CSci 8980: Advanced Topics in Graphical Models MCMC, Gibbs Sampling

Instructor: Arindam Banerjee

September 27, 2007

Problems	Basics	МСМС	Gibbs Sampling	Auxiliary Variable Samplers
	Problems			

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• Primarily of two types: Integration and Optimization

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• Optimization, Model Selection, etc.

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Monte Carlo Principle

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- For finite σ_f^2 , central limit theorem implies

$$\sqrt{n}(I_n(f) - I(f)) \Longrightarrow_{n \to \infty} \mathcal{N}(0, \sigma_f^2)$$

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Rejection Sampling

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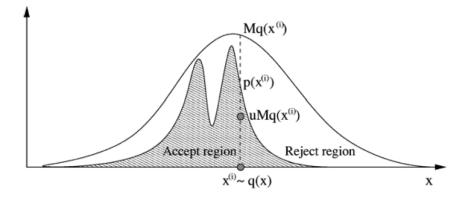
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 - If M is too large, acceptance probability is small

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Rejection Sampling (Contd.)



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Importance Sampling

• For a proposal distribution q(x), with w(x) = p(x)/q(x)

$$I(f) = \int_{x} f(x)w(x)q(x)dx$$

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• The estimator is unbiased, and converges to I(f) a.s.

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Importance Sampling (Contd.)

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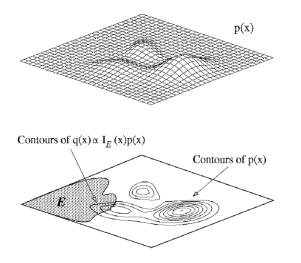
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Markov C	hains		

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- MCMC samplers, invariant distribution = target distribution
- Design of samplers for fast convergence

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Markov Chains (Contd.)

• Random walker on the web

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- Continuous spaces, T becomes an integral kernel K

$$\int_{x_i} p(x_i) \mathcal{K}(x_{i+1}|x_i) dx_i = p(x_{i+1})$$

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• p(x) is the corresponding eigenfunction

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The Metropolis-Hastings Algorithm

• Most popular MCMC method

Basics

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- Most popular MCMC method
- Based on a proposal distribution $q(x^*|x)$

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 - Sample $u \sim \mathcal{U}(0, 1)$
 - Sample $x^* \sim q(x^*|x_i)$
 - Then

$$x_{i+1} = \begin{cases} x^* & \text{if } u < A(x_i, x^*) = \min\left\{1, \frac{p(x^*)q(x_i|x^*)}{p(x_i)q(x^*|x_i)}\right\}\\ x_i & \text{otherwise} \end{cases}$$

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• The transition kernel is

 $K_{MH}(x_{i+1}|x_i) = q(x_{i+1}|x_i)A(x_i, x_{i+1}) + \delta_{x_i}(x_{i+1})r(x_i)$

where $r(x_i)$ is the term associated with rejection

$$r(x_i) = \int_X q(x|x_i)(1 - A(x_i, x))dx$$

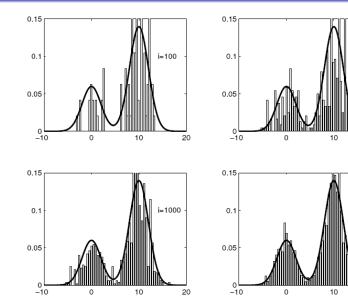
i=500

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i=5000

The Metropolis-Hastings Algorithm (Contd.)



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Basics

The Metropolis-Hastings Algorithm (Contd.)

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 - Irreducibility, ensure support of *q* contains support of *p*
 - Aperiodicity, ensured since rejection is always a possibility
- Independent sampler: $q(x^*|x_i) = q(x^*)$ so that

$$A(x_i, x^*) = \min\left\{1, \frac{p(x^*)q(x_i)}{q(x^*)p(x_i)}\right\}$$

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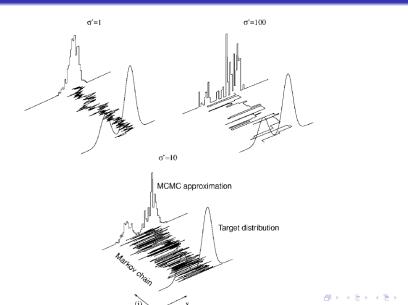
$$A(x_i, x^*) = \min\left\{1, \frac{p(x^*)q(x_i)}{q(x^*)p(x_i)}\right\}$$

• Metropolis sampler: symmetric $q(x^*|x_i) = q(x_i|x^*)$

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The Metropolis-Hastings Algorithm (Contd.)



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Simulated Annealing

• Problem: To find global maximum of p(x)

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Simulated Annealing

- Problem: To find global maximum of p(x)
- Initial idea: Run MCMC, estimate $\hat{p}(x)$, compute max

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Simulated Annealing

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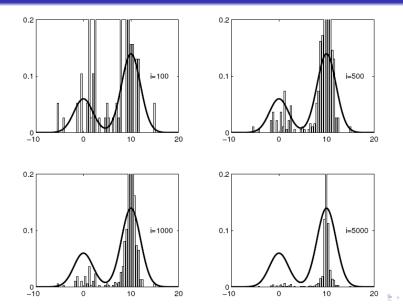
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- T_i decreases following a cooling schedule, $\lim_{i\to\infty} T_i = 0$
- Cooling schedule needs proper choice, e.g., $T_i = \frac{1}{C \log(i + T_0)}$

Simulated Annealing (Contd.)



• E-step involves computing an expectation

$$Q(\theta, \theta_n) = \int_x \log p(x, z|\theta) p(z|x, \theta_n) dx$$

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- Estimate the expectation using MCMC
- Draw samples using MH with acceptance probability

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Mixtures of MCMC Kernels

• Powerful property of MCMC: Combination of Samplers

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- Example: Target has many narrow peaks
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 - Local proposals get the neighborhood of peaks (random walk)

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Cycles of MCMC Kernels

• Split a multi-variate state into blocks

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- Gibbs sampling effectively uses block size of 1

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The Gibbs Sampler

• For a *d*-dimensional vector *x*, assume we know

$$p(x_j|x_{-j}) = p(x_j|x_1, \ldots, x_{j-1}, x_{j+1}, \cdots, x_d)$$

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$$q(x^*|x^{(i)}) = egin{cases} p(x_j^*|x_{-j}^{(i)}) & ext{if} \ \ x_{-j}^* = x_{-j}^{(i)} \\ 0 & ext{otherwise} \end{cases}$$

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• Deterministic scan: All samples are accepted

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The Gibbs Sampler (Contd.)

• Initialize
$$x^{(0)}$$
. For $i = 0, ..., (N - 1)$

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• Possible to have MH steps inside a Gibbs sampler

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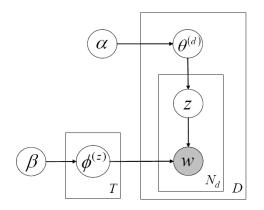
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- For d = 2, Gibbs sampler is the data augmentation algorithm

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- Possible to have MH steps inside a Gibbs sampler
- For d = 2, Gibbs sampler is the data augmentation algorithm
- For Bayes nets, the conditioning is on the Markov blanket

$$p(x_j|x_{-j}) = p(x_j|x_{pa(j)}) \prod_{k \in ch(j)} p(x_k|pa(k))$$

Bayesian LDA



Gibbs Sampler for Bayesian LDA

• The conditional distribution

 $p(z_\ell = h | \mathbf{z}_{-\ell}, \mathbf{w}) \propto p(z_\ell = h | z_{-\ell}) p(w_\ell | z_\ell = h, \mathbf{z}_{-\ell}, \mathbf{w}_{-\ell})$



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 - $C_{(d-\ell,h)}^{DT}$ = words from d assigned to h, excluding current word

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 C^{WT}_(w-ℓ,h) = w_ℓ assigned to h, excluding current word

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Notation:

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Then, the first term

$$p(z_{\ell} = h|z_{-\ell}) = \frac{C_{(d_{-\ell},h)}^{DT} + \alpha}{\sum_{t=1}^{T} C_{(d_{-\ell},t)}^{DT} + T\alpha}$$

Gibbs Sampler for Bayesian LDA

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The second term

$$p(w_{\ell}|z_{\ell} = h, \mathbf{z}_{-\ell}, \mathbf{w}_{-ell}) = \frac{C_{(w_{-\ell},h)}^{WT} + \beta}{\sum_{w=1}^{W} C_{(w_{-\ell},h)}^{WT} + W\beta}$$

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Basic Idea

• Sometimes easier to sample from p(x, u) rather than p(x)

- Sometimes easier to sample from p(x, u) rather than p(x)
- Sample (x_i, u_i) , and then ignore u_i

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Hybrid Monte Carlo

• Uses gradient of the target distribution

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• Gradient vector $\Delta(x) = \partial \log p(x) / \partial x$, step-size ρ

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- Gradient descent for L steps to get proposal candidate
- When L = 1, one obtains the Langevin algorithm

$$x^* = x_0 + \rho u_0 = x^{(i-1)} + \rho(u^* + \rho \Delta(x^{(i-1)})/2)$$

• Initialize
$$x^{(0)}$$
. For $i = 0, ..., (n-1)$

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• For
$$\ell = 1, \dots, L$$
, with $\rho_\ell = \rho, \ell < L$, $\rho_L = \rho/2$

$$x_{\ell} = x_{\ell-1} + \rho u_{\ell-1}$$
 $u_{\ell} = u_{\ell-1} + \rho_{\ell} \Delta(x_{\ell})$

Hybrid Monte Carlo (Contd.)

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• For $\ell = 1, ..., L$, with $\rho_\ell = \rho, \ell < L, \rho_L = \rho/2$
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Set

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Hybrid Monte Carlo (Contd.)

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- Tradeoffs for ρ, L
 - $\bullet\,$ Large ρ gives low acceptance, small ρ needs many steps
 - Large L gives candidates far from x_0 , but expensive

The Slice Sampler

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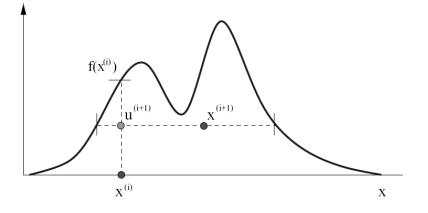
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- Algorithm is easy is A is easy to figure out
- Otherwise, several auxiliary variables need to be introduced

The Slice Sampler (Contd.)



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