Stochastic MCMC techniques

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Deep|Bayes

What stochasticity we are talking about?

We want to sample from posterior distribution

$$p(\theta|X) \propto p(\theta) \prod_{i=1}^{N} p(x_i|\theta)$$

Full dataset!

How to use minibatches instead of full dataset?

Minibatch MCMC techniques

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DeepBayes

Variational Bayes vs. MCMC

	MCMC	IPM	Variational Bayes
Bias	No	??	Strong
Sampling/Ensembling	Inefficient	??	Efficient
Density	No	??	Yes
Likelihood	Needed	??	Needed

Metropolis-Hastings

$$\alpha(\theta, \theta') = \frac{p(\theta'|X)q(\theta|\theta')}{p(\theta|X)q(\theta'|\theta)}$$

$$\alpha(\theta, \theta') = \frac{p_0(\theta') \prod_{i=1}^{N} p(x_i|\theta')q(\theta|\theta')}{p_0(\theta) \prod_{i=1}^{N} p(x_i|\theta)q(\theta'|\theta)}$$

Full dataset!

$p_0(\theta)$ – prior distribution

Accept θ' if

$$\alpha(\theta, \theta') > u, \qquad u \sim \text{Uniform}[0,1]$$

An Efficient Minibatch Acceptance Test for Metropolis-Hastings

Deniel Seita, Xinlei Pan, Haoyu Chen, Jhon Canny

Barker lemma

$$\Delta(\theta, \theta') = \log \frac{p_0(\theta') \prod_{i=1}^{N} p(x_i|\theta') q(\theta|\theta')}{p_0(\theta) \prod_{i=1}^{N} p(x_i|\theta) q(\theta'|\theta)}$$

For any function $g(s)$ such that $g(s) = \exp(s)\, g(-s)$,
$\alpha(\theta, \theta') \triangleq g(\Delta(\theta, \theta'))$ satisfies detailed balance.

What does it mean?

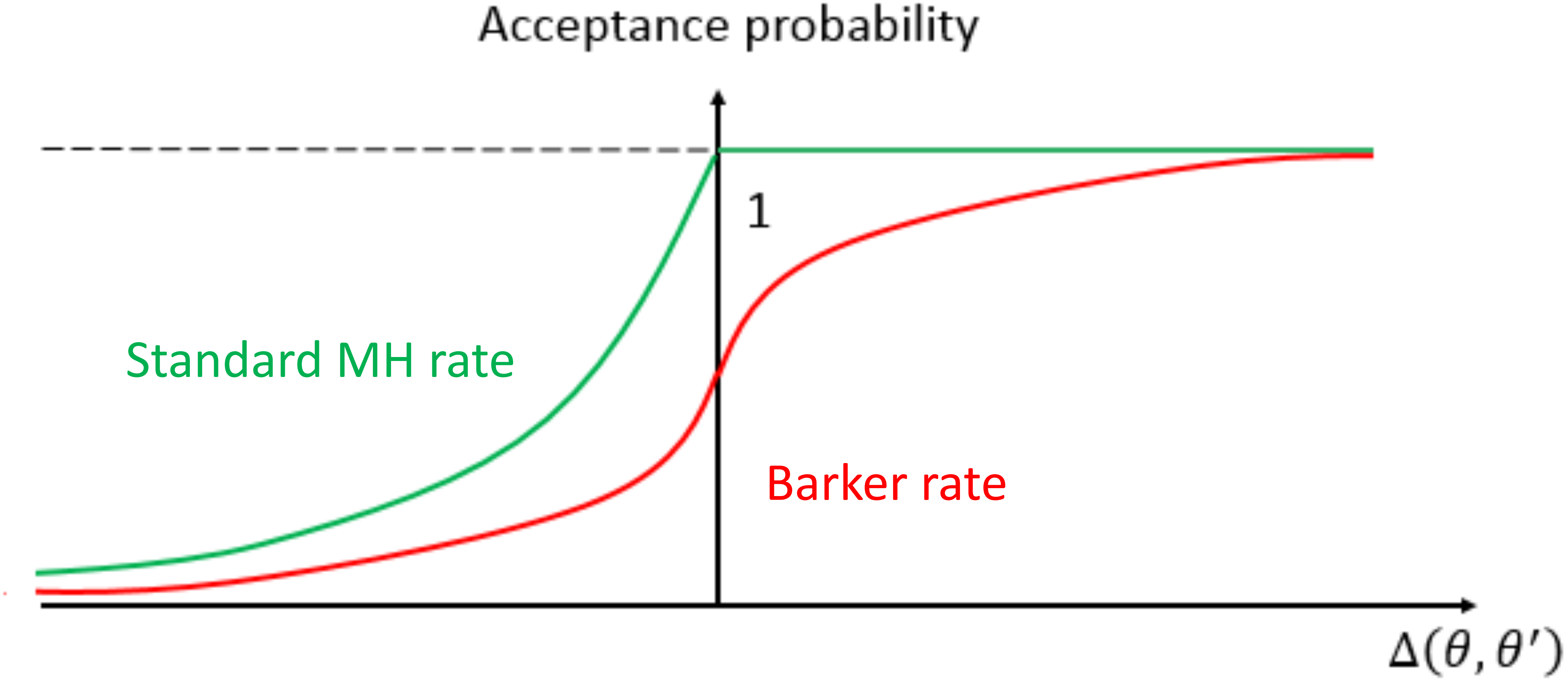
$$\Delta(\theta, \theta') = \log \frac{p_0(\theta') \prod_{i=1}^{N} p(x_i|\theta') q(\theta|\theta')}{p_0(\theta) \prod_{i=1}^{N} p(x_i|\theta) q(\theta'|\theta)}$$

If g satisfies Barker lemma, then performing the test

$$g(\Delta(\theta, \theta')) > u, \qquad u \sim \text{Uniform}[0,1]$$

we sample from true posterior distribution!

Acceptance rate



Barker acceptance function

Let $g(s) = \frac{1}{1+\exp(-s)}$, then test

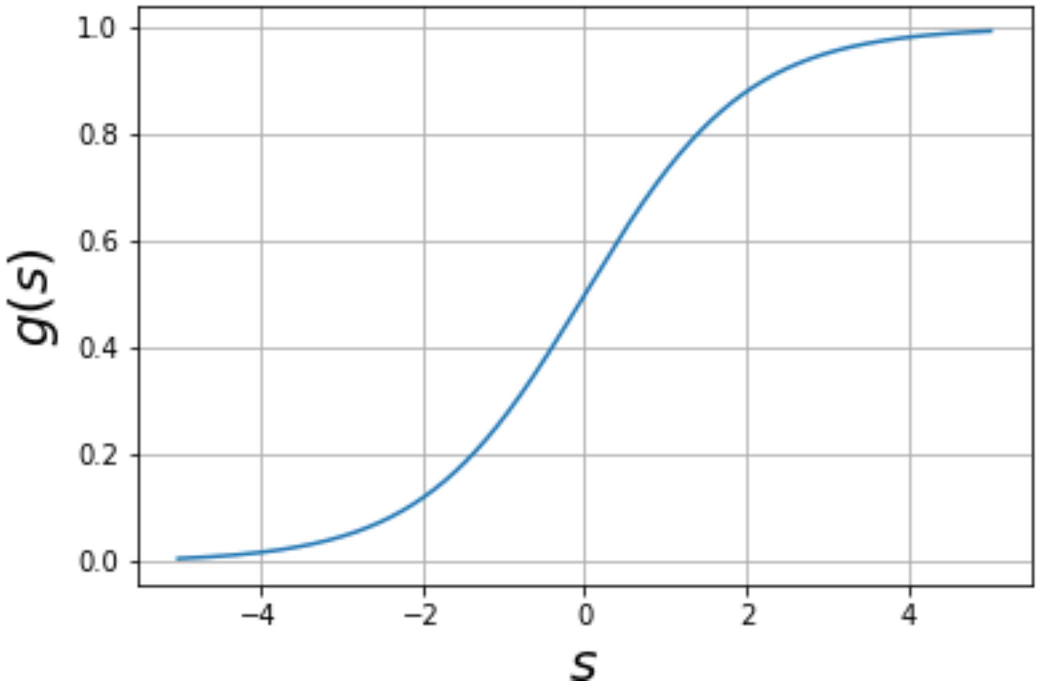
$$g\big(\Delta(\theta, \theta')\big) > u, \qquad u \sim \mathrm{Uniform}[0,1]$$

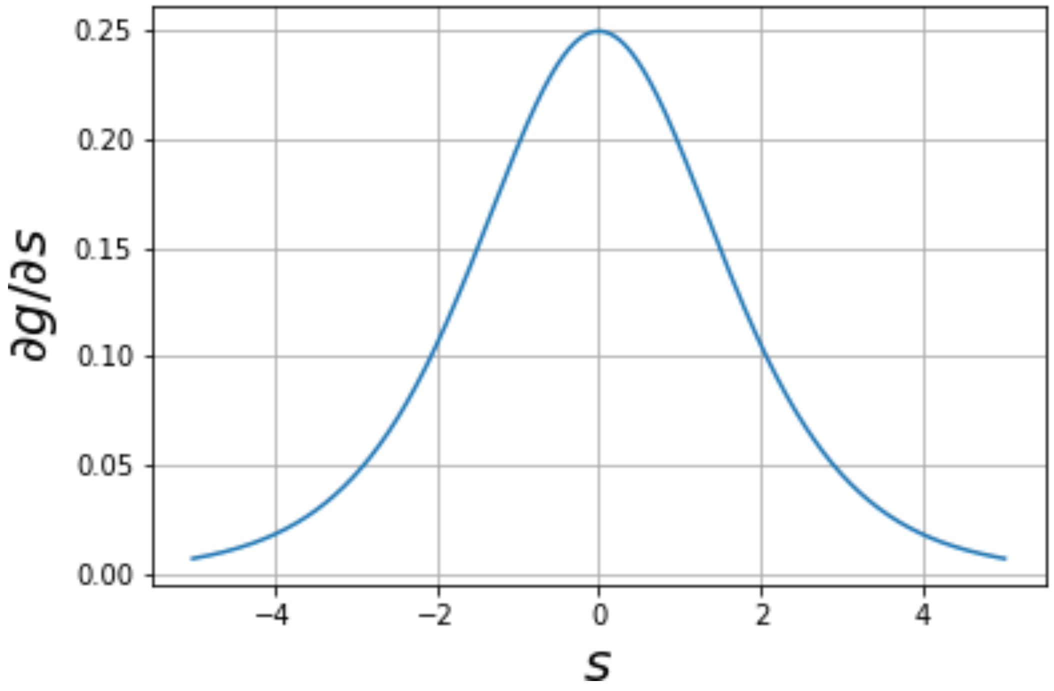
satisfies detailed balance and

$$\Delta(\theta, \theta') > X = g^{-1}(u), \qquad u \sim \mathrm{Uniform}[0,1]$$

also satisfies detailed balance

$g^{-1}(u)$ – sample from logistic distribution





$$X = X_{log} \sim \text{Logistic}(0,1)$$

$$-X_{log} \sim \text{Logistic}(0,1)$$

New acceptance test

$$\Delta(\theta,\theta') = \sum_i^N \log\frac{p(x_i|\theta')}{p(x_i|\theta)} + \log\frac{p_0(\theta')q(\theta|\theta')}{p_0(\theta)q(\theta'|\theta)}$$

Accept θ' if

$$\Delta(\theta,\theta') > X = g^{-1}(u), \qquad u \sim \text{Uniform}[0,1]$$

Or equivalently

$$\Delta(\theta,\theta') + X_{log} > 0, \qquad X_{log} \sim \text{Logistic}(0,1)$$

Exact, but we still use full dataset to sample one point

Minibatch acceptance test

$$\Delta^*(\theta, \theta') = \frac{N}{b} \sum_{i=1}^{b} \log \frac{p(x_i|\theta')}{p(x_i|\theta)} + \log \frac{p_0(\theta')q(\theta|\theta')}{p_0(\theta)q(\theta'|\theta)}$$

$$\Delta^* = \Delta + \mathrm{X}_{\mathrm{norm}}, \qquad \mathrm{X}_{\mathrm{norm}} \sim \overline{\mathcal{N}}\left(0, \sigma^2(\Delta^*)\right)$$

$\mathrm{X}_{\mathrm{norm}}$ – approximately normal distribution (Central Limit Theorem)

$$\Delta_i = N \log \frac{p(x_i|\theta')}{p(x_i|\theta)} + \log \frac{p_0(\theta')q(\theta|\theta')}{p_0(\theta)q(\theta'|\theta)}$$

$$\sigma^2(\Delta^*) = \sum_{i=1}^{b} \left(\Delta_i - \overline{\Delta}\right)^2$$

How to use Δ^* instead of Δ?

$$\Delta(\theta,\theta') = \sum_{i}^{N} \log \frac{p(x_i|\theta')}{p(x_i|\theta)} + \log \frac{p_0(\theta')q(\theta|\theta')}{p_0(\theta)q(\theta'|\theta)}$$

Accept θ' if

$$\Delta(\theta,\theta') + X_{log} > 0, \qquad X_{log} \sim \mathrm{Logistic}(0,1)$$

Our current test

But for minibatches we have value

$$\Delta^* = \Delta + \mathrm{X}_{\mathrm{norm}}, \qquad \mathrm{X}_{\mathrm{norm}} \sim \overline{\mathcal{N}}\left(0, \sigma^2(\Delta^*)\right)$$

Logistic noise decomposition

Let's decompose

$$X_{log} = X_{norm} + X_{corr}, \qquad X_{norm} \sim \mathcal{N}(0, \sigma^2),$$

where X_{corr} – correction distribution with PDF $C_\sigma(x)$

Not true!

If

$$\Delta^* = \Delta + X_{norm}, \qquad X_{norm} \sim \mathcal{N}(0, \sigma^2),$$

Then

$$\Delta + X_{log} = \underbrace{\Delta + X_{norm}}_{\Delta^*} + X_{corr} = \Delta^* + X_{corr}$$

Big picture

1. Evaluate

$$\Delta^*(\theta, \theta') = \frac{N}{b} \sum_{i=1}^{b} \log \frac{p(x_i|\theta')}{p(x_i|\theta)} + \log \frac{p_0(\theta')q(\theta|\theta')}{p_0(\theta)q(\theta'|\theta)}$$

2. Sample

$$X_{corr} \sim \text{Correction Distribution}\big(\sigma^2(\Delta^*)\big)$$

3. Accept θ' if

$$\Delta^* + X_{corr} > 0$$

4. Otherwise repeat θ

We still have some questions

- How to sample from correction distribution?
- What error we have if we assume that

$$\Delta^* = \Delta + X_{norm}, \qquad X_{norm} \sim \mathcal{N}\left(0, \sigma^2(\Delta^*)\right)$$

Instead of

$$\Delta^* = \Delta + X_{norm}, \qquad X_{norm} \sim \overline{\mathcal{N}}\left(0, \sigma^2(\Delta^*)\right)$$

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PDF of the correction distribution

$$X_{log} = X_{norm} + X_{corr}, \qquad X_{norm} \sim \mathcal{N}(0, \sigma^2)$$

Φ_σ – CDF of $\mathcal{N}(0, \sigma^2)$

C_σ – PDF of corresponding correction distribution

$. * .$ – convolution operation

$$CDF(X_{norm} + X_{corr}) = \Phi_\sigma * C_\sigma$$

$$\mathbb{P}\{X + Y < t\} = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{t-x} p_x(x) p_y(y) dy = \int_{-\infty}^{+\infty} dx p_x(x) F_y(t - x)$$

PDF of the correction distribution

$$C_\sigma^* = \operatorname*{argmin}_{C_\sigma} \sup |\Phi_\sigma * C_\sigma - S|$$

S −CDF of Logistic Distribution

After discretization on the uniform grid [-20,20]

$$C_\sigma^* = \operatorname*{argmin}_{C_\sigma} \max_{\mathrm{i} \in \mathrm{I}} \left| \sum_{j \in J} \Phi_\sigma(X_i - Y_j) C_\sigma(Y_j) - S(X_i) \right|$$

Define

$$M_{ij} = \Phi_\sigma(X_i - Y_j), \qquad u_j = C_\sigma(Y_j), \qquad v_i = S(X_i)$$

Then

$$u^* = (M^T M + \lambda I)^{-1} M^T v$$

PDF of the correction distribution

S —CDF of Logistic Distribution

After discretization on the uniform grid [-20, 20]

$$C_\sigma^* = \underset{C_\sigma}{\operatorname{argmin}} \left\| \sum_{j \in J} \Phi_\sigma(X_i - Y_j) C_\sigma(Y_j) - S(X_i) \right\|_2^2 + \lambda \sum_j C_\sigma(Y_j)^2$$

Define

$$M_{ij} = \Phi_\sigma(X_i - Y_j), \qquad u_j = C_\sigma(Y_j), \qquad v_i = S(X_i)$$

Then

$$u^* = (M^T M + \lambda E)^{-1} M^T v$$

PDF of the correction distribution

Bu instead of solving

$$u^* = \underset{u}{\operatorname{argmin}} \max_{\mathrm{i} \in \mathrm{I}} |Mu - v|, \qquad u > 0$$

Let’s solve

$$u^* = \underset{u}{\operatorname{argmin}} \|Mu - v\|_2^2 + \lambda \|u\|_2^2$$

$$u^* = (M^T M + \lambda I)^{-1} M^T v$$

And show empirically that error is negligible

Precomputing correction distribution

Note that PDF $C_\sigma(x)$ depends on variance σ^2 of normal distribution $\mathcal{N}(0, \sigma^2)$

$$\underbrace{\Delta + \mathcal{N}(0, \sigma^2(\Delta^*))}_{\approx \Delta^*} + X_{corr}\left(\sigma^2(\Delta^*)\right) =$$

$$\Delta + \underbrace{\mathcal{N}\left(0, \sigma^2(\Delta^*)\right) + \mathcal{N}\left(0{,}1 - \sigma^2(\Delta^*)\right)}_{\mathcal{N}(0{,}1)} + X_{corr}(\sigma^2 = 1)$$

We can imitate standard normal noise by adding $\mathrm{X_{nc}} \sim \mathcal{N}\left(0{,}1 - \sigma^2(\Delta^*)\right)$

Good We can use precomputed $X_{corr}(\sigma^2 = 1)$

Bad We need to sample minibatches until $\sigma^2(\Delta^*) < 1$

We still have some questions

- How to sample from correction distribution?
- What error we have if we assume that

$$\Delta^* = \Delta + X_{norm}, \qquad X_{norm} \sim \mathcal{N}\left(0, \sigma^2(\Delta^*)\right)$$

Instead of

$$\Delta^* = \Delta + X_{norm}, \qquad X_{norm} \sim \overline{\mathcal{N}}\left(0, \sigma^2(\Delta^*)\right)$$

Bounding acceptance probability error

$$X_i = N \log \frac{p(x_i|\theta')}{p(x_i|\theta)} - \sum_i^N \log \frac{p(x_i|\theta')}{p(x_i|\theta)}$$

$$\approx N \log \frac{p(x_i|\theta')}{p(x_i|\theta)} - \frac{N}{b} \sum_i^b \log \frac{p(x_i|\theta')}{p(x_i|\theta)}$$

Authors bound error of acceptance probability

$$\sup_y |\mathbb{P}\{\Delta^* + X_{nc} + X_{corr} < y\} - S(y - \Delta)| \leq \frac{6.4\mathbb{E}|X|^3 + 2\mathbb{E}|X|}{\sqrt{b}} = \varepsilon$$

S −CDF of Logistic Distribution

Bounds stationary distribution

$\hat{p}$, p – stationary distributions of true and approximate transition operators $\hat{\tau}$ and τ

If

$$|\widehat{\mathbb{P}}\{\text{acceptance}\} - \mathbb{P}\{\text{acceptance}\}| < \varepsilon$$

And true operator has contraction property

$$d(\tau q, p) < \eta d(q, p),$$

Where $d(q, p)$ – total variation distance

Then

$$d(\hat{p}\ , p) < \frac{\varepsilon}{1 - \eta}$$

Korattikara, Anoop, Yutian Chen, and Max Welling. "Austerity in MCMC land: Cutting the Metropolis-Hastings budget." *International Conference on Machine Learning*. 2014.

Algorithm

1. Sample candidate $\theta' \sim \mathrm{q}(\theta'|\theta)$
2. Increase minibatch until

$$\sigma^2(\Delta^*) < 1 \qquad \text{and} \qquad \varepsilon < \delta$$

3. Accept θ' if

$$\Delta^* + X_{nc} + X_{corr} > 0$$

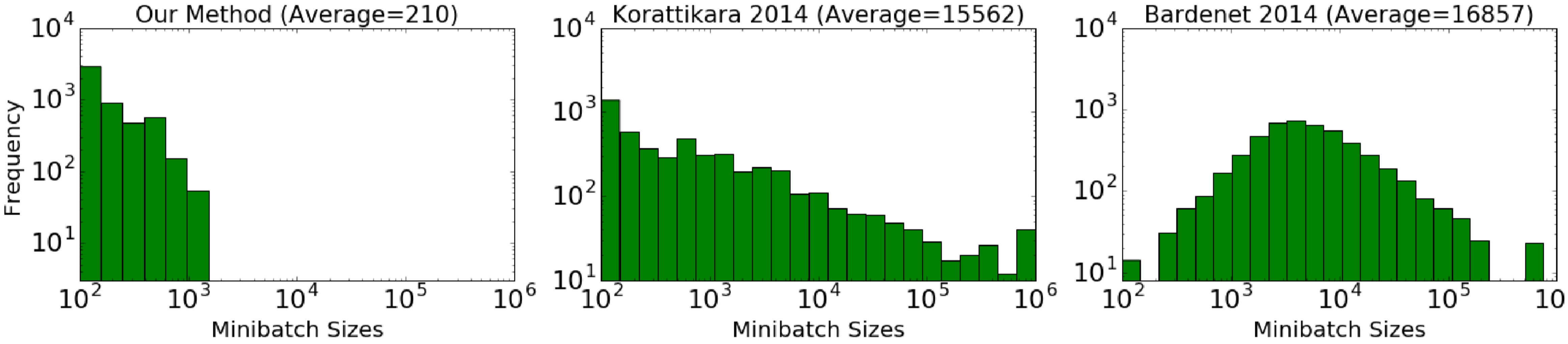
$$X_{nc} \sim \mathcal{N}(0,1 - \sigma^2(\Delta^*))$$

$$X_{corr} \sim \text{Correction Distribution}(\sigma^2 = 1)$$

4. Otherwise keep old θ

Efficiency

Dataset of 10^6 points sampled from mixture of Gaussians



5 min break

Langevin Dynamics

Makes use of the gradient of log-density

$$\Delta\theta_t = \frac{\varepsilon}{2}\nabla \log p(\theta) + \eta_t, \qquad \eta_t \sim \mathcal{N}(0, \varepsilon)$$

In Bayesian Inference

$$\Delta\theta_t = \frac{\varepsilon}{2}\left(\nabla \log p(\theta_t) + \boxed{\sum_{i=1}^{N} \nabla \log p(x_i|\theta_t)}\right) + \eta_t, \qquad \eta_t \sim \mathcal{N}(0, \varepsilon)$$

Full dataset!

Bayesian Learning via Stochastic Gradient Langevin Dynamics

Max Welling, Yee Whye Teh

Stochastic Gradient Langevin Dynamics

Estimate gradient in Langevin Dynamics on minibatch $= \{x_{t_1}, \dots, x_{t_n}\}$

$$\Delta\theta_t = \frac{\varepsilon_t}{2}\left(\nabla \log p(\theta_t) + \frac{N}{n}\sum_{i=1}^{n} \nabla \log p\left(x_{t_i} \middle| \theta_t\right)\right) + \eta_t, \qquad \eta_t \sim \mathcal{N}(0, \varepsilon_t)$$

~~Proof~~ Intuitive Analysis of SGLD

True gradient

$$\mathrm{g}(\theta) = \nabla \log p(\theta) + \sum_{i=1}^{N} \nabla \log p(x_i|\theta)$$

Deviations

$$\mathrm{h_t}(\theta) = \nabla \log p(\theta) + \frac{N}{n} \sum_{i=1}^{n} \nabla \log p\left(x_{t_i} \middle| \theta\right) - g(\theta),$$

$$h_t(\theta) \sim \overline{\mathcal{N}}(0, V_t(\theta))$$

Intuitive Analysis of SGLD

Given

$$\sum_{t=1}^{\infty} \varepsilon_t = \infty \qquad \sum_{t=1}^{\infty} \varepsilon_t^2 < \infty$$

We can find subsequence $t_1 < t_2 < \cdots$ such that

$$\lim_{s \to \infty} \sum_{t=t_s+1}^{t_{s+1}} \varepsilon_t = \varepsilon_0,$$

Where $0 < \varepsilon_0 < 1$ is initial step

After one step

$$\Delta\theta_t = \frac{\varepsilon_t}{2}\big(g(\theta_t) + h_t(\theta_t)\big) + \eta_t, \qquad \eta_t \sim \mathcal{N}(0, \varepsilon_t)$$

After several steps

$$\Delta\theta = \sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2}\big(g(\theta_t) + h_t(\theta_t)\big) + \mathcal{N}\left(0, \sum_{t=t_s+1}^{t_{s+1}} \varepsilon_t\right) =$$

$$\sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2}\Big(g(\theta_t) - g\big(\theta_{t_s}\big) + g\big(\theta_{t_s}\big)\Big) + \sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2} h_t(\theta_t) + \mathcal{N}\left(0, \sum_{t=t_s+1}^{t_{s+1}} \varepsilon_t\right)$$

For s big enough

One step of Langevin dynamics

Langevin noise

Has order of $O\left(\sqrt{\varepsilon_0}\right)$

$$\Delta\theta = \overbrace{\frac{\varepsilon_0}{2} g\left(\theta_{t_s}\right) + \mathcal{N}(0, \varepsilon_0)} + \sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2}\left(g(\theta_t) - g\left(\theta_{t_s}\right)\right) + \sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2} h_t(\theta_t)$$

Systematic error

Non-zero mean

Has order of $O(\varepsilon_0^2)$

"Random" error

Zero-mean

Has order of $O(\varepsilon_0)$

Bounding systematic error

Firstly we bound $\left\|\theta_t - \theta_{t_s}\right\|_2 \ \forall\, t \in [t_s + 1, t_{s+1}]$

$$\left\|\theta_t - \theta_{t_s}\right\|_2 \le \left\| \sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2}\big(g(\theta_t) + h_t(\theta_t)\big) + \mathcal{N}\left(0, \sum_{t=t_s+1}^{t_{s+1}} \varepsilon_t\right) \right\|_2$$

$$\le \sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2} \|g(\theta_t)\|_2 + \left\| \sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2} h_t(\theta_t) \right\|_2 + \|\mathcal{N}(0, \varepsilon_0)\|_2 = O(\varepsilon_0)$$

Assuming that $\|\mathrm{g}(\theta)\|_2$ and $\|h_t(\theta_t)\|$ have some upper bounds

Bounding systematic error

Assuming gradient Lipschitz continuity $\left\|g(\theta_t) - g\left(\theta_{t_s}\right)\right\|_2 \leq L\left\|\theta_t - \theta_{t_s}\right\|_2$

$$\left\|\sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2}\left(g(\theta_t) - g\left(\theta_{t_s}\right)\right)\right\| \leq O(\varepsilon_0) \sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2} = O(\varepsilon_0^2)$$

$O(\varepsilon_0^2)$ is negligible compared to $\frac{\varepsilon_0}{2} g\left(\theta_{t_s}\right)$

$$\sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2}\left(g(\theta_t) - g\left(\theta_{t_s}\right)\right) \ll \frac{\varepsilon_0}{2} g\left(\theta_{t_s}\right)$$

Systematic error True gradient

Analysis of "random" error

$$\sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2} h_t(\theta_t) \sim \overline{\mathcal{N}}\left(0, \sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t^2}{4} V_t(\theta_t)\right)$$

$$\sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t^2}{4} V_t(\theta_t) \leq V\left(\sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2}\right)^2 = V\varepsilon_0^2$$

Variance $V\varepsilon_0^2$ is negligible compared to ε_0

$$\underbrace{\sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2} h_t(\theta_t)}_{\text{“Random” error}} \ll \underbrace{\mathcal{N}(0, \varepsilon_0)}_{\text{Langevin dynamics noise}}$$

Several steps of SGLD ≈ one step of LD

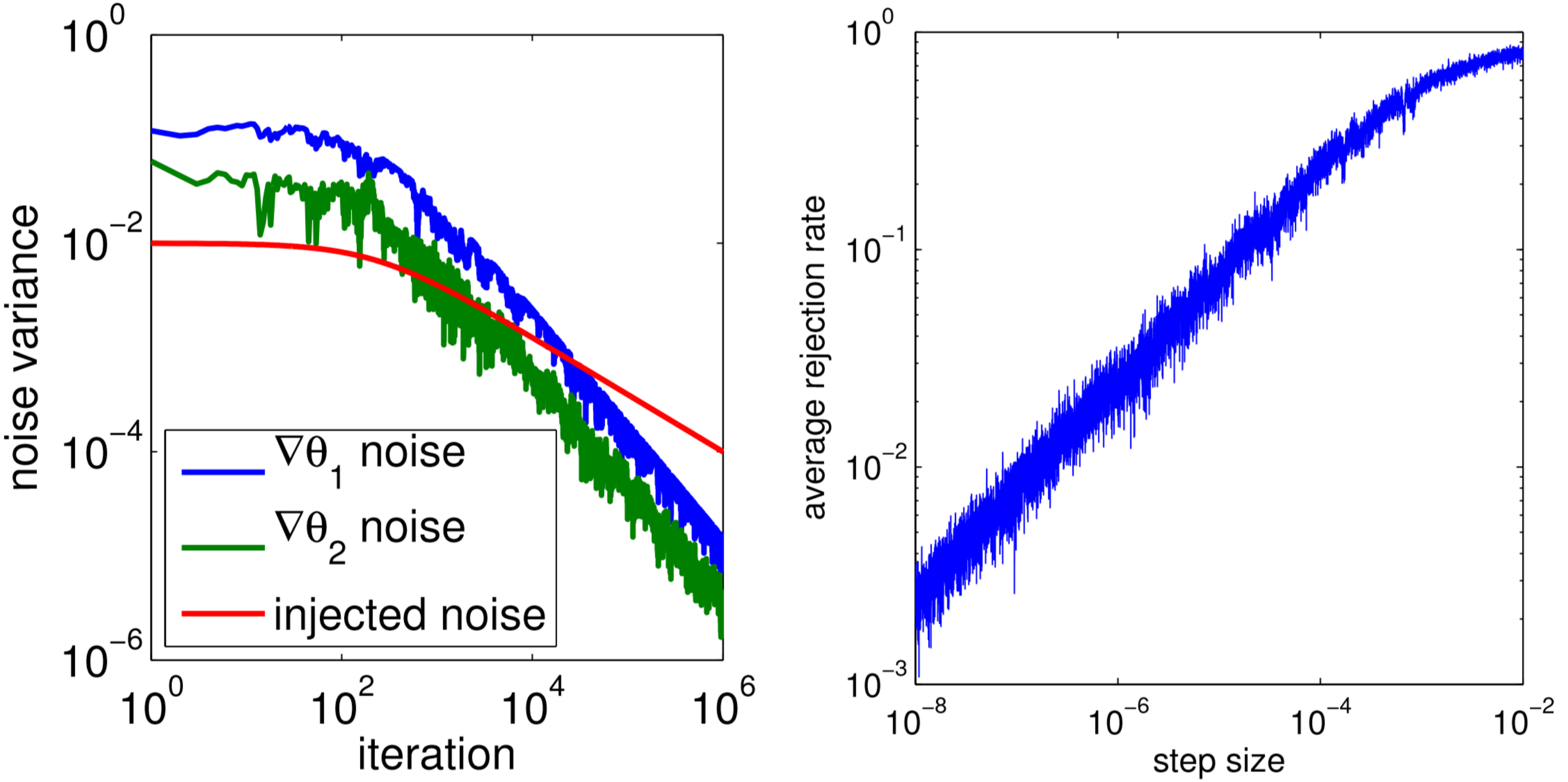
$$\Delta\theta = \sum_{t=t_s+1}^{t_{s+1}} \frac{\varepsilon_t}{2}\big(g(\theta_t) + h_t(\theta_t)\big) + \mathcal{N}\left(0, \sum_{t=t_s+1}^{t_{s+1}} \varepsilon_t\right) \approx$$
$$\approx \frac{\varepsilon_0}{2} g\left(\theta_{t_s}\right) + \mathcal{N}(0, \varepsilon_0)$$

For ε_0 small enough we can ignore M-H test

OR

Perform minibatch M-H test!

Empirical analysis on toy problem



Conclusion

- Stochastic MCMC is a new-generation methods of sampling from posterior conditioned on large dataset
- Makes use of mini-batching and stochastic optimization
- Higher rejection rates but MUCH cheaper iterations

Acceptance rate