theta}$). The right plot of Figure 4 shows the approximation of $\partial U/\partial \beta_j$ by $\partial U_0/\partial \beta_j$.

4 Experiments

In this section, we use simulated and real data to compare our proposed methods to the standard HMC.

For each problem, we set the number of leapfrog steps to $L = 20$ for the standard HMC, and find $\epsilon$ such that the acceptance probability (AP) is close to 0.65 [Neal, 2010]. We set $L$ and $\epsilon$ for the Split HMC methods such that the trajectory length, $\epsilon L$, remains the same, but with a larger stepsize and hence a smaller number of steps. We try to choose $\epsilon$ for the Split HMC methods such that the acceptance probability is equal to that of standard HMC. However, increasing the stepsize beyond a certain point leads to instability of trajectories, in which the error of the Hamiltonian grows rapidly with $L$ [Neal, 2010], so that proposals are rejected with very high probability. This sometimes limits the stepsize of Split HMC to values at which the acceptance probability is greater than the 0.65 aimed at for standard HMC.

When splitting the data in order to use Split HMC Algorithm 2, we always use the 30% of the data with highest entropy MAP class predictions (ie, class probabilities closest to 0.5) to define $U_0$. We always set the number of inner leapfrog steps in Algorithm 2 to $M = 3$. 

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To measure the efficiency of each sampling method, we use the autocorrelation time (ACT) by dividing the $N$ posterior samples into batches of size $B$, and estimating ACT as follows (Neal, 1993; Geyer, 1992):

$$\tau = BS_b^2S^2$$

Here, $S^2$ is the sample variance and $S_b^2$ is the sample variance of batch means. Following Thompson (2010), we divide the posterior samples into $N^{1/3}$ batches of size $B = N^{2/3}$. Throughout this section, we set the number of Markov chain Monte Carlo (MCMC) iterations for simulating posterior samples to $N = 100000$.

The autocorrelation time can be roughly interpreted as the number of MCMC transitions required to produce samples that can be considered as independent. For the logistic regression problems discussed in this section, we find the autocorrelation times for each regression parameter separately, and then compare different methods using the maximum autocorrelation time (i.e., the autocorrelation time of the slowest parameter in the chain), denoted as $\tau_{\text{max}}$, over all regression parameters.

We adjust $\tau_{\text{max}}$ to account for the varying computation time needed by the different methods in two ways. One is to compare different methods using $\tau_{\text{max}} \times s$, where $s$ is the CPU time per iteration, using an implementation written in R. This measures the CPU time required to produce samples that can be regarded as independent samples. We also compare in terms of $\tau_{\text{max}} \times g$, where $g$ is the number of gradient computations on the number of cases in the full data set required for each trajectory simulated by HMC. This will be equal to the number of leapfrog steps, $L$, for standard HMC or Split HMC using a normal approximation. When using data splitting with a fraction $f$ of data in $R_0$ and $M$ inner leapfrog steps, $g$ will be $(fM + (1 - f)) \times L$, which is $1.6L$ when $f = 0.3$ and $M = 3$, as for these experiments. In general, we expect that computation time will be dominated by the gradient computations counted by $g$, so that $\tau_{\text{max}} \times g$ will provide a measure of performance independent of any particular implementation. In our experiments, $s$ was close to being proportional to $g$, except for slightly larger than expected times for Split HMC with data splitting.
Table 1: Split HMC (with normal approximation and data splitting) compared to standard HMC using simulated data, on a data set with \( n = 10000 \) observations and \( p = 100 \) covariates.

|                  | HMC | Split HMC |
|------------------|-----|-----------|
|                  |     | Normal Appr. | Data Splitting |
| \( L \)          | 20  | 11         | 11             |
| \( g \)          | 20  | 11         | 17.6           |
| \( s \)          | 0.401 | 0.228     | 0.370          |
| \( AP \)         | 0.58 | 0.73       | 0.70           |
| \( \tau_{\text{max}} \) | 281.7 | 170.0      | 212.2          |
| \( \tau_{\text{max}} \times g \) | 5634 | 1870       | 3735           |
| \( \tau_{\text{max}} \times s \) | 113.03 | 38.78     | 78.57          |

4.1 Simulated data

We first tested the methods on a simulated data set with 100 covariates and 10000 observations. The covariates were sampled as \( x_{ij} \sim N(0, \sigma_j^2) \), for \( i = 1, \ldots, 10000 \) and \( j = 1, \ldots, 100 \), with \( \sigma_j \) set to 5 for the first five variables, to 1 for the next five variables, and to 0.2 for the remaining 90 variables. We sampled true parameter values, \( \alpha \) and \( \beta_j \), independently from \( N(0, 1) \) distributions. Finally, we sampled the class labels according to the model, as \( y_i \sim \text{Bernoulli}(p_i) \) with \( \text{logit}(p_i) = \alpha + x_i^T \beta \).

For the Bayesian logistic regression model, we assumed normal priors with mean zero and standard deviation 5 for \( \alpha \) and \( \beta_j \), where \( j = 1, \ldots, 100 \). We ran standard HMC, Split HMC with normal approximation, and Split HMC with data splitting for \( N = 100000 \) iterations. For the standard HMC, we set \( L = 20 \) and \( \epsilon = 0.02 \), so the trajectory length was \( 20 \times 0.015 = 0.3 \). For Split HMC with normal approximation and Split HMC with data splitting, we reduce the number of leapfrog steps to 11, while increasing the stepsizes so that the trajectory length remained 0.3.

Table 1 shows the results for the three methods. The CPU times (in seconds) per iteration, \( s \), and \( \tau_{\text{max}} \times s \) for the Split HMC methods are substantially lower than for standard HMC. Especially, the Split HMC with normal approximation is almost three times faster compared to the standard HMC, in terms of generating samples that can be considered independent. The comparison is similar looking at \( \tau_{\text{max}} \times g \).
4.2 Results on real data sets

In this section, we evaluate our proposed method using four real binary classification problems. The data for these four problems are available from the UCI Machine Learning Repository (http://archive.ics.uci.edu/ml/index.html). For all data sets, we standardized the numerical variables to have mean zero and standard deviation 1. Further, we assumed normal priors with mean zero and standard deviation 5 for the regression parameters. We used the setup described at the beginning of Section 4, running each Markov chain for $N = 100000$ iterations. Table 2 summarizes the results using the three sampling methods.

The first problem, StatLog, involves using multi-spectral values of pixels in a satellite image in order to classify the associated area into soil or cotton crop. (In the original data, different types of soil are identified.) The sample size for this data set is $n = 4435$, and the number of features is $p = 37$. For the standard HMC, we set $L = 20$ and $\epsilon = 0.075$. For the two Split HMC methods with normal approximation and data splitting, we reduce $L$ to 14 and 8 respectively while increasing $\epsilon$ so $\epsilon \times L$ remains the same as that of the standard HMC. As seen in the table, the Split HMC methods substantially reduce $\tau_{\text{max}} \times s$ (and $\tau_{\text{max}} \times g$), with the data splitting method performing somewhat better than the normal approximation method.

The second example, Gisette, is a handwritten digit recognition problem (Guyon et al., 2004) constructed based on the MNIST data (http://yann.lecun.com/exdb/mnist). The objective is to separate the highly confusable digits “4” and “9”. The data include $n = 6000$ observations and a set of 5000 highly sparse features. Here, we use the projections of original covariates onto the first 100 principal components as predictors. We set $L = 20$ and $\epsilon = 0.11$ for the standard HMC. We reduced the number of leapfrog steps to 14 and 11 for Split HMC with normal approximation and data splitting respectively. Again, a substantial improvement is achieved over standard HMC, with the normal approximation method performing best on this data set.

The third problem, CTG, involves analyzing 2126 fetal cardiotocograms along with their respective diagnostic features (de Campos et al., 2000). The objective is to determine whether the fetal state class is “pathologic” or not. The data include 2126 observations and 21 features. For the standard HMC, we set $L = 20$ and $\epsilon = 0.075$. We reduced the number of leapfrog steps to 14 and 8 for Split HMC with normal approximation and data splitting respectively. Both zsplitting methods improved performance significantly.
| Data Set  | HMC | Split HMC |
|-----------|-----|-----------|
|           | Normal Appr. | Data Splitting |
| StatLog   | L 20 | 14 | 8 |
| n = 4435, p = 37 | g 20 | 14 | 12.8 |
|           | s 0.055 | 0.040 | 0.039 |
|           | AP 0.63 | 0.70 | 0.78 |
|           | $\tau_{\text{max}}$ 11.0 | 10.4 | 8.2 |
|           | $\tau_{\text{max}} \times g$ 220 | 146 | 105 |
|           | $\tau_{\text{max}} \times s$ 0.61 | 0.41 | 0.32 |
| Gisette   | L 20 | 14 | 11 |
| n = 600, p = 100 | g 20 | 14 | 17.6 |
|           | s 0.233 | 0.169 | 0.201 |
|           | AP 0.70 | 0.85 | 0.78 |
|           | $\tau_{\text{max}}$ 21.0 | 20.7 | 20.6 |
|           | $\tau_{\text{max}} \times g$ 420 | 290 | 363 |
|           | $\tau_{\text{max}} \times s$ 4.88 | 3.50 | 4.11 |
| CTG       | L 20 | 14 | 8 |
| n = 2126, p = 21 | g 20 | 14 | 12.8 |
|           | s 0.016 | 0.012 | 0.013 |
|           | AP 0.65 | 0.82 | 0.79 |
|           | $\tau_{\text{max}}$ 64.1 | 54.1 | 54.6 |
|           | $\tau_{\text{max}} \times g$ 1282 | 757 | 699 |
|           | $\tau_{\text{max}} \times s$ 1.03 | 0.63 | 0.71 |
| Chess     | L 20 | 13 | 9 |
| n = 3196, p = 36 | g 20 | 13 | 14.4 |
|           | s 0.035 | 0.024 | 0.031 |
|           | AP 0.69 | 0.82 | 0.84 |
|           | $\tau_{\text{max}}$ 28.4 | 25.2 | 36.6 |
|           | $\tau_{\text{max}} \times g$ 568 | 328 | 527 |
|           | $\tau_{\text{max}} \times s$ 1.00 | 0.61 | 1.12 |

Table 2: HMC and Split HMC (normal approximation and data splitting) on four real data sets.
The objective of the last problem, Chess, is to predict chess endgame outcomes — either “white can win” or “white cannot win”. This data set includes \( n = 3196 \) instances, where each instance is a board-description for the chess endgame. There are \( p = 36 \) attributes describing the board. For the standard HMC, we set \( L = 20 \) and \( \epsilon = 0.08 \). For the two Split HMC methods with normal approximation and data splitting, we reduced \( L \) to 13 and 9 respectively. Using the normal approximation method, \( \tau_{\text{max}} \times s \) and \( \tau_{\text{max}} \times g \) were substantially reduced compared to standard HMC. For the Split HMC with data splitting, however, the reduction in \( s \) and \( g \) coincides with an increase in \( \tau_{\text{max}} \) so there was little or no improvement compared to standard HMC. The failure of data splitting on this problem is puzzling. (One possible explanation might be that the overall high acceptance probability with this method might conceal a low acceptance probability in some regions of the parameter space.)

5 Discussion

We have proposed two new methods for improving the efficiency of HMC, both based on splitting the Hamiltonian in a way that allows much of the movement around the state space to be performed at low computational cost.

While we have focused on the application of our methods to logistic regression models for binary classification problems, they can be extended to more complex models, such as multinomial logistic (MNL) models for multiple classes. For MNL models, the regression parameters for \( p \) covariates and \( J \) classes form a matrix of \((p + 1)\) rows and \( J \) columns, which we can vectorize so that the model parameters, \( \theta \), become a vector of \((p + 1) \times J \) elements. For Split HMC with normal approximation, we define \( U_0(\theta) \) using an approximate multivariate normal \( N(\hat{\theta}, J^{-1}(\hat{\theta})) \) as before. For Split HMC with data splitting, we still construct \( U_0(\theta) \) using a small subset of data with the highest entropy class distributions, with the entropy is calculated as

\[
\sum_{j=1}^{J} P(y = j|x, \hat{\theta}) \log[1 / P(y = j|x, \hat{\theta})]
\]

The data splitting method could be further extended to any model for which it is feasible to find a MAP estimate, and then divide the data into two parts based on “residuals” of some form.

We (Lan and Shahbaba [2011]) have recently extended our Split HMC method to Gaussian process models for regression and classifications problems. These nonparametric Bayesian models
tend to be computationally intensive, with the computational cost being a major factor limiting their application. We have shown that splitting the Hamiltonian function can reduce the computational cost (measured in terms of $\tau_{\text{max}} \times s$) of sampling from the posterior distribution of hyperparameters by up to 10 fold, by handling a quadratic part of the Hamiltonian analytically.

Future research in this area could involve finding tractable approximations to the posterior distribution other than normal distributions. One could also investigate other methods for splitting the Hamiltonian dynamics by splitting the data — for example, fitting a support vector machine (SVM) to binary classification data, and using the support vectors for constructing $U_0$.

While the results on simulated data and real classification problems presented in this paper have demonstrated the advantages of splitting the Hamiltonian dynamics in terms of improving the sampling efficiency, our proposed methods do require preliminary analysis of data, mainly, finding the MAP estimate. The performance of our approach obviously depends on how well the corresponding normal distribution based on MAP estimates approximates the posterior distribution, or how well a small subset of data found using this MAP estimate captures the overall patterns in the whole data set. This preliminary analysis involves some computational overhead, but the computational cost associated with finding the MAP estimate is often negligible compared to the potential improvement in sampling efficiency for the full Bayesian model.

Another approach to improving HMC has recently been proposed by Girolami and Calderhead (2011). Their method, Riemannian Manifold HMC (RMHMC), can also substantially improve performance. RMHMC utilizes the geometric properties of the parameter space to explore the best direction, typically at higher computational cost, to produce distant proposals with high probability of acceptance. In contrast, our method attempts to find a simple approximation to the Hamiltonian to reduce the computational time required for reaching distant states. It is possible that these approaches could be combined, to produce a method that performs better than either method alone. The recent proposals of Hoffman and Gelman (2011) for automatic tuning of HMC could also be combined with our Split HMC methods.
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