Implementation of Stochastic Gradient Hamiltonian Monte Carlo

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Abstract

The Stochastic Gradient Hamiltonian Monte Carlo (SGHMC) algorithm is proposed to address the limitations of Hamiltonian Monte Carlo (HMC) sampling methods, which is not suitable for solving the problems of computing the gradient of streaming data or large sample size. SGHMC takes the advantage of noisy gradient estimates based on the subsets of data. This project implements the algorithm from the paper Stochastic Gradient Hamiltonian Monte Carlo and optimizes the performance by using Numba and C++. The algorithm was applied on both simulated data and real data and was compared to other competing algorithms.

Background

Description of algorithm

This part contains two parts: Hamiltonian Monte Carlo and Stochastic Gradient Hamiltonian Monte Carlo.

Hamiltonian Monte Carlo

HMC provides momentum variables (r) to establish a new joint distribution (θ, r) so that it can draw samples from the posterior distribution.

Let U be the potential energy function described in the article, we have

$$\pi(\theta, r) \propto \exp(-U(\theta) - \frac{1}{2} r^T M^{-1} r)$$

$$U = \sum_{x \in D} ln[p(x|D)] - ln[p(\theta)]$$

In physical field, the Hamilton function can be described as

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

Therefore, we have

$$d\theta = M^{-1} r dt \quad and \quad dr = -\nabla U(\theta) dt$$

Stochastic Gradient Hamiltonian Monte Carlo

Instead of computing the ∇U in $dr = -\nabla U(\theta)dt$, SGHMC uniformly chooses $\tilde{D}$ (minibatch) from the dataset and compute $\tilde{U}$. The equattion can be shown as the following:

$$\nabla \tilde{U}(\theta) = -\frac{|D|}{|\tilde{D}|} \sum_{x \in \tilde{D}} \nabla logp(x|\theta) - \nabla logp(\theta)$$

From the article, we can approximate the above equation by

$$\nabla U(\theta) + N(0, V(\theta))$$

Since the equation can be regarded as a discreted system, we may want to introduce Metroplis-Hasting sampling. Let ϵ be the step term in in Metroplis-Hasting sampling, we can rewrite the dr as following:

$$dr = -\nabla U(\theta)dt = -\nabla U(\theta) + N(0, 2B(\theta)dt)$$

where $B(\theta) = \frac{1}{2}\epsilon V(\theta)$ (positive semi-definite). In addition, the article shows we need to add a friction term because $\pi(\theta, r)$ is not invariant in this case. Finally, the dynamic equations become the following:

$$d\theta = M^{-1}rdt \quad and \quad dr = -\nabla U(\theta)dt - BM^{-1}rdt + N(0, 2B(\theta)dt)$$

$$dr = -\nabla U(\theta)dt - BM^{-1}rdt + N(0, 2B(\theta)dt) \quad (10)$$

Optimization for performance

In this part, we create a new mixture normal model for the optimization. With the true $\mu = [-3, 3]$, we have $p(x|\mu_1, \mu_2) = \frac{1}{2}N(\mu_1, 1) + \frac{1}{2}N(\mu_2, 1)$. The parameters are shown as following:

ϵ	C	V	Batch Size	Epochs	Burns
0.1	4	4	1	4000	200

Four different functions for optimization are plain python using numpy, python function with cholesky decomposition and cholesky based sampling, JIT (numba) and cpp. The running time are show in the following table:

Algorithm	Running Time
plain python (numpy)	7.91 s ± 140 ms
python with cholesky decomposition	7.51 s ± 140 ms
numba	7.38 s ± 321 ms
cpp	316 ms ± 6.25 ms

We first found that using Numba did not improve the performance a lot, so we decided to use C++ to optimize the algorithm. The main reasons that Python is slower than C++ are Python is an interpreted language and supports Garbage Collection. We use the package pybind11 to wrap C++ code for Python, which provides an automatic conversion for NumPy arrays and the C++ Eigen linear algebra library. In our experiment, we re-write the gradient function and SGHMC function in C++.

Except using cpp, the other three methods provide similar results regarding the mixture normal example. We can see that using Cholesky decomposition or using JIT compilation (numba) only improves the algorithm a little, from 7.91 s $\pm$ 140 ms per loop to 7.51 s $\pm$ 140 ms per loop and 7.38 s $\pm$ 321 ms per loop. One noteworthy point is that we use the `jacobian` function from the autograd package o calculate the auto-gradient. However, this function takes more time than expected. To implement SGHMC, a function to calculate the gradients of log densities are necessary. Therefore, we encourage users to write a gradient function by themselves and then use it as an argument in the sghmc function (our sghmc function allows users to use their gradient functions).

Applications to simulated data sets

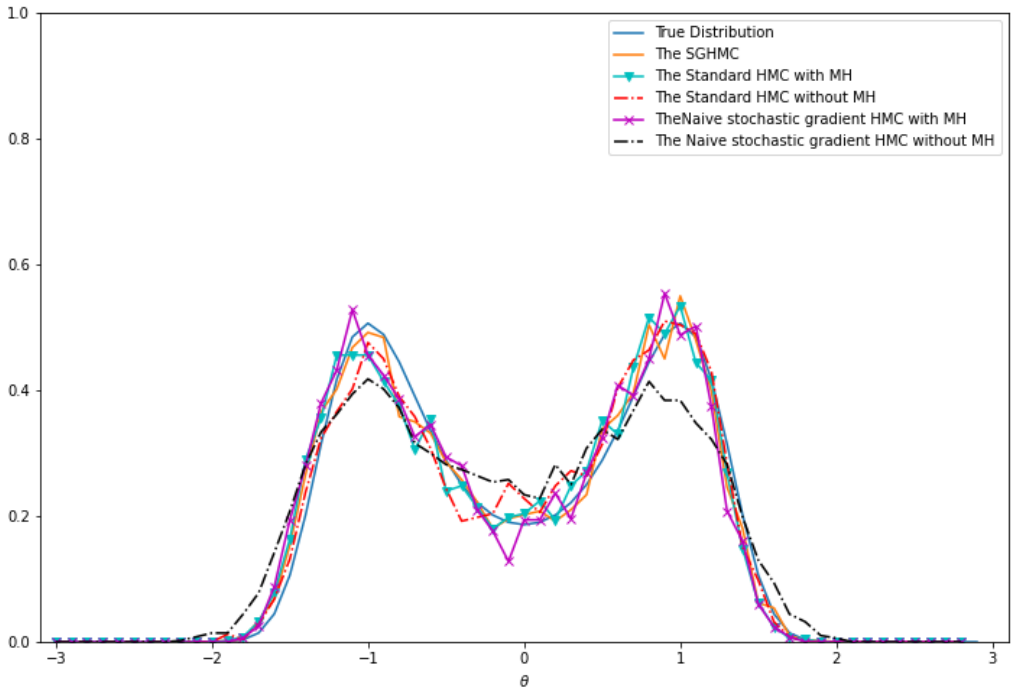
This part compares the distribution among five different algorithms (listed below) and the true distribution of the simulated data set in the original paper $U(\theta) = -2\theta^2 + \theta^4$.

- the distribution from the Stochastic Gradient Hamiltonian Monte Carlo algorithm $\nabla\tilde{U}(\theta) = \nabla U(\theta) + N(0, 4)$ with following argument:

ϵ	C	V	Batch Size	Epochs	Burns
0.1	3	4	1	5000	200

- The standard HMC with MH
- The standard HMC witthout MH
- The Naive stochastic gradient HMC with MH
- The Naive stochastic gradient HMC without MH

And a comparison figure shown as below:

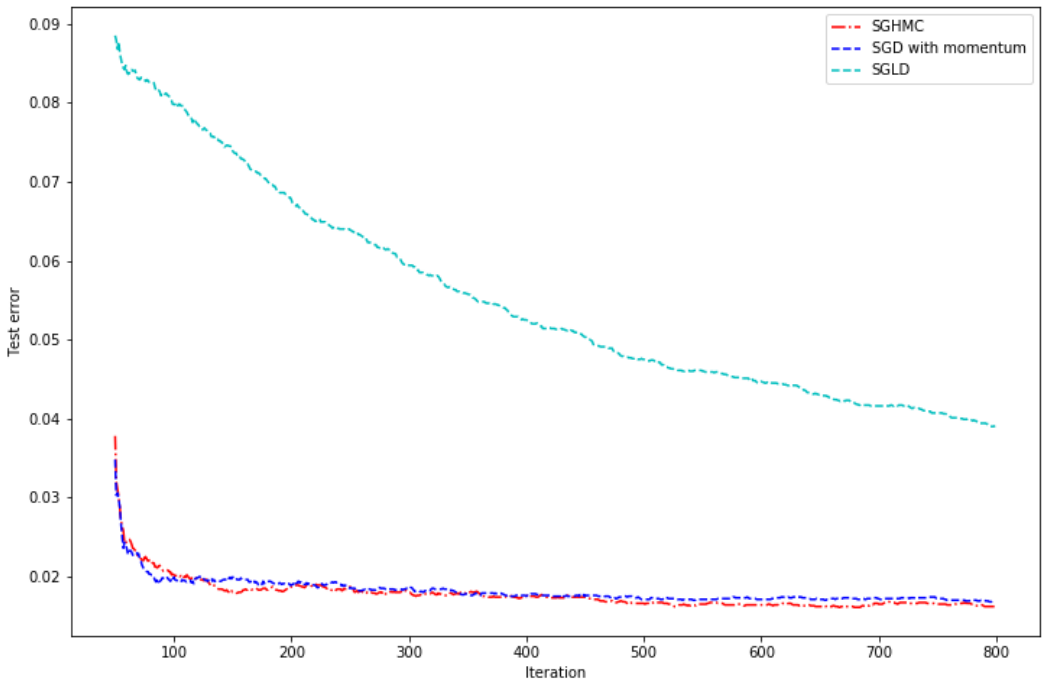


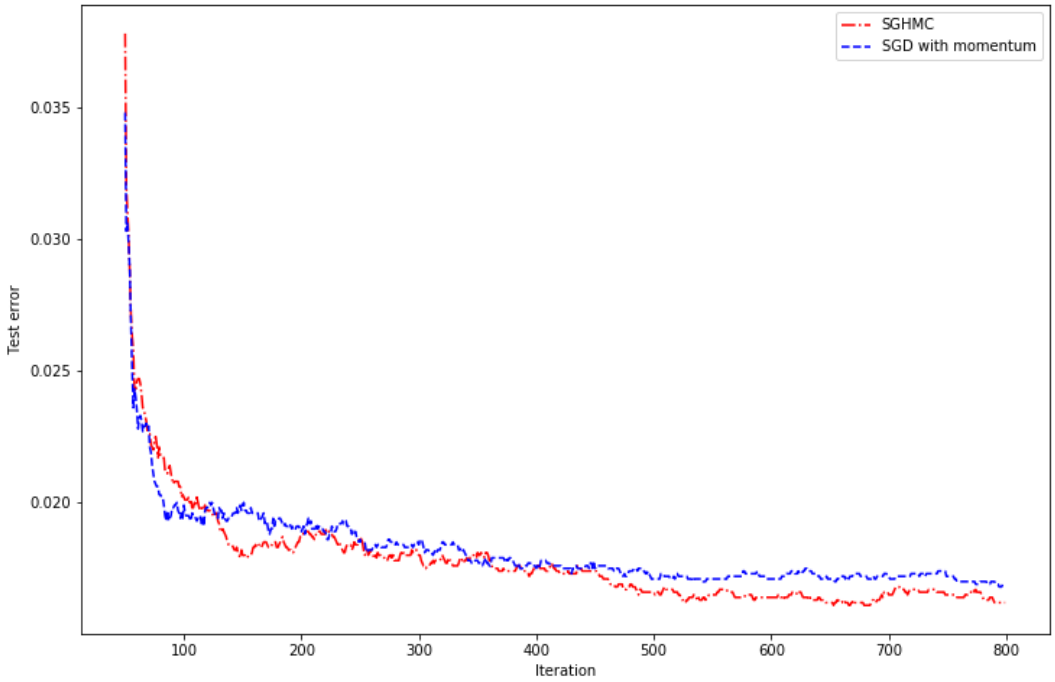
All five algorithms perform similarly to the distribution of simulated data except the naive stochastic gradient HMC without MH. Theoretically, SGHMC and HMC have the invariance of Hamiltonian function for a ϵ value close to 0. However, the naive stochastic gradient HMC without MH does not unless the MH step is added. That is the reason why the naive stochastic gradient HMC without MH is barely satisfactory in the figure. Then, the MH step will be costly, so that users may need a tradeoff between the accuracy and the cost. Our focus, the distribution of SGHMC, gives a similar result as the distribution of simulated data.

Applications to real data sets

Real data sets

In addition to the application on the simulated datasets, we also applied the SGHMC on the real datasets MNIST, which was used in the paper. MNIST is a large database of handwritten digits that is commonly used for training various image processing systems, consists of 60,000 training instances and 10,000 test instances. We utilized the author's code to train a two-layer Bayesian neural network with 100 hidden variables using a sigmoid unit and an output layer using softmax. To select training parameters, the training data is split out 10,000 instances to form a validation set and the remaining 50,000 instances are used for training. We run the samplers for 800 iterations and discard the initial 50 samples as burn-in. Three methods are tested in this experiment, SGD with momentum, SGLD and SGHMC. Fig 3 is the test result of the methods. It is shown that, based on our experiment results, both SGHMC and SGD with momentum converge to the lower test error compared to SGLD. But in Fig 4 we can see that SGHMC has the better result than SGD with momentum. However, according to the running time, SGHMC is much faster than SGD with momentum.





Competing algorithms

Discussion

References

Chen, Tianqi, Fox, Emily, and Guestrin, Carlos. Stochastic gradient hamiltonian monte carlo. ICML 2014.

Appendix

URL

https://github.com/yimi97/sghmc

Installation

```
pip install -i https://test.pypi.org/simple/ sghmc-2021
```