Statistical Models & Computing Methods

Lecture 6: Scalable MCMC

Cheng Zhang

School of Mathematical Sciences, Peking University

November 12, 2020

Motivation

- Large scale datasets are becoming more commonly available across many fields. Learning complex models from these datasets is the future
- While many modern MCMC methods have been proposed in recent years, they usually require expensive computation when the data size is large
- In this lecture, we will discuss recent development on Markov chain Monte Carlo methods that are applicable to large scale datasets
  - Best of both worlds: scalability, and Bayesian protection against overfitting

- Stochastic differential equations are widely used to model dynamical systems with noise

$$dX_t = \mu(X_t, t)dt + \sigma(X_t, t)dB_t$$

  where B denotes a Wiener process/Brownian motion
- Now suppose the probability density for X_t is $p(x,t)$, we are interested in how $p(x,t)$ evolves along time
- For example, does it converge to some distribution? If it does, how can we find it out?

- It turns out the $p(x,t)$ satisfies the Fokker-Planck equation (also known as the Kolmogorov forward equation)

$$\frac{\partial p(x,t)}{\partial t} = -\sum_i \frac{\partial}{\partial x_i}(\mu_i(x,t)p(x,t)) + \sum_{i,j} \frac{\partial^2}{\partial x_i \partial x_j}(D_{ij}(x,t)p(x,t))$$

where $D = \frac{1}{2}\sigma\sigma^T$ is the diffuse tensor

- Example: Weiner process $dX_t = dB_t$

$$\frac{\partial p(x,t)}{\partial t} = \frac{1}{2}\frac{\partial^2}{\partial x^2}p(x,t)$$

If $p(x,0) = \delta(x)$, the solution is $p(x,t) = \frac{1}{\sqrt{2\pi t}}e^{-\frac{x^2}{2t}}$

Challenges From Massive Datasets

- Suppose that we have a large number of data items

$$\mathcal{D} = \{x_1, x_2, \ldots, x_N\}$$

where $N \gg 1$

- The log-posterior (up to a constant) is

$$\log p(\theta|X) = \log p(\theta) + \sum_{i=1}^{N} \log p(x_i|\theta) \sim \mathcal{O}(N)$$

- How to reduce this computation in MCMC without damaging the convergence to the target distribution?

Stochastic Gradient Ascent

- Also known as stochastic approximation
- At each iteration
  - Get a subset (minibatch) $x_{t_1}, \ldots, x_{t_n}$ of data items where $n \ll N$
  - Approximate gradient of log-posterior using the subset

$$\nabla \log p(\theta_t | X) \approx \nabla \log p(\theta_t) + \frac{N}{n} \sum_{i=1}^{n} \nabla \log p(x_{t_i} | \theta_t)$$

  - Take a gradient step

$$\theta_{t+1} = \theta_t + \frac{\epsilon_t}{2} \left(\nabla \log p(\theta_t) + \frac{N}{n} \sum_{i=1}^{n} \nabla \log p(x_{t_i} | \theta_t) \right)$$

Stochastic Gradient Ascent

- Major requirement for convergence on step-sizes

$$\sum_{t=1}^{\infty} \epsilon_t = \infty, \quad \sum_{t=1}^{\infty} \epsilon_t^2 < \infty$$

- Intuition
  - Step sizes cannot decrease too fast, otherwise will not be able to explore parameter space
  - Step sizes must decrease to zero, otherwise will not converge to a local mode

- **First order Langevin dynamics** can be described by the following stochastic differential equation

$$d\theta_t = \frac{1}{2}\nabla \log p(\theta_t|X)dt + dB_t$$

- The above dynamical system converges to the target distribution $p(\theta|X)$ (easy to verify via the Fokker-Planck equation)
- Intuition
  - Gradient term encourages dynamics to spend more time in high probability areas
  - Brownian motion provides noise so that dynamics will explore the whole parameter space

- First order Euler discretization

$$\theta_{t+1} = \theta_t + \frac{\epsilon}{2}\nabla \log p(\theta_t|X) + \eta_t, \quad \eta_t = \mathcal{N}(0, \epsilon)$$

- Amount of noise is balanced to gradient step size
- With finite step size, there will be discretization errors. We can add MH correction step to fix it, and this is MALA!
- As step size $\epsilon \to 0$, acceptance rate goes to 1

Stochastic Gradient Langevin Dynamics

- Introduced by Welling and Teh (2011)
- **Idea**: use stochastic gradients in Langevin dynamics

$$\theta_{t+1} = \theta_t + \frac{\epsilon_t}{2} g(\theta_t) + \eta_t, \quad \eta_t = \mathcal{N}(0, \epsilon_t)$$

$$g(\theta_t) = \nabla \log p(\theta_t) + \frac{N}{n} \sum_{i=1}^{n} \nabla \log p(x_{t_i} | \theta_t)$$

- Update is just stochastic gradient ascent plus Gaussian noise
- Noise variance is balanced with gradient step sizes
- require step size ϵ_t decrease to 0 slowly

Why SGLD Works?

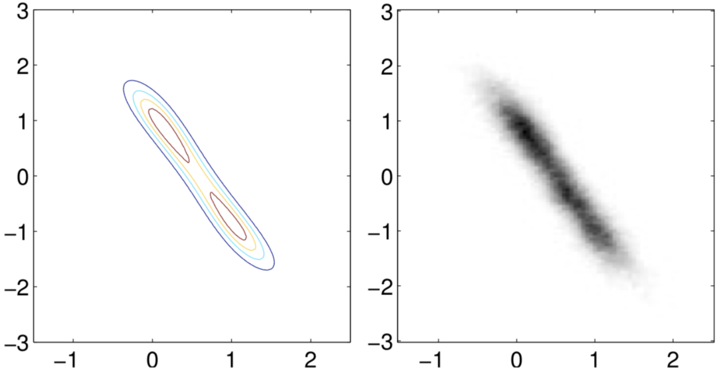
- Controllable stochastic gradient noise. The stochastic gradient estimate $g(\theta_t)$ is unbiased, but it introduces noise

$$g(\theta_t) = \nabla \log p(\theta|X) + \mathcal{N}(0, V(\theta_t))$$

  - Stochastic gradient noise $\sim \mathcal{N}(0, \mathcal{O}(\epsilon_t^2))$
  - Injected noise $\eta_t \sim \mathcal{N}(0, \epsilon_t)$
- When $\epsilon_t \to 0$
  - Stochastic gradient noise will be dominated by injected noise η_t, so can be ignored. SGLD then recovers Langevin dynamics updates with decreasing step sizes
  - MH acceptance probability approaches 1, so we can ignore the expensive MH correction step
  - If ϵ_t approaches 0 slowly enough, the discretized Langevin dynamics is still able to explore the whole parameter space

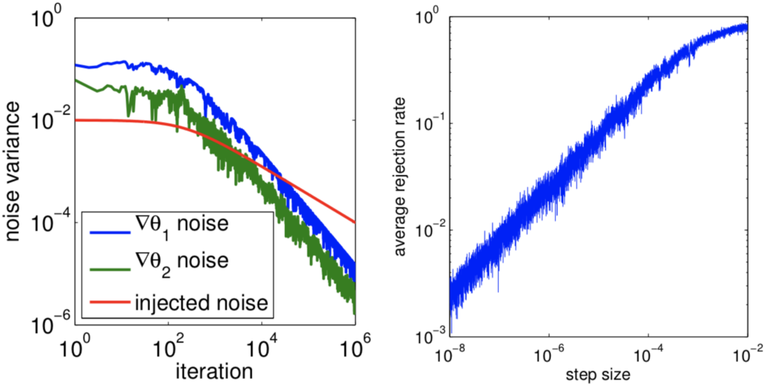
Examples: Mixture of Gaussian

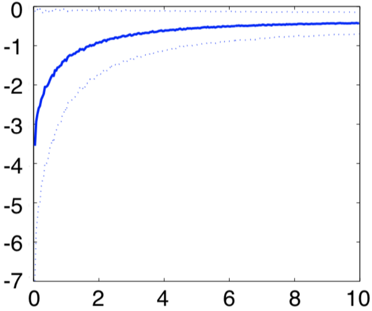
$$\theta_1 \sim \mathcal{N}(0, \sigma_1^2), \quad \theta_2 \sim \mathcal{N}(0, \sigma_2^2)$$
$$x_i \sim \frac{1}{2}\mathcal{N}(\theta_1, \sigma_x^2) + \frac{1}{2}\mathcal{N}(\theta_1 + \theta_2, \sigma_x^2)$$



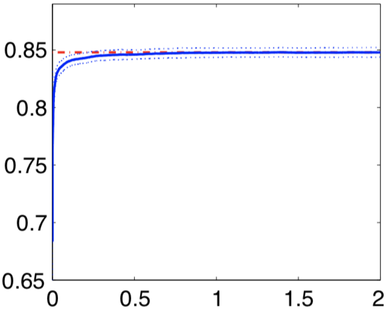
Examples: Mixture of Gaussian

Noise and rejection probability





Log probability vs epoches



Test accuracy vs epoches

Naive Stochastic Gradient HMC

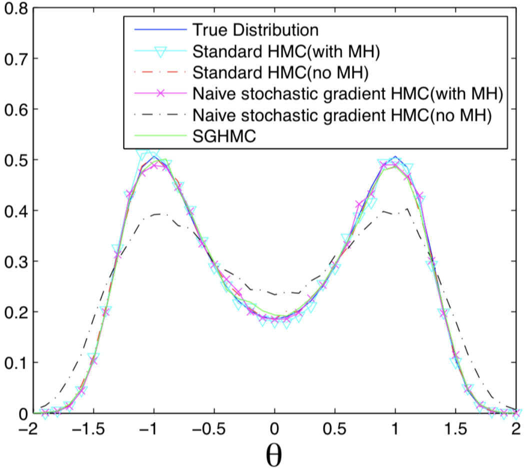
- Now that stochastic gradient scales MALA, it seems straightforward to use stochastic gradient for HMC

$$d\theta = M^{-1} r dt$$
$$dr = g(\theta)dt = -\nabla U(\theta)dt + \sqrt{\epsilon V(\theta)}dB_t$$

- However, the resulting dynamics does not leave $p(\theta, r)$ invariant (can be verified via Fokker-Planck equation)
- This deviation can be saved by MH correction, but that leads to a complex computation vs efficiency trade-off
  - Short runs reduce deviation, but requires more expensive HM steps and does not full utilize the exploration of the Hamiltonian dynamics
  - Long runs lead to low acceptance rates, waste of computation

Example: Naive Stochastic Gradient HMC Fails

$$U(\theta) = -2\theta^2 + \theta^4$$



- We can introduce friction into the dynamical system to reduce the influence of the gradient noise, which leads to the **second order Langevin dynamics**

$$\begin{aligned} d\theta &= M^{-1} r dt \\ dr &= -\nabla U(\theta) dt - C M^{-1} r dt + \sqrt{2C} dB_t \end{aligned} \tag{1}$$

- Consider the joint space $z = (\theta, r)$, rewrite (1)

$$dz = -[D + G] \nabla H(z) dt + \sqrt{2D} dB_t$$

where

$$G = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix}, \quad D = \begin{bmatrix} 0 & 0 \\ 0 & C \end{bmatrix}$$

- $p(\theta, r) \propto \exp(-H(\theta, r))$ is the unique stationary distribution of (1)

Stochastic Gradient HMC

- Introduced by Chen et al (2014)
- Use stochastic gradient in the second order Langevin dynamics. In each iteration
  - resample momentum $r^{(t)} \sim \mathcal{N}(0, M)$ (optional), $(\theta_0, r_0) = (\theta^{(t)}, r^{(t)})$
  - simulate dynamics in (1)

$$\begin{aligned}
\theta_i &= \theta_{i-1} + \epsilon_t M^{-1} r_{i-1} \\
r_i &= r_{i-1} + \epsilon_t g(\theta_i) - \epsilon_t C M^{-1} r_{i-1} + \mathcal{N}(0, 2C\epsilon_t)
\end{aligned}$$

  - update the parameter $(\theta^{(t+1)}, r^{(t+1)}) = (\theta_m, r_m)$, no MH correction step
- Similarly, the stochastic gradient noise is controllable, and when $\epsilon_t \to 0$, **SGHMC** recovers the second order Langevin dynamics

- Let $v = \epsilon M^{-1} r$, we can rewrite the update rule in SGHMC

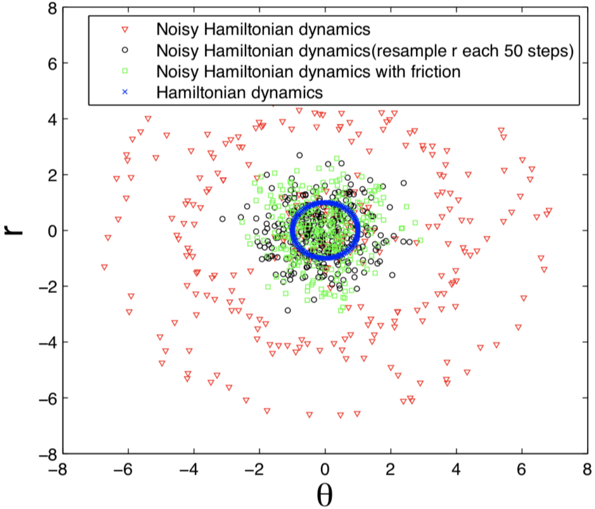
$$\Delta v = \epsilon^2 M^{-1} g(\theta) - \epsilon M^{-1} C v + \mathcal{N}(0, 2\epsilon^3 M^{-1} C M^{-1})$$
$$\Delta \theta = v$$

- Define $\eta = \epsilon^2 M^{-1}, \alpha = \epsilon M^{-1} C$, the update rule becomes

$$\Delta v = \eta g(\theta) - \alpha v + \mathcal{N}(0, 2\alpha\eta)$$
$$\Delta \theta = v$$

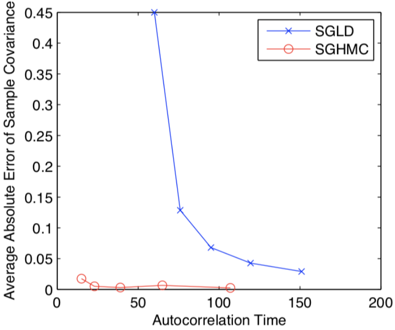
- If we ignore the noise term, this is basically SGD with momentum where η is the learning rate and $1 - \alpha$ the momentum coefficient
- This connection can be used to guide our choices of SGHMC hyper-parameters

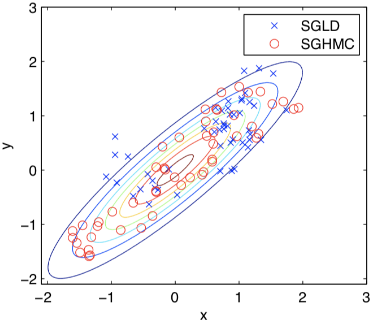
Examples: Univariate Standard Normal



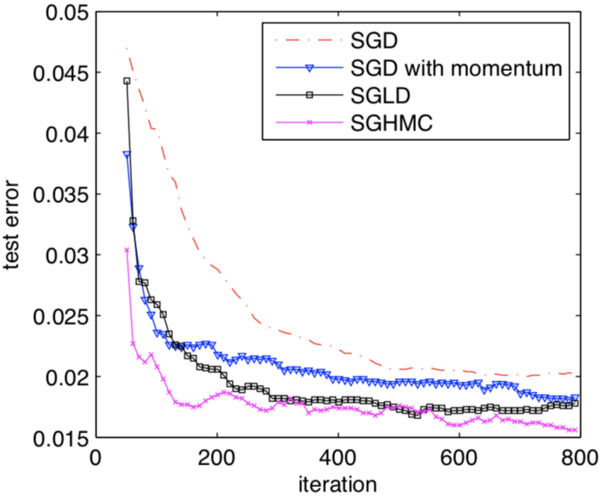
SGHMC vs SGLD on a bivariate Gaussian with correlation

$$U(\theta) = \frac{1}{2}\theta^T \Sigma^{-1}\theta, \quad \Sigma^{-1} = \begin{pmatrix} 1 & 0.9 \\ 0.9 & 1 \end{pmatrix}$$





Examples: MNIST Dataset



- Stochastic gradient in SGHMC introduces noise. With step size ϵ, the corresponding dynamics is

$$d\theta = M^{-1} r dt$$

$$dr = -\nabla U(\theta)dt - CM^{-1}dt + \sqrt{2(C + \frac{1}{2}\epsilon V(\theta))}dB_t$$

- If somehow we correct the mismatch between friction coefficient and the real noise level, we can improve the approximation accuracy for a finite ϵ
- But how can we do that given that the noise $V(\theta)$ is unknown?

Nosé-Hoover Thermostat

- One missing key fact is the thermal equilibrium condition:

$$p(\theta, r) \propto \exp\left(-(U(\theta) + K(r))/T\right) \Rightarrow T = \frac{1}{d}\mathbb{E}(r^T r)$$

- Unfortunately, using stochastic gradients destroys the thermal equilibrium condition
- We can introduce an additional variable ξ that adaptively controls the mean kinetic energy, and use the following dynamics

$$d\theta = r dt, \quad dr = g(\theta)dt - \xi r dt + \sqrt{2A}dB_t$$
$$d\xi = (\frac{1}{d}r^T r - 1)dt \tag{2}$$

- (2) is known as the Nosé-Hoover thermostat in statistical physics.

Stochastic Gradient Nosé-Hoover Thermostat

- Introduced by Ding et al (2014)
- The algorithm
  - Initialized $\theta_0, r_0 \sim \mathcal{N}(0, I)$, and $\xi_0 = A$
  - For $t = 1, 2, \ldots$

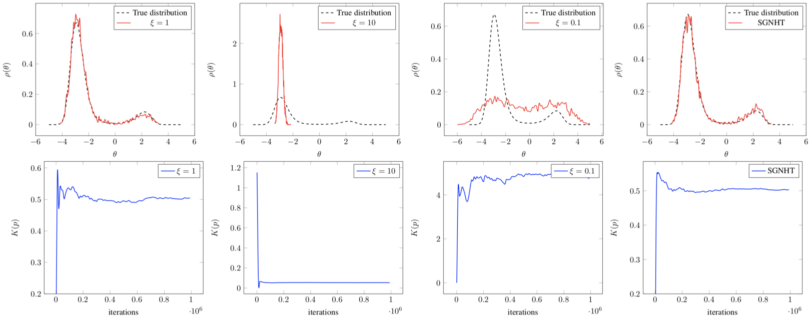
$$
\begin{aligned}
r_t &= r_{t-1} + \epsilon_t g(\theta_{t-1}) - \epsilon_t \xi_{t-1} r_{t-1} + \sqrt{2A}\mathcal{N}(0, \epsilon) \\
\theta_t &= \theta_{t-1} + \epsilon_t r_t \\
\xi_t &= \xi_{t-1} + \epsilon_t ((r^{(t)})^T r^{(t)}/d - 1)
\end{aligned}
$$

- The thermostat ξ helps to adjust the friction according to the real noise level, and maintains the right mean kinetic energy
  - When mean kinetic energy is high, ξ get bigger, increasing friction to cool down the system
  - When mean kinetic energy is low, ξ get smaller, reducing friction to heat up the system

Example: A Double-well Potential

$$U(\theta) = (\theta+4)(\theta+1)(\theta-1)(\theta-3)/14 + 0.5$$
$$g(\theta)\epsilon = -\nabla U(\theta)\epsilon + \mathcal{N}(0, 2B\epsilon), \quad \epsilon = 0.01, B = 1$$

For SGNHT, we set $A = 0$



- Consider the following stochastic differential equation
$$d\Gamma = v(\Gamma)dt + \mathcal{N}(0, 2D(\theta)dt)$$
where $\Gamma = (\theta, r, \xi)$.
- $p(\Gamma) \propto \exp(-H(\Gamma))$ is the stationary distribution if
$$\nabla \cdot (p(\Gamma)v(\Gamma)) = \nabla\nabla^T : (p(\Gamma)D)$$
We can construct H such that the marginal distribution is $p(\theta) \propto \exp(-U(\theta))$.
- For SGNHT, $H(\Gamma) = U(\theta) + \frac{1}{2}r^T r + \frac{d}{2}(\xi - A)^2$
$$v(\Gamma) = \begin{bmatrix} r \\ -\nabla U(\theta) - \xi r \\ r^T r/d - 1 \end{bmatrix}, \quad D(\theta) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

A Recipe for Continuous Dynamics MCMC

- Introduced by Ma et al (2015)
- Assume target distribution $p(\theta|X)$ is the marginal distribution of $p(z) \propto \exp(-H(z))$
- We consider the following stochastic differential equation

$$dz = -(D(z) + Q(z))\nabla H(z)dt + \Gamma(z)dt + \sqrt{2D(z)}dB_t$$

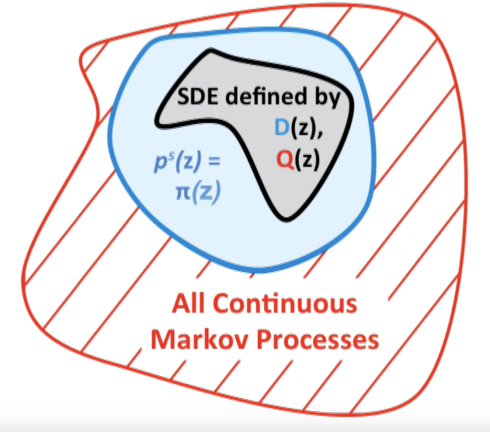
$$\Gamma_i(z) = \sum_{j=1}^{d} \frac{\partial}{\partial z_j}(D_{ij}(z) + Q_{ij}(z))$$

  - $Q(z)$ is a skew-symmetric curl matrix
  - $D(z)$ denotes the positive semidefinite diffusion matrix
- The above dynamics leaves $p(z)$ invariant

The Recipe is Complete

All existing samplers can be written in framework

- HMC
- Riemannian HMC
- Langevin Dynamics (LD)
- Riemannian LD

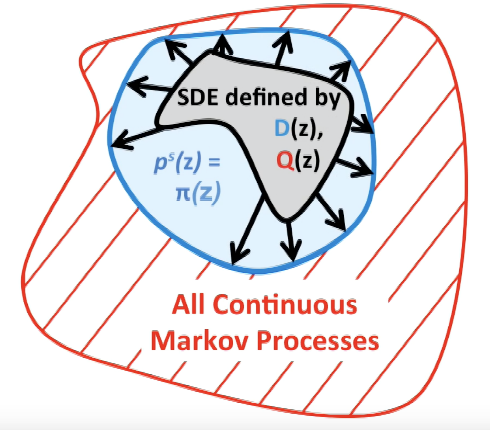


Adapted from Emily Fox 2017

All existing samplers can be written in framework

- HMC
- Riemannian HMC
- Langevin Dynamics (LD)
- Riemannian LD

Any valid sampler has a D and Q in the framework



Adapted from Emily Fox 2017

A Practical Algorithm

- Consider ϵ-discretization

$$z_{t+1} = z_t - \epsilon_t((D(z_t) + Q(z_t))\nabla H(z_t) + \Gamma(z_t)) + \mathcal{N}(0, 2\epsilon_t D(z_t))$$

- The gradient computation in $\nabla H(z_t)$ could be expansive, can be replaced with stochastic gradient $\nabla \tilde{H}(z_t)$

$$z_{t+1} = z_t - \epsilon_t((D(z_t) + Q(z_t))\nabla \tilde{H}(z_t) + \Gamma(z_t)) + \mathcal{N}(0, 2\epsilon_t D(z_t))$$

- The gradient noise is still controllable

$$\nabla \tilde{H}(z_t) = \nabla H(z_t) + (\mathcal{N}(0, V(\theta)), 0)^T$$

  - stochastic gradient noise $\sim \mathcal{N}(0, \epsilon_t^2 V(\theta))$
  - injected noise $\sim \mathcal{N}(0, 2\epsilon_t D(z_t))$

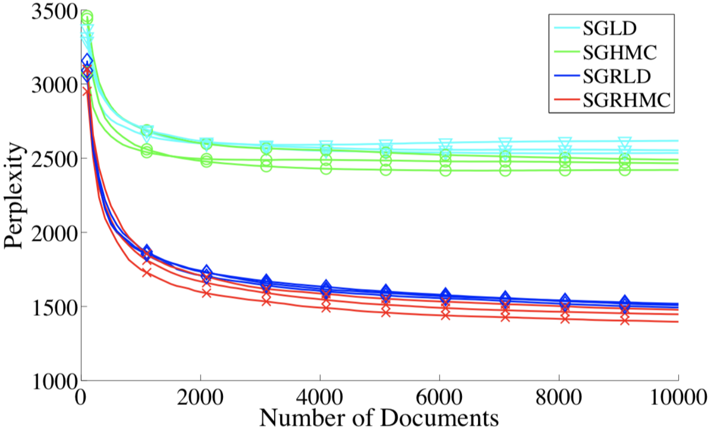
- As shown before, previous stochastic gradient MCMC algorithms all cast into this framework
- Moreover, the framework helps to develop new samplers without requiring significant physical intuition
- Consider $H(\theta, r) = U(\theta) + \frac{1}{2}r^T r$, modify D and Q to account for the geometry

$$D(\theta, r) = \begin{pmatrix} 0 & 0 \\ 0 & G(\theta)^{-1} \end{pmatrix}, \quad Q(\theta, r) = \begin{pmatrix} 0 & -G(\theta)^{-1/2} \\ G(\theta)^{-1/2} & 0 \end{pmatrix}$$

Note that this works for any positive definite $G(\theta)$, not just the fisher information metric

Applied SGRHMC to online LDA

- each entry was analyzed on the fly



Alternative Methods for Scalable MCMC

- Reduce the computation in MH correction step via subsets of data (Korattikara et al 2014)
- Divide and conquer: divide the entire data set into small chunks, run MCMC in parallel for these subsets of data, and merge the results for the true posterior approximation (Scott et al 2016)
- Using deterministic approximation instead of stochastic gradients. This may introduce some bias, but remove the unknown noise for gradient estimation, allowing for better exploration efficiency
  - Gaussian processes: Rasmussen 2003, Lan et al 2016
  - Reproducing kernel Hilbert space: Strathmann et al 2015
  - Random Bases: Zhang et al 2017

- M. Welling and Y.W. Teh. Bayesian learning via stochastic gradient Langevin dynamics. In Proceedings of the 28th International Conference on Machine Learning (ICML'11), pages 681–688, June 2011.
- T. Chen, E.B. Fox, and C. Guestrin. Stochastic gradient Hamiltonian Monte Carlo. In Proceeding of 31st International Conference on Machine Learning (ICML'14), 2014.
- N. Ding, Y. Fang, R. Babbush, C. Chen, R.D. Skeel, and H. Neven. Bayesian sampling using stochastic gradient thermostats. In Advances in Neural Information Processing Systems 27 (NIPS'14). 2014.

- Ma, Y.A., Chen, T. and Fox, E. (2015). A complete recipe for stochastic gradient MCMC. In Advances in Neural Information Processing Systems 2917–2925.
- A. Korattikara, Y. Chen, and M. Welling. Austerity in MCMC land: Cutting the Metropolis-Hastings budget. In Proceedings of the 30th International Conference on Machine Learning (ICML'14), 2014.
- Scott, S. L., Blocker, A. W., Bonassi, F. V., Chipman, H. A., George, E. I. and McCullogh, R. E. (2016). Bayes and Big Data: The Consensus Monte Carlo Algorithm. International Journal of Management Science and Engineering Management 11 78-88.

- Rasmussen, C. E. (2003). "Gaussian Processes to Speed up Hybrid Monte Carlo for Expensive Bayesian Integrals." Bayesian Statistics, 7: 651–659.
- Lan, S., Bui-Thanh, T., Christie, M., and Girolami, M. (2016). Emulation of higher-order tensors in manifold Monte Carlo methods for Bayesian inverse problems. J. Comput. Phys., 308:81–101.
- Strathmann, H., Sejdinovic, D., Livingstone, S., Szabo, Z., and Gretton, A. Gradient-free Hamiltonian monte carlo with efficient kernel exponential families. In Advances in Neural Information Processing Systems, pp. 955–963, 2015

References

- Zhang, C., Shahbaba, B., and Zhao, H. (2017). "Hamiltonian Monte Carlo acceleration using surrogate functions with random bases." Statistics and Computing, 1–18.