LECTURE 16: MARKOV CHAIN MONTE CARLO (CONTD)

STAT 545: Intro. to Computational Statistics

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Markov chain Monte Carlo

We are interested in a distribution $\pi(x) = \frac{f(x)}{Z}$

(e.g. want the mean, quantiles etc.)

Monte Carlo: approximate with independent samples from π

MCMC: produce dependent samples via a Markov chain

$$x_0 \to x_1 \to x_2 \to x_3 \to \cdots \to x_{N-1} \to x_N$$

Use dependent samples to approximate integrals w.r.t. $\pi(x)$:

$$\frac{1}{N}\sum_{i=1}^{N} g(x_i) \approx \mathbb{E}_\pi[g] \quad \text{as}$$

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Finally, for infinite state-spaces (e.g. the real line), need an additional condition:

- positive recurrent: revisits every neighborhood infinitely often

Ergodicity

With these conditions, our chain is *ergodic*

For any initialization:

$$\frac{1}{N}\sum_{i=1}^{N} g(x_i) \to \mathbb{E}_\pi[g] \quad \text{as } N \to \infty \qquad \text{(Ergodicity)}$$

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A good transition kernel has:

- A short burn-in period.
- Fast mixing (small dependence across samples).

The Markov transition kernel $\mathcal{T}$ must satisfy

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Usually, we enforce the stronger condition of detailed balance:

$$\pi(x_{n+1})\mathcal{T}(x_n|x_{n+1}) = \pi(x_n)\mathcal{T}(x_{n+1}|x_n)$$

(Sufficient but not necessary)

The problem

Given some probability density $\pi(x) = f(x)/Z$:

- How do you construct a transition kernel $\mathcal{T}$ with π as it's stationary distribution?
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Focus of a huge literature.

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One approach: the Metropolis-Hastings algorithm

The Metropolis-Hastings algorithm

The simplest and most widely applicable MCMC algorithm. Featured in Dongarra & Sullivan (2000)'s list of top 10 algoirithms.

1. Metropolis Algorithm for Monte Carlo
2. Simplex Method for Linear Programming
3. Krylov Subspace Iteration Methods
4. The Decompositional Approach to Matrix Computations
5. The Fortran Optimizing Compiler
6. QR Algorithm for Computing Eigenvalues
7. Quicksort Algorithm for Sorting
8. Fast Fourier Transform
9. Integer Relation Detection
10. Fast Multipole Method

The Metropolis-Hastings algorithm

A random walk algorithm

Choose a proposal distrib. $q(x_{new}|x_{old})$. E.g. $x_{new} \sim \mathcal{N}(x_{old}, \sigma^2 I)$

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Initialize chain at some starting point x_0.

Repeat:

- Propose a new point x^* according to $q(x^*|x_n)$.
- Define $\alpha = \min\left(1, \frac{\pi(x^*)q(x_n|x^*)}{\pi(x_n)q(x^*|x_n)}\right) = \min\left(1, \frac{f(x^*)q(x_n|x^*)}{f(x_n)q(x^*|x_n)}\right)$
- Set $x_{n+1} = x^*$ with probability α, else $x_{n+1} = x_n$.

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- Accept/reject steps ensure this has the correct distribution.

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- Accept/reject steps ensure this has the correct distribution.
- On rejection, keep old sample (i.e. there will be repetition)

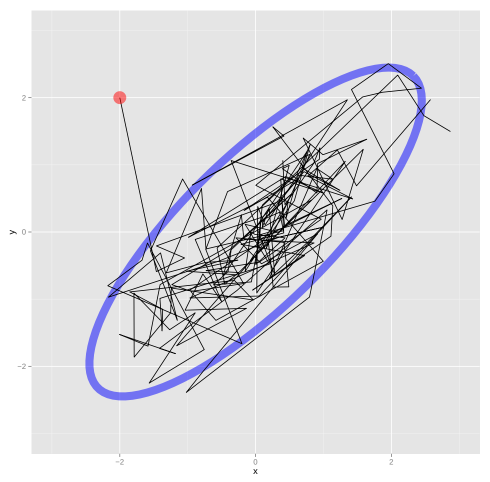
For a symmetric proposal ($q(x^*|x_n) = q(x_n|x^*)$):

$$\alpha = \min\left(1, \frac{f(x^*)}{f(x_n)}\right)$$

The Metropolis algorithm.

The Metropolis-Hastings algorithm

How do we chose the proposal variance?



$$\sigma^2 = 1$$

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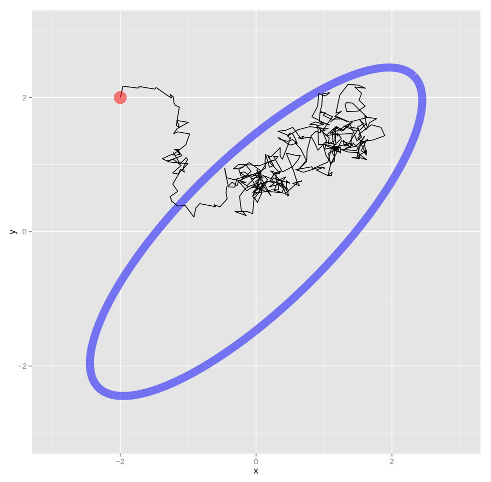

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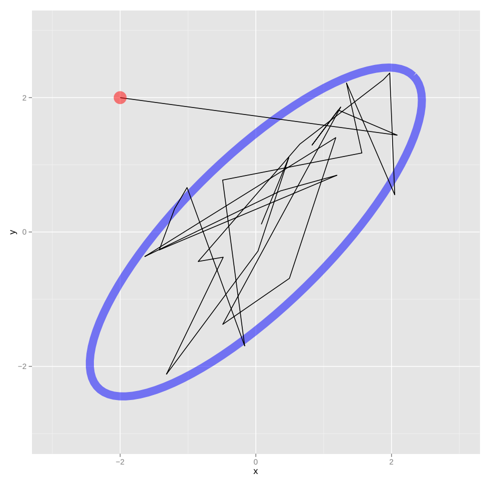

$$\sigma^2 = 5$$

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We then have:

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We want to show detailed balance:

$$\pi(x_n)\mathcal{T}(x_{n+1}|x_n) = \pi(x_{n+1})\mathcal{T}(x_n|x_{n+1})$$

The Metropolis-Hastings algorithm

Detailed balance: $\pi(x_n)\mathcal{T}(x_{n+1}|x_n) = \pi(x_{n+1})\mathcal{T}(x_n|x_{n+1})$

Consider the LHS:

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The first term is: $$\frac{f(x_n)}{Z}\min\left(1, \frac{f(x_{n+1})q(x_n|x_{n+1})}{f(x_n)q(x_{n+1}|x_n)}\right)q(x_{n+1}|x_n)$$

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Thus, $\pi(x_n)\mathcal{T}(x_{n+1}|x_n) = \pi(x_{n+1})\mathcal{T}(x_n|x_{n+1})$

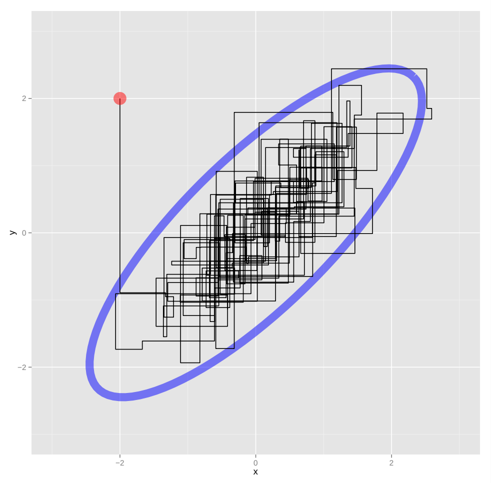
Consider a Markov chain on over a set of variables $(x_1, \cdots, x_d)$.

Gibbs sampling cycles though these sequentially (or randomly). At the ith step, it updates x_i conditioned on the the rest:

$$x_i \sim \pi(x_i | x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n) = \pi(x_i | \mathbf{x}_{\setminus i})$$

Often these conditionals have a much simpler form than the joint.

Gibbs sampling



Detailed balance for the sequential Gibbs sampler

Does it satisfy stationarity?

Does it satisfy irreducibility?

Is it aperiodic?

Detailed balance for the randomized Gibbs sampler

Suppose we update component i with prob. ρ_i. Let $\mathbf{x}$ and $\mathbf{x}'$ differ only in component i. Then:

$$\mathcal{T}(\mathbf{x}'|\mathbf{x}) = \rho_i \pi(x_i'|\mathbf{x}_{\setminus i})$$

Also

$$\begin{aligned}\pi(\mathbf{x})\mathcal{T}(\mathbf{x}'|\mathbf{x}) &= \pi(\mathbf{x})\rho_i\pi(x_i'|\mathbf{x}_{\setminus i}) \\ &= \pi(\mathbf{x}_{\setminus i})\pi(x_i|\mathbf{x}_{\setminus i})\rho_i\pi(x_i'|\mathbf{x}_{\setminus i})\end{aligned}$$

From symmetry (or by calculating RHS), we have detailed balance.

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Often, conditional independencies in a model along with suitable conjugate priors allow efficient 'blocked-Gibbs samplers'.