Stochastic Gradient Descent Hamiltonian Monte Carlo Applied to Bayesian Logistic Regression

Sta663 Final Project

Gilad Amitai and Beau Coker

Abstract

Hamiltonian Monte Carlo (HMC) is a Markov chain Monte Carlo algorithm for drawing samples from a probability distribution where proposed values are computed using Hamiltonian dynamics to find values of high acceptance probabilities. They allow us to explore sample states more efficiently than random walk proposals, but are limited by the expensive computation of the gradient of the potential energy function. Chen, Fox, and Guestrin propose the method Stochastic Gradient Hamiltonian Monte Carlo (SGHMC), a HMC algorithm that uses a subset of the data to compute the gradient. The authors find that the stochastic gradient is noisy and correct this with a friction term.

In this project, we adapt the SGHMC to be used for Bayesian Logistic regression, implement this method in Python, optimize the code for computational efficiency, validate our approach using simulated data, and apply the algorithm to real world classification problems.

Keywords: Hamiltonian Monte Carlo, Stochastic Gradient Hamiltonian Monte Carlo, Pima Indians Diabetes Dataset, Hockey Puck, Logistic Regression, Markov chain Monte Carlo

1 Background

Because this is a project about Hamiltonian Monte Carlo, imagine a frictionless puck on an icy surface of varying heights. The state of this puck is given by it's momentum $\boldsymbol{q}$ and position $\boldsymbol{p}$. The potential energy of the puck U will be a function of only its height, while the kinetic energy will be a function of its momentum $K(q) = \frac{|\boldsymbol{q}|^2}{2m}$. If the ice is flat, the puck will move with a constant velocity. If the ice slopes upwards, the kinetic energy will decrease as the potential energy increases until it reaches zero, at which point it will slide back down. In the context of Bayesian statistics, we can think of the position as the posterior distribution we want to sample from, and the momentum variable are artificial constructs that allow us to efficiently move around our space. The Hamiltonian $H(q, p)$ will be the sum of the potential and kinetic energy, and its partial derivatives will determine how q and p change overt ime t

$$\frac{dp_i}{dt} = \frac{\partial H}{\partial q_i}$$

Input: Starting position $\theta^{(1)}$ and step size ϵ.
for *t=1, 2, ...* **do**
  Sample momentum $r^{(1)} \sim \mathcal{N}(0, M)$
  $r_0 = r_0 + \frac{\epsilon}{2}\Delta U(\theta_0)$
  for *i=1,...,m* **do**
    $\theta_i = \theta_{i-1} + \epsilon M^{-1} r_{i-1}$
    $r_i = r_{i-1} - \epsilon \Delta U(\theta_i)$
  end
  $r_m = r_m - \frac{\epsilon}{2}\Delta U(\theta_m)$
  $(\hat{\theta}, \hat{r}) = (\theta_m, r_m)$
  Sample $u \sim$ Uniform$[0, 1]$
  $\rho = \exp\left\{H(\hat{\theta}, \hat{r}) - H(\theta^{(t)}, r^{(t)})\right\}$
  if $u < \min(1, \rho)$ **then**
    $\theta^{(t+1)} = \hat{\theta}$
  end
end

2 Description of Algorithm

In their *Stochastic Gradient Hamiltonian Monte Carlo*, Chen, Fox, and Guestrin propose using a subset $\tilde{\mathcal{D}}$ of the entire dataset $\mathcal{D}$ to compute

$$\Delta\tilde{U}(\theta) = -\frac{|\mathcal{D}|}{|\tilde{\mathcal{D}}|}\sum_{x\in\tilde{\mathcal{D}}} \Delta \log p(x|\theta) - \Delta \log p(\theta)$$

which can then be used in the Hamiltonian Monte Carlo equations in the stead of the gradient $\Delta U(\theta)$. Logistic regression assigns the probability of success to a dichotomous response variable

$$\Pr\left(y_i = 1|\boldsymbol{x}_i, \boldsymbol{\beta}\right) = \frac{\exp\left\{\boldsymbol{x}_i^T\boldsymbol{\beta}\right\}}{1 + \exp\left\{\boldsymbol{x}_i^T\boldsymbol{\beta}\right\}}$$

where $\boldsymbol{x}_i$ is a vector of length p covariates for data point i and $\boldsymbol{\beta}$ is a vector of regression coefficients of length p. In a Bayesian framework, we would assign the a prior distribution on our unknown parameters $P(\boldsymbol{\beta}) \sim \mathcal{N}(0, \sigma^2)$ where, for the purposes of our project, σ^2 is known. The corresponding posterior will be proportional to $P(\theta)\prod_{i=1}^n \Pr\left(y_i|\boldsymbol{x}_i, \boldsymbol{\beta}\right)$, which would give us the potential energy function

$$U(\boldsymbol{\beta}) = -\log\left[P(\boldsymbol{\beta})\right] - \sum_{i=1}^n \log\left[\Pr\left(y_i|\boldsymbol{x}_i, \boldsymbol{\beta}\right)\right] = \sum_{j=1}^p \frac{\beta_j^2}{2\sigma^2} - \sum_{i=1}^n \left[y_i(\boldsymbol{x}_i^T\boldsymbol{\beta}) - \log(1 + \exp\left\{\boldsymbol{x}_i^T\boldsymbol{\beta}\right\})\right]$$

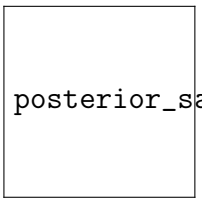
and gradient components

$$\frac{\partial U}{\partial \beta_j} = \frac{\beta_j}{\sigma^2} - \sum_{i=1}^n x_{ij}\left[y_i - \frac{\exp\left\{\boldsymbol{x}_i^T\boldsymbol{\beta}\right\}}{1 + \exp\left\{\boldsymbol{x}_i^T\boldsymbol{\beta}\right\}}\right].$$

In practice, the stochastic gradient is noisy since it is an approximation of the gradient. The paper suggests introducing a friction term to the momentum to dampen the movement of the chain. The

algorithm will take a user specified friction term C that is element-wise bigger than the noise model B. The noise model is unknown but can be set to zero for simplicity. The final algorithm will be:

Input: Starting position $\theta^{(1)}$ and step size ϵ.
for *t=1, 2, ...* **do**
  Sample momentum $r^{(1)} \sim \mathcal{N}(0, M)$
  for *i=1,...,m* **do**
    $\theta_i = \theta_{i-1} + \epsilon M^{-1} r_{i-1}$
    $r_i = r_{i-1} + \epsilon \Delta \tilde{U}(\theta_i) - \epsilon C M^{-1} r_{i-1} + \mathcal{N}(0, 2(C - \hat{B})\epsilon)$
  end
  $(\theta^{t+1}, r^{t+1}) = (\theta_m, r_m)$
end



3 Optimization

blah blah blah

4 Application to Simulated Data

describe how to create data show that it returns something close to the MLE

5 Application to Real Data

traceplots coefficients description of pima dataset

6 Comparative Analysis

blah blah blah

7 Discussion and Conclusion

blah blah blah

8 Bibliography