hdtg: An R package for high-dimensional truncated normal simulation

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Abstract

Simulating from the multivariate truncated normal distribution (MTN) is required in various statistical applications yet remains challenging in high dimensions. Currently available algorithms and their implementations often fail when the number of parameters exceeds a few hundred. To provide a general computational tool to efficiently sample from high-dimensional MTNs, we introduce the hdtg package that implements two state-of-the-art simulation algorithms: harmonic Hamiltonian Monte Carlo (Harmonic-HMC) and zigzag Hamiltonian Monte Carlo (Zigzag-HMC). Both algorithms exploit analytical solutions of the Hamiltonian dynamics under a quadratic potential energy with hard boundary constraints, leading to rejection-free methods. We compare their efficiencies against another state-of-the-art algorithm for MTN simulation, the minimax tilting accept-reject sampler (MET). The run-time of these three approaches heavily depends on the underlying multivariate normal correlation structure. Zigzag-HMC and Harmonic-HMC both achieve 100 effective samples within 3,600 seconds across all tests with dimension ranging from 100 to 1,600, while MET has difficulty in several high-dimensional examples. We provide guidance on how to choose an appropriate method for a given situation and illustrate the usage of hdtg.
1 Introduction

Sampling from a multivariate truncated normal (MTN) distribution is a recurring problem in many statistical applications. The MTN distribution of a \( d \)-dimensional random vector \( \mathbf{x} \in \mathbb{R}^d \) has the form

\[
\mathbf{x} \sim \mathcal{N}(\mu, \Sigma) \text{ with } l \leq \mathbf{x} \leq u \text{ bounded,}
\]

where \( \mu \) and \( \Sigma \) are the mean vector and covariance matrix, and \( l, u \in \mathbb{R}^d \) denote the lower and upper truncation bounds. MTNs arise in various context including probit and tobit models (Albert and Chib, 1993; Tobin, 1958), latent Gaussian models (Bolin and Lindgren, 2015), copula regression (Pitt et al., 2006), spatial models (Tsionas and Michaelides, 2016; Baltagi et al., 2018; Zareifard and Khaledi, 2021), Bayesian metabolic flux analysis (Heinonen et al., 2019), and many others. When the dimension \( d \) is small, a standard rejection sampler (Geweke, 1991; Kotecha and Djuric, 1999) works well and is a common choice. However, simulation from a larger MTN with hundreds or thousands of correlated dimensions remains a computational challenge. Work towards this goal include harmonic Hamiltonian Monte Carlo (Pakman and Paninski, 2014, Harmonic-HMC), rejection sampling based on minimax (saddle point) exponential tilting (Botev, 2017, MET), and the most recent Zigzag Hamiltonian Monte Carlo (Nishimura et al., 2020, 2021, Zigzag-HMC) methods.

The MET method provides independent samples but can suffer from low acceptance rates and becomes impractical with \( d > 100 \), except in special cases like when the MTN has a strongly positive correlation structure (Botev, 2017). Both Harmonic-HMC and Zigzag-HMC are Markov chain Monte Carlo (MCMC) approaches that generate correlated samples, but can nonetheless be highly efficient and scale to thousands or more dimensions. To our knowledge, however, there is no general-purpose implementation of either method; the \texttt{tmg} package provided by Pakman and Paninski (2014) is no longer available on CRAN, and Zhang et al. (2022) implement Zigzag-HMC for their phylogenetics applications in the specialized software BEAST (Suchard et al., 2018). Therefore, we have developed the \texttt{hdtg} R package for efficient MTN simulation. The package implements tuning-free Zigzag-HMC and Harmonic-HMC. We provide performance comparisons among these two methods and a MET implementation from the \texttt{TruncatedNormal} package (Botev and Belzile, 2021). In most of the test cases with \( d > 100 \), Harmonic-HMC and Zigzag-HMC outperform MET. We then conclude with some empirical guidance on which method to use in different scenarios.

2 Algorithm

We begin by briefly introducing Harmonic-HMC and Zigzag-HMC, both of which are variants of HMC, an effective proposal generation mechanism exploiting the properties of Hamiltonian dynamics (Neal, 2011). Harmonic-HMC and Zigzag-HMC follow the same general framework. To sample \( \mathbf{x} = (x_1, \ldots, x_d) \in \mathbb{R}^d \) from the target distribution...
π(x), the HMC variants introduce an auxiliary momentum variable $p$ and define an augmented target distribution $\pi(x, p) = \pi(x)\pi(p)$ in the joint space. They then propose the next state by first re-sampling the momentum variable from its marginal and then simulating the solution of Hamiltonian dynamics governed by the differential equations

$$\frac{dx}{dt} = \nabla K(p), \quad \frac{dp}{dt} = -\nabla U(x),$$

where $U(x) = -\log \pi(x)$ and $K(p) = -\log \pi(p)$ are referred to as potential and kinetic energies. The dynamics are simulated for a pre-set time duration $T$ and the end state constitutes a valid Metropolis proposal to be accepted or rejected according to the standard formula (Metropolis et al., 1953; Hastings, 1970).

The most common versions of HMC use the momentum distribution $\pi(p) \sim N(0, I)$ and rely on the leapfrog integrator to numerically solve (2), as its solutions are analytically intractable in general settings. Harmonic-HMC takes advantage of the fact that (2) admits analytical solutions when the target $\pi(x)$ is an MTN. The solution follows independent harmonic oscillations along the principal components of the covariance/precision matrix (Pakman and Paninski, 2014); we thus refer to the algorithm as Harmonic-HMC. Truncation boundaries are handled via elastic “bounces” against hard “potential energy walls” (Neal, 2011). We refer interested readers to Pakman and Paninski (2014) for details on Harmonic-HMC.

Zigzag-HMC differs from the common HMC versions in that it deploys a Laplace momentum (Nishimura et al., 2020, 2021)

$$\pi(p) \propto \prod_i \exp (-|p_i|), i = 1, \ldots, d.$$  

The Hamiltonian dynamics then become

$$\frac{dx}{dt} = \text{sign}(p), \quad \frac{dp}{dt} = -\nabla U(x),$$

where $\text{sign}(p_i)$ returns 1 if $p_i$ is positive and -1 otherwise. Because the velocity $\frac{dx}{dt} \in \{\pm 1\}^d$ remains constant until one of the $p_i$ flips its sign, the trajectory of these Hamiltonian dynamics has a zigzag pattern, hence the name Zigzag-HMC. The zigzag dynamics also admit analytical solutions under an MTN target and can handle the truncation in the same manner as in Harmonic-HMC. We refer interested readers to Nishimura et al. (2021) and Zhang et al. (2022) for Zigzag-HMC algorithm details, including how to determine the time of a momentum sign change and of a bounce against truncation boundaries.

The simulation duration $T$, i.e. how long Hamiltonian dynamics is simulated for each proposal generation, critically affects efficiencies of both Harmonic and Zigzag-HMC. For Harmonic-HMC, Pakman and Paninski (2014) suggest setting $T = \pi/2$; when using this fixed $T$, however, we observe inefficiencies in some of our examples in Section 4 due to Hamiltonian dynamics’ periodic behaviors (Neal, 2011). We therefore
randomize the duration \( T \), as recommended by Neal (2011), and draw it from a uniform distribution on \([\pi/8, \pi/2]\). For Zigzag-HMC, we adopt the choice \( T = \sqrt{2\lambda_{\text{min}}^{-1/2}} \) based on the heuristics of Nishimura et al. (2021), where \( \lambda_{\text{min}} \) is the minimal eigenvalue of the precision matrix \( \Omega = \Sigma^{-1} \). We compute \( \lambda_{\text{min}} \) using the Lanczos algorithm (Demmel, 1997) as in the mgcv package (Wood, 2017). We further implement the no-U-turn algorithm (NUTS) of Hoffman and Gelman (2014) to automatically determine the integration time. With NUTS, we only need to pick a base integration time \( \Delta T \) which we set to \( 0.1\lambda_{\text{min}}^{-1/2} \) as recommended by Nishimura et al. (2021).

3 Using hdtg

The hdtg package allows users to draw MCMC samples from an MTN with fixed or random mean and covariance/precision matrix. In our current implementation, Zigzag-HMC accepts the most commonly seen element-wise truncations as in Equation (1) while Harmonic-HMC can handle a more general constraint

\[
(Fx + g)_i \geq 0, \text{ for } i = 1, \ldots, m.
\]  

(5)

Here the \( m \times d \) matrix \( F \) and \( m \)-dimensional vector \( g \) specify the truncations and \( (\cdot)_i \) denotes the \( i \)th vector element. As an example, one may use the following code to generate 1,000 samples from a 10-dimensional MTN with zero mean and an identity covariance matrix truncated to the positive orthant:

```r
# set the random seed
set.seed(1)
# draw MTN samples using Zigzag-HMC
samplesZHMC <- zigzagHMC(n = 1000, mean = rep(0, 10), prec = diag(10),
                        init = rep(0.1, 10), lowerBounds = rep(0, 10),
                        upperBounds = rep(Inf, 10))
# draw MTN samples using Harmonic-HMC
samplesHHMC <- harmonicHMC(n = 1000, mean = rep(0, 10),
                        choleskyFactor = diag(10), precFlg = TRUE,
                        init = rep(0.1, 10), F = diag(10), g = rep(0, 10))
```

The arguments are:

- \( n \): number of samples.
- \( \text{mean} \): a \( d \)-dimensional mean vector.
- \( \text{prec} \): the precision matrix.
- \( \text{init} \): a vector of the initial value that must satisfy all constraints.
- \( \text{lowerBounds} \): a \( d \)-dimensional vector specifying the lower bounds.
• upperBounds: a \(d\)-dimensional vector specifying the upper bounds.

• choleskyFactor: upper triangular matrix \(U\) from Cholesky decomposition of precision or covariance matrix into \(U^T U\).

• precFlg: whether choleskyFactor is from precision (TRUE) or covariance matrix (FALSE).

• \(F\): the \(F\) matrix.

• \(g\): the \(g\) vector.

With a random \(\mu\) or \(\Omega\), one can simply call \texttt{zigzagHMC} or \texttt{harmonicHMC} and pass the updated \(\mu\) and \(\Omega\) as arguments. But a more efficient usage of Zigzag-HMC exists. \texttt{zigzagHMC} calls the function \texttt{createEngine} (or \texttt{createNutsEngine} if using NUTS) to create a C++ object that sets up truncation boundaries and SIMD (single instruction-stream, multiple data-stream) vectorization. Therefore, we can avoid repeated calls of \texttt{createEngine} by reusing the C++ object, as in the following example where the 10-dimensional target MTN has a random mean and precision:

```r
set.seed(1)
n <- 1000
d <- 10
samples <- array(0, c(n, d))
# initialize MTN mean and precision
m <- rnorm(d, 0, 1)
prec <- rWishart(n = 1, df = d, Sigma = diag(d))[, , 1]

# call createEngine once
engine <- createEngine(dimension = d, lowerBounds = rep(0, d),
                         upperBounds = rep(Inf, d), seed = 1, mean = m, precision = prec)

HZZtime <- sqrt(2) / sqrt(min(mgcv::slanczos(A = prec, k = 1,
                                         kl = 1)[["values"]]))

currentSample <- rep(0.1, d)
for (i in 1:n) {
  m <- rnorm(d, 0, 1)
  prec <- rWishart(n = 1, df = d, Sigma = diag(d))[, , 1]
  setMean(sexp = engine$engine, mean = m)
  setPrecision(sexp = engine$engine, precision = prec)
  currentSample <- getZigzagSample(position = currentSample, nutsFlg = F,
                                   engine = engine, stepZZHMC = HZZtime)
  samples[i, ] <- currentSample
}
```
4 Efficiency comparison and method choice

To assess the performance of Harmonic-HMC, Zigzag-HMC and MET, we compare them on MTNs with a variety of correlation structures. The three examples are:

1) MTNs with its covariance matrix $\Sigma$ drawn from the uniform LKJ distribution (Lewandowski et al., 2009) as implemented in the `rlkjcorr` function from package `trialr` (Brock, 2020); 2) MTNs with a compound symmetric covariance matrix such that $\Sigma_{i,i} = 1$ and $\Sigma_{i,j} = 0.9$ for $i \neq j$; and 3) a real-world MTN that arises as a posterior conditional distribution in a statistical phylogenetics model of HIV evolution (Zhang et al., 2021, 2022). For simplicity, we assume the truncation $x_i > 0$ for $i = 1, \ldots, d$ in the first two examples. For the HIV example, the truncation is determined by the signs of observed binary biological features.

We now specify our comparison criteria and the rationale behind them. A more efficient MCMC algorithm takes shorter time to achieve a certain effective sample size (ESS). For all three samplers considered, we compare their run-time to obtain the first one or 100 effectively independent samples ($t_1$ and $t_{100}$). We include both $t_1$ and $t_{100}$ because $t_{100}$ reflects a practical run-time for simulation from a fixed MTN and $t_1$ better captures the pre-processing overhead that remains relevant in cases where $\Sigma$ is random. Recall that the main pre-processing costs are the Cholesky decomposition of $\Sigma$ or $\Omega$ (Harmonic-HMC), calculating the minimal precision matrix eigenvalue $\lambda_{\text{min}}$ (Zigzag-HMC), and solving the minimax optimization problem (MET). Therefore we have

$$t_1 = t_0 + c$$
$$t_{100} = t_0 + 100c,$$

(6)

where $t_0$ and $c$ are the pre-processing time required for each $\Sigma$ update and the average run-time per one effective sample. For simulation from a fixed MTN, $t_0$ is a one-time cost and so $t_{100}$ serves as a better efficiency criterion. When $\Sigma$ is random (e.g. the second example in Section 3), if $\Sigma$ changes its value $k$ times, the total run-time to obtain one effective sample for each $\Sigma$ is $kt_1$ and so the $t_1$ criterion would be more informative.

For Harmonic-HMC and Zigzag-HMC, we estimate the ESS using the `coda` package (Plummer et al., 2006) and define $n_1$ as the average number of MCMC iterations required for one effectively independent sample. We approximate $n_1$ by $L/\text{ESS}_{\text{min}}$, where $\text{ESS}_{\text{min}}$ is the minimal ESS across all dimensions and $L$ is the chain length. We fix $n_1 = 1$ for MET as it generates independent samples. Therefore $c$ in Equation (6) equals the average time to complete $n_1$ iterations after pre-processing. Table 1 reports our efficiency comparison in terms of $t_1$ and $t_{100}$. We run each test on a quad-core Intel i7 4 GHZ equipped machine with 32GB of memory.

The efficiency of all three methods strongly depends on the correlation structure. MET fails to generate 100 effectively independent samples within two hours in a few higher dimensional tests, while Harmonic-HMC and Zigzag-HMC/NUTS enjoy a $t_{100} < 3600$ seconds across all tests. In the LKJ example, Zigzag-HMC/NUTS become more
Table 1: Efficiency comparison of Harmonic-HMC, Zigzag-HMC, Zigzag-HMC with NUTS (Zigzag-NUTS), and MET sampling approaches across three example correlation structures. We report $t_1$ and $t_{100}$ (in seconds), the run-time to obtain one or 100 effective samples. In some cases MET takes more than two hours to generate 100 effective samples so the results are not shown. We benchmark each test for three replications and report the average run-time. Bold numbers are column minimums in each test.

| Correlation Structure | $d = 100$ | 400 | 800 | 1600 |
|-----------------------|------------|-----|-----|------|
|                       | $t_1$ | $t_{100}$ | $t_1$ | $t_{100}$ | $t_1$ | $t_{100}$ | $t_1$ | $t_{100}$ |
| LKJ                   | Harmonic-HMC | 0.004 | 0.34 | 0.17 | 13 | 0.95 | 82 | 16 | 1567 |
|                       | Zigzag-HMC | 0.028 | 1.8 | 0.37 | 20 | 2.1 | 136 | 15 | 1098 |
|                       | Zigzag-NUTS | 0.029 | 1.3 | 0.39 | 20 | 1.7 | 94 | 13 | 975 |
|                       | MET | 4.3 | 42 | 13 | 975 |
| CS0.9                 | Harmonic-HMC | 0.001 | 0.026 | 0.009 | 0.18 | 0.056 | 0.84 | 0.40 | 4.8 |
|                       | Zigzag-HMC | 0.010 | 0.63 | 0.33 | 29 | 1.8 | 147 | 10 | 895 |
|                       | Zigzag-NUTS | 0.035 | 3.2 | 1.3 | 129 | 6.9 | 689 | 20 | 1759 |
|                       | MET | 0.13 | 0.20 | 5.1 | 5.7 | 39 | 40 | 296 | 302 |
| HIV                   | Harmonic-HMC | 0.008 | 0.74 | 0.23 | 20 | 1.7 | 137 | 22 | 2185 |
|                       | Zigzag-HMC | 0.013 | 0.65 | 0.22 | 14 | 0.98 | 40 | 3.9 | 225 |
|                       | Zigzag-NUTS | 0.020 | 1.0 | 0.30 | 19 | 1.3 | 69 | 10 | 626 |
|                       | MET | 0.060 | 0.084 | 2.7 | 3.5 | 22 | 10 | 626 |
efficient than Harmonic-HMC when $d$ reaches 1600. Zigzag-HMC and Zigzag-NUTS tend to share similar performance. While Zigzag-NUTS is the most efficient choice for the LKJ test ($d = 1600$), Zigzag-HMC wins the test on an MTN from the HIV example ($d = 800, 1600$). On the other hand, when $\Sigma$ is compound symmetric with a high correlation of 0.9, Harmonic-HMC consistently outperforms the other methods. When MET does function for a target MTN, its $t_{100}$ is close to $t_1$, as solving the initial minimax optimization problem takes most of its run-time.

In practice, we recommend running a quick efficiency comparison to decide which method to use. Nevertheless we provide some general guidance on method choice for high-dimensional MTN simulation:

- If $d \leq 100$ or the correlation structure is strongly positive, use MET or Harmonic-HMC. Harmonic-HMC may run faster but MET has the advantage of generating independent samples.

- For all other cases, Zigzag-HMC/NUTS is presumably more efficient, although Harmonic-HMC may outperform them when $d < 1000$.

- It is always worth trying MET which is free of MCMC convergence concerns. Since our simulation only examines a few correlation structures, it is possible that MET can handle other large MTNs.

A final point that needs consideration is that Zigzag-HMC/NUTS require $\Omega$ and if only $\Sigma$ is available, the method first inverts $\Sigma$. This is a one-time operation and likely negligible cost when $\Sigma$ is constant. The approaches does become expensive if $\Sigma$ is random, as the $O(d^3)$ inversion is necessary for each value of $\Sigma$. In practice, statistical models may be parameterized in terms of $\Sigma$ (Lachaab et al., 2006; Molstad et al., 2021) or $\Omega$ (Balaghi et al., 2018; Lehnert et al., 2019; Li et al., 2020). Harmonic-HMC carries a similar limitation since it requires a $O(d^3)$ Cholesky decomposition of $\Sigma$ or $\Omega$, whichever is provided. Therefore, when $d$ is large and the target MTN has a random correlation structure, one may favor Zigzag-HMC/NUTS over Harmonic-HMC especially if a closed-form $\Omega$ is at hand.

5 Conclusion

This article introduces the hdtg package oriented for efficient MTN simulation. In most of our high-dimensional tests the implemented Harmonic-HMC and Zigzag-HMC algorithms outperform the current best approach available in the TruncatedNormal package. To our best knowledge, hdtg is the first tool that can generate samples from an arbitrary MTN with thousands of dimensions. We discuss the usage of functions and provide practical suggestions on method choice. We expect to see future large-scale statistical applications utilizing the efficiency of hdtg.
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