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:

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

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

Optimization for performance

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

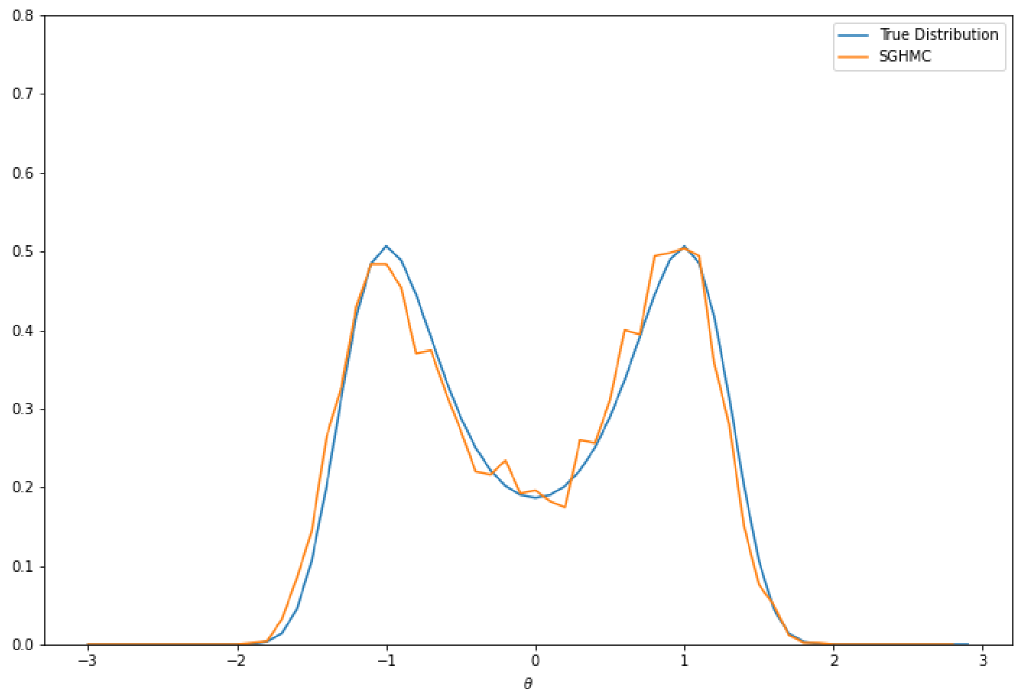
Algorithm	Running Time
Plain python (numpy)	8.27 s ± 216 ms per loop
Numba	8.04 s ± 259 ms per loop

Applications to simulated data sets

This part shows the comparison of thhe distribution between the simulated data set in the original paper $U(\theta) = -2\theta^2 + \theta^4$ and the distribution from the Stochastic Gradient Hamiltonian Monte Carlo algorithm $\nabla \tilde{U}(\theta) = \nabla U(\theta) + N(0, 4)$ with following argument:

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

And a comparison figure shown as below:



Applications to real data sets

Real data sets

Competing algorithms

Discussion

References