Markov Chain Monte Carlo Methods

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Outline

Historical facts

Dongarra and Sullivan (2000) list the top algorithms with the greatest influence on the development and practice of science and engineering in the 20th century (in chronological order):

- Metropolis Algorithm for Monte Carlo
- Simplex Method for Linear Programming
- Krylov Subspace Iteration Methods
- The Decompositional Approach to Matrix Computations
- The Fortran Optimizing Compiler
- QR Algorithm for Computing Eigenvalues
- Quicksort Algorithm for Sorting
- Fast Fourier Transform

70s and 80s

Metropolis-Hastings:
Hastings (1970) and his student Peskun (1973) showed that Metropolis and the more general Metropolis-Hastings algorithm are particular instances of a larger family of algorithms.

Gibbs sampler:

Besag (1974) Spatial Interaction and the Statistical Analysis of Lattice Systems.
Geman and Geman (1984) Stochastic relaxation, Gibbs distributions and the Bayesian restoration of images.
Pearl (1987) Evidential reasoning using stochastic simulation.
Tanner and Wong (1987). The calculation of posterior distributions by data augmentation.
Gelfand and Smith (1990) Sampling-based approaches to calculating marginal densities.

MH algorithms

A sequence $\{\theta^{(0)}, \theta^{(1)}, \theta^{(2)}, \ldots\}$ is drawn from a Markov chain whose *limiting equilibrium distribution* is the posterior distribution, $\pi(\theta)$.

Algorithm

1. Initial value: $\theta^{(0)}$
2. Proposed move: $\theta^* \sim q(\theta^*|\theta^{(i-1)})$
3. Acceptance scheme:

$$\theta^{(i)} = \begin{cases} \theta^* & \text{com prob. } \alpha \\ \theta^{(i-1)} & \text{com prob. } 1-\alpha \end{cases}$$

where

$$\alpha = \min\left\{1, \frac{\pi(\theta^*)}{\pi(\theta^{(i-1)})} \frac{q(\theta^{(i-1)}|\theta^*)}{q(\theta^*|\theta^{(i-1)})}\right\}$$

Special cases

1. Symmetric chains: $q(\theta|\theta^*) = q(\theta^*|\theta)$

$$\alpha = \min\left\{1, \frac{\pi(\theta^*)}{\pi(\theta)}\right\}$$

2. Independence chains: $q(\theta|\theta^*) = q(\theta)$

$$\alpha = \min\left\{1, \frac{\omega(\theta^*)}{\omega(\theta)}\right\}$$

where $\omega(\theta^*) = \pi(\theta^*)/q(\theta^*)$.

Random walk Metropolis

The most famous symmetric chain is the random walk Metropolis:

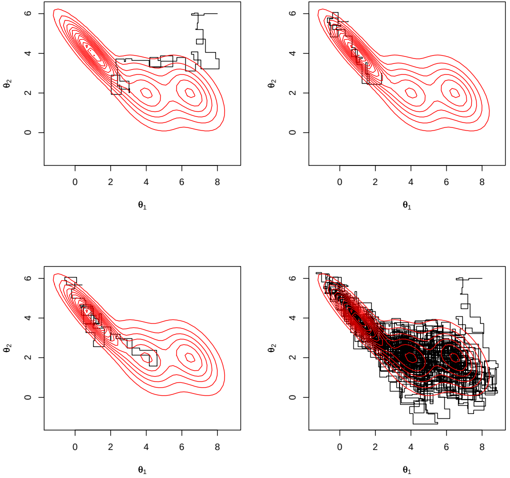
$$q(\theta|\theta^*) = q(|\theta - \theta^*|)$$

Hill climbing: when

$$\alpha = \min\left\{1, \frac{\pi(\theta^*)}{\pi(\theta)}\right\}$$

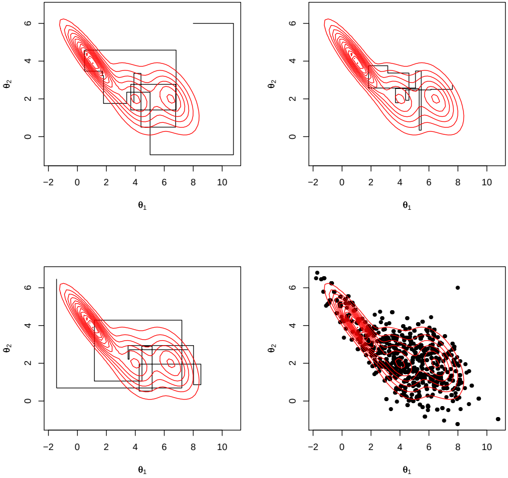
a value θ^* with higher density $\pi(\theta^*)$ greater than $\pi(\theta)$ is automatically accepted.

Example iv. RW Metropolis



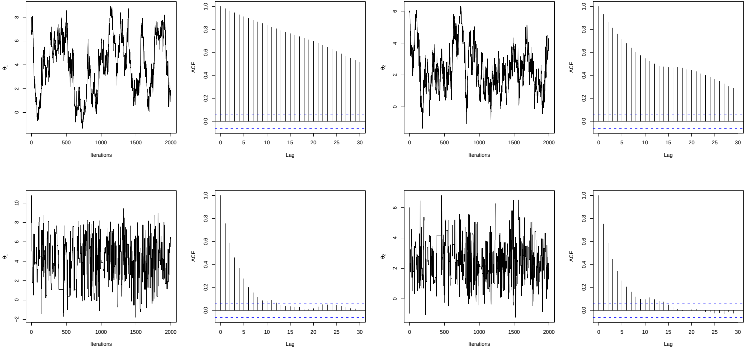
$$q(\theta|\theta_i) \sim N(\theta_i, 0.25\Sigma_2).$$

Example iv. Ind. Metropolis

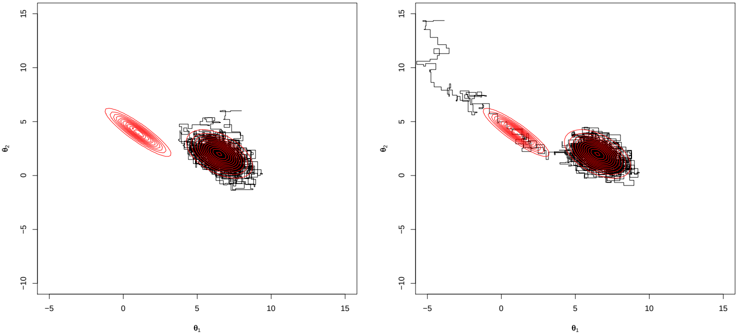


$$q(\theta) \equiv q_{SIR}(\theta) \sim N(\mu, \Sigma).$$

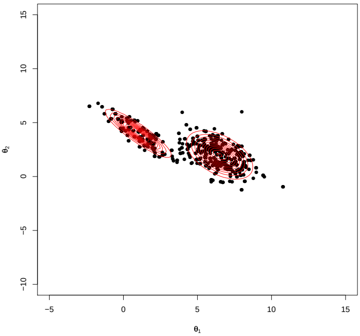
Example iv. Autocorrelations

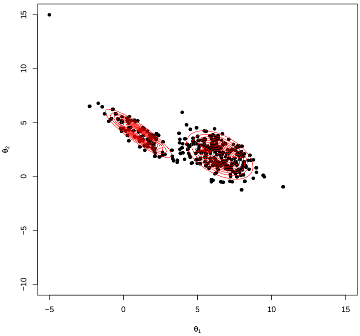


Example v. RW Metropolis

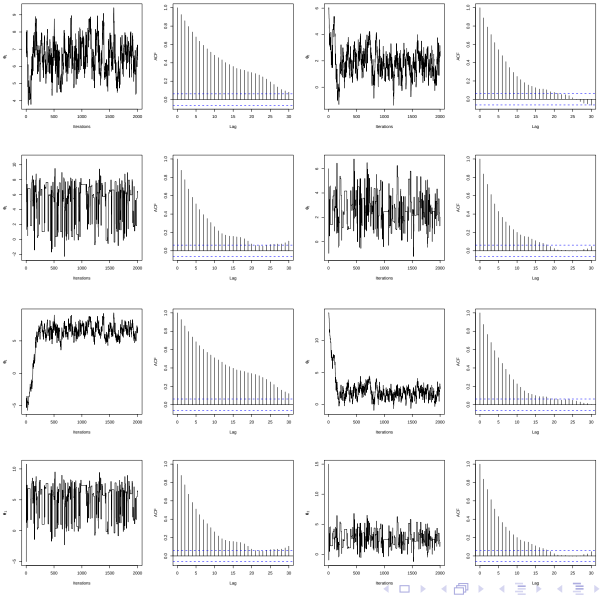


Example v. Ind. Metropolis





Example v. Autocorrelations



Example vi. tuning selection

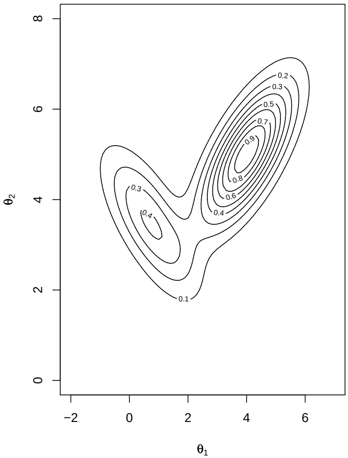
Tthe target distribution is a two-component mixture of bivariate normal densities, ie:

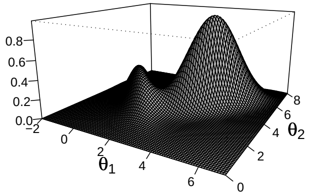
$$\pi(\theta) = 0.7 f_N(\theta; \mu_1, \Sigma_1) + 0.3 f_N(\theta; \mu_2, \Sigma_2).$$

where

$$\begin{aligned}
\mu_1' &= (4.0, 5.0) \\
\mu_2' &= (0.7, 3.5) \\
\Sigma_1 &= \begin{pmatrix} 1.0 & 0.7 \\ 0.7 & 1.0 \end{pmatrix} \\
\Sigma_2 &= \begin{pmatrix} 1.0 & -0.7 \\ -0.7 & 1.0 \end{pmatrix}.
\end{aligned}$$

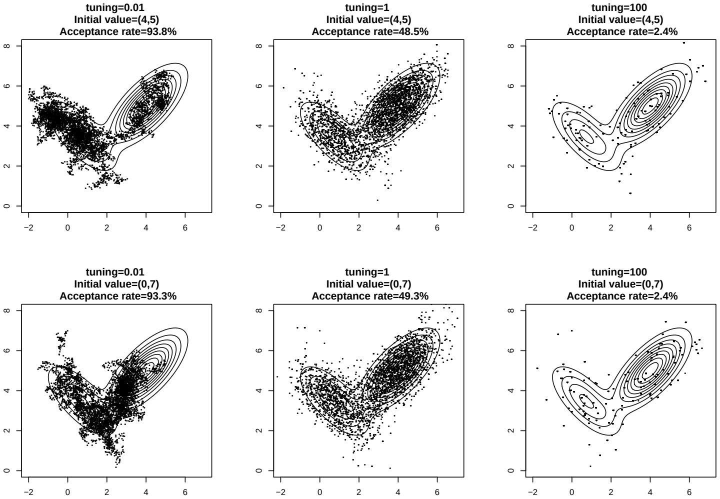
Target distribution



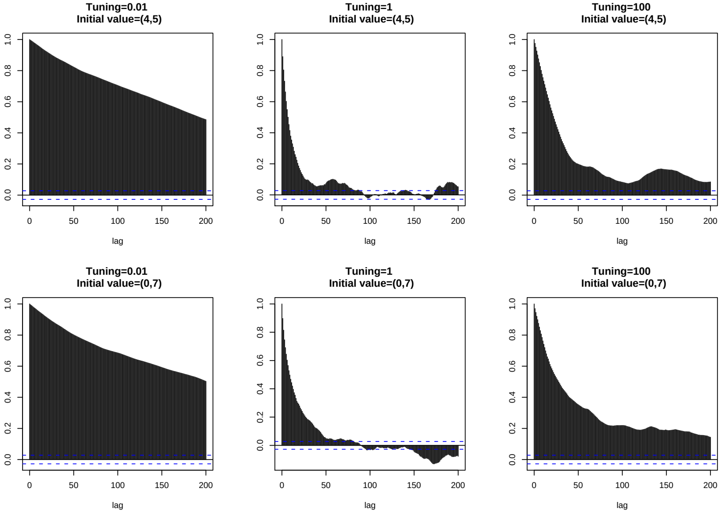


RW Metropolis

$q(\theta, \phi) = f_N(\phi; \theta, \nu I_2)$ and ν =tuning.

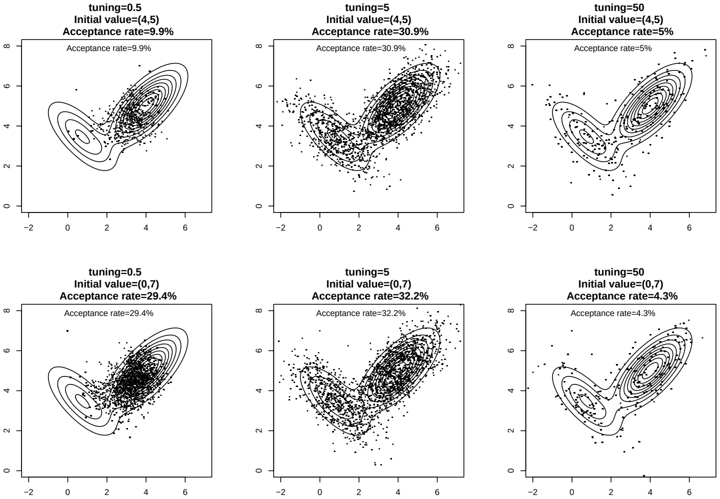


Autocorrelations

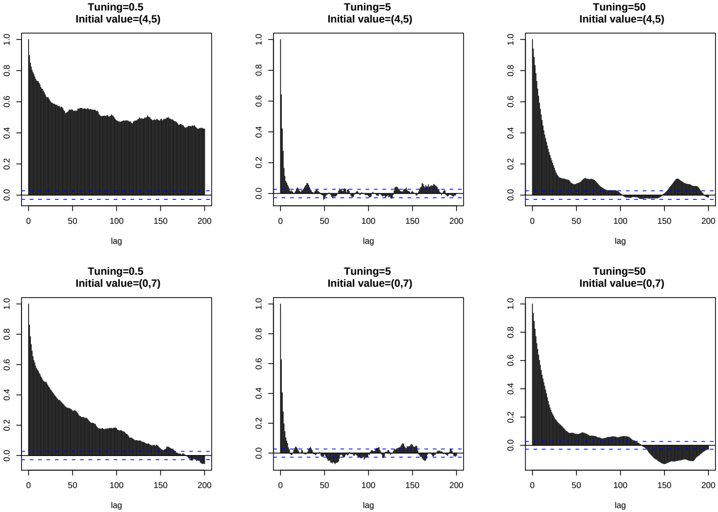


Independent Metropolis

$q(\theta, \phi) = f_N(\phi; \mu_3, \nu I_2)$ and $\mu_3 = (3.01, 4.55)'$.



Autocorrelations



Gibbs sampler

Technically, the Gibbs sampler is an MCMC scheme whose transition kernel is the product of the full conditional distributions.

Algorithm

1. Start at $\theta^{(0)} = (\theta_1^{(0)}, \theta_2^{(0)}, \ldots)$
2. Sample the components of $\theta^{(j)}$ iteratively:

$$\begin{aligned}
\theta_1^{(j)} &\sim \pi(\theta_1 | \theta_2^{(j-1)}, \theta_3^{(j-1)}, \ldots) \\
\theta_2^{(j)} &\sim \pi(\theta_2 | \theta_1^{(j)}, \theta_3^{(j-1)}, \ldots) \\
\theta_3^{(j)} &\sim \pi(\theta_3 | \theta_1^{(j)}, \theta_2^{(j)}, \ldots) \\
&\vdots
\end{aligned}$$

The Gibbs sampler opened up a new way of approaching statistical modeling by combining simpler structures (the full conditional models) to address the more general structure (the full model).

Example: Bivariate normal

Assume that the target distribution is the bivariate normal with mean vector and covariance matrix given by

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \quad \text{and} \quad \Sigma = \begin{pmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{pmatrix},$$

respectively.

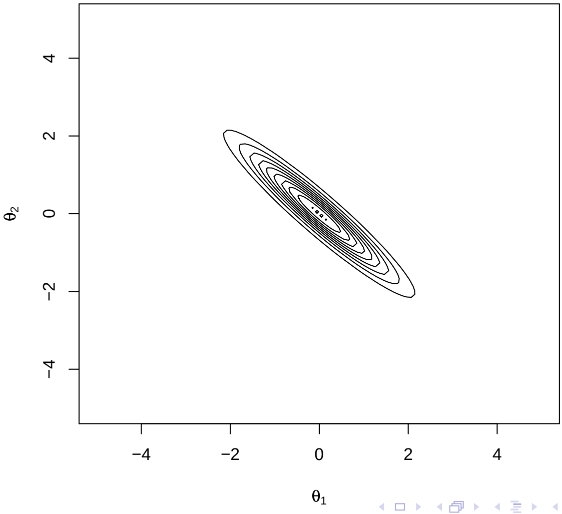
In this case, the two full conditionals are given by

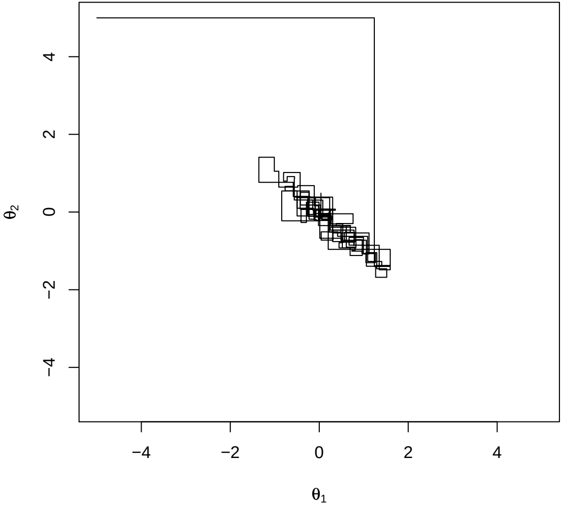
$$\theta_1|\theta_2 \sim N\left(\mu_1 + \frac{\sigma_{12}}{\sigma_2^2}(\theta_2 - \mu_2), \sigma_1^2 - \frac{\sigma_{12}^2}{\sigma_2^2}\right)$$

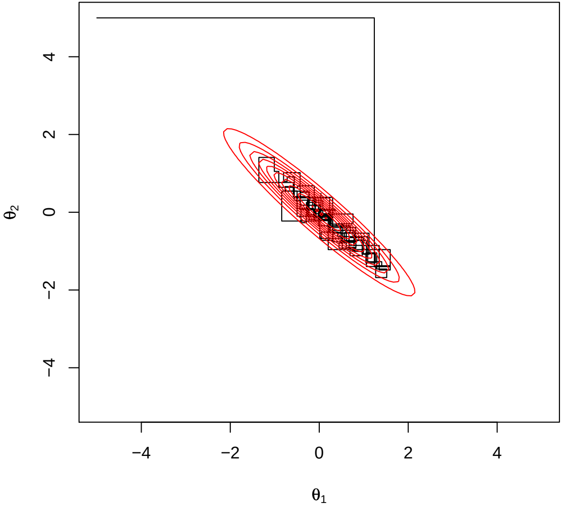
and

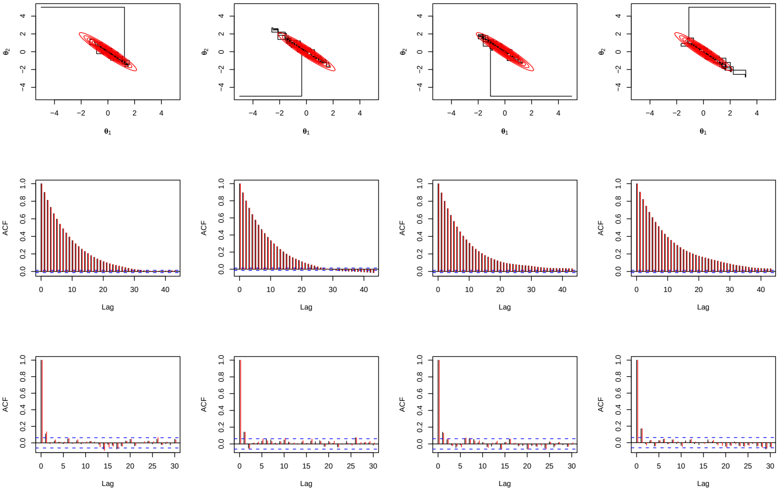
$$\theta_2|\theta_1 \sim N\left(\mu_2 + \frac{\sigma_{12}}{\sigma_1^2}(\theta_1 - \mu_1), \sigma_2^2 - \frac{\sigma_{12}^2}{\sigma_1^2}\right)$$

$\mu_1 = \mu_2 = 0$
$\sigma_1^2 = \sigma_2^2 = 1$
$\sigma_{12} = -0.95$

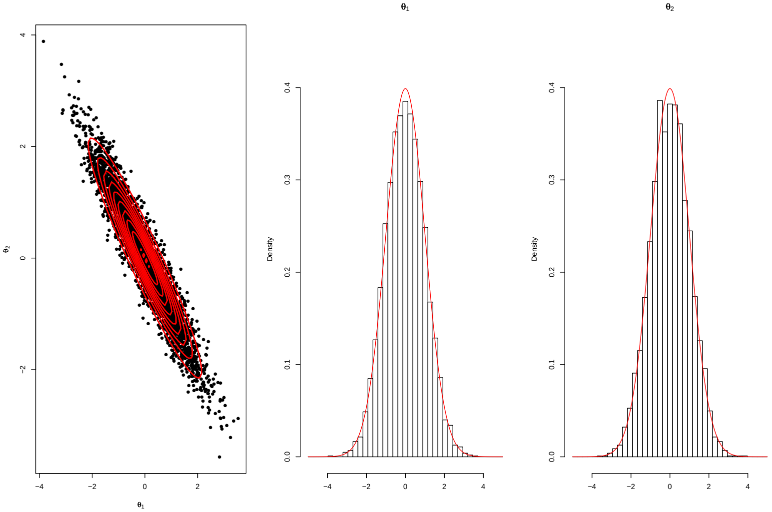



4
2
0
−2
−4
θ_2
−4
−2
0
2
4
θ_1


4
2
0
−2
−4
θ2
−4
−2
0
2
4
θ1



Middle frame: Based on $M = 21,000$ consecutive draws.
Bottom frame: Based on $M = 1000$ draws, after initial $M_0 = 1000$ draws and saving every 20th draws.


θ1
θ2
Density
Density
θ1
θ2
−4
−2
0
2
4
0.0
0.1
0.2
0.3
0.4

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