

# MONTE CARLO METHODS

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Date	Time	Topic
Monday 23rd	16:45-18:00	Basic Monte Carlo Methods
Tuesday 24th	16:25-17:40	Markov Chain Monte Carlo Methods

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# MC in the 40s and 50s

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**Stan Ulam** soon realized that computers could be used in this fashion to answer questions of **neutron diffusion** and **mathematical physics**;

He contacted **John Von Neumann** and they developed many Monte Carlo algorithms (importance sampling, rejection sampling, etc);

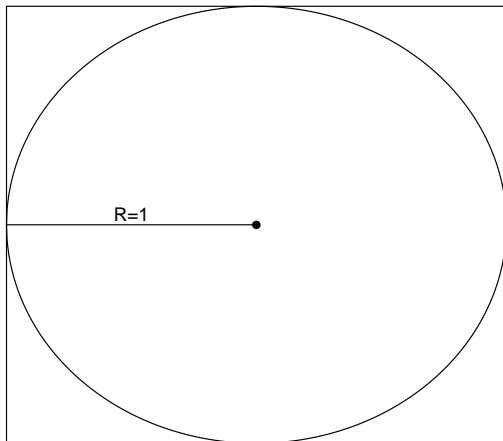
In the 1940s **Nick Metropolis** and **Klari Von Neumann** designed new controls for the state-of-the-art computer (ENIAC);

**Metropolis and Ulam (1949)** The Monte Carlo method. *Journal of the American Statistical Association*.  
**Metropolis et al. (1953)** Equations of state calculations by fast computing machines. *Journal of Chemical Physics*.

## Example 0. $\pi = ?$

Draw a square of side  $L = 2$  (area=4).

Draw a circle of radius  $R = 1$  inside the square (area= $\pi$ ).



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# Monte Carlo idea

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Randomly toss a bunch of (black) beans in the square.

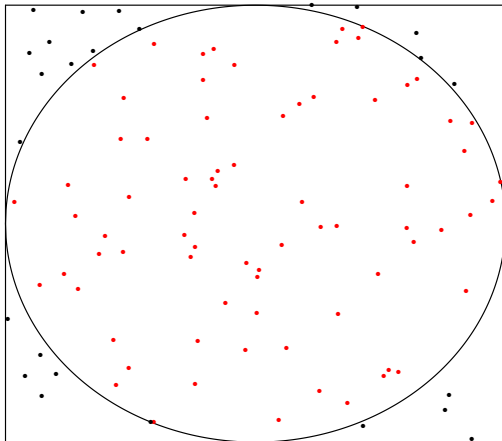
Let  $p$  be the proportion of beans in the circle.

Simple rule:

	<i>Area</i>	<i>Total</i>
<i>Square</i>	4	1
<i>Circle</i>	$\pi$	$p$

Therefore  $4p$  should converge to  $\pi$ .

## MC approximation to $\pi=3$ Based on 100 draws



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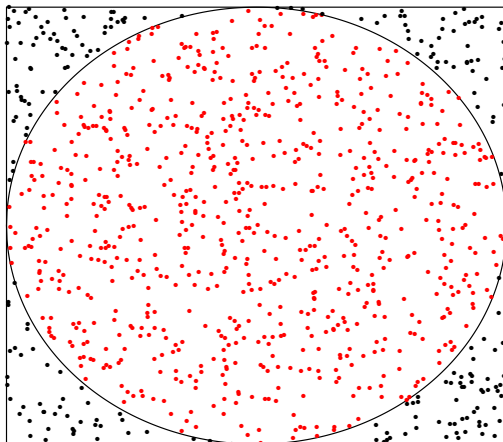
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## MC approximation to $\pi=3.112$ Based on 1000 draws



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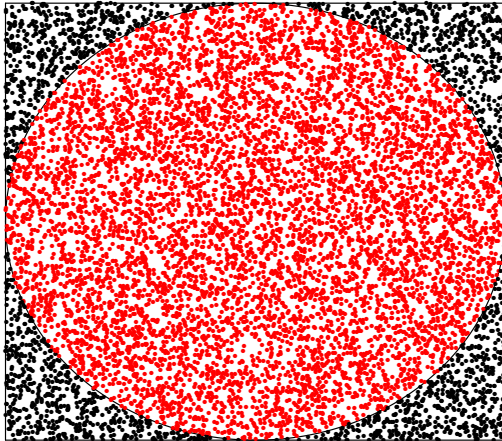
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## MC approximation to $\pi=3.1392$ Based on 10000 draws



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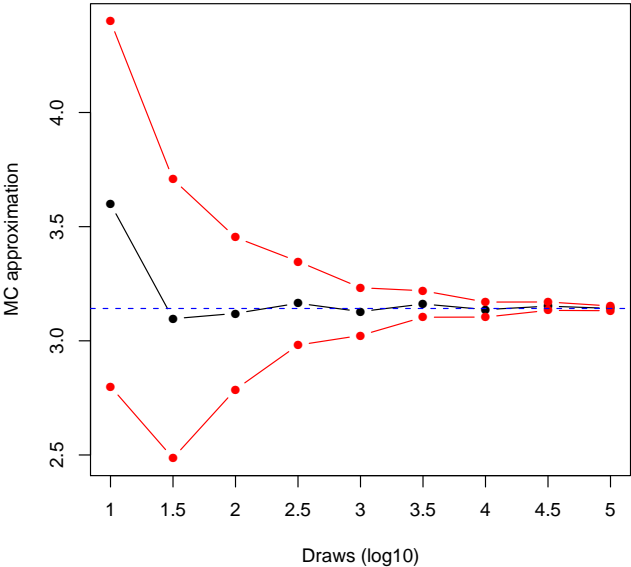
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## Riemann sum

From the standard normal density

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\{-0.5x^2\} dx = 1$$

it is easy to see that

$$\pi = 2 \left\{ \int_0^{\infty} \exp\{-0.5x^2\} dx \right\}^2$$

Then, assuming that 10 is pretty close to  $\infty$ , a simple Reimann sum approximation to  $\pi$  is

$$2 \left\{ h \sum_{i=1}^N \exp\{-0.5x_i^2\} \right\}^2$$

with  $x_1 = h/2$ ,  $x_N = 10 - h/2$  and  $h = x_2 - x_1$ .

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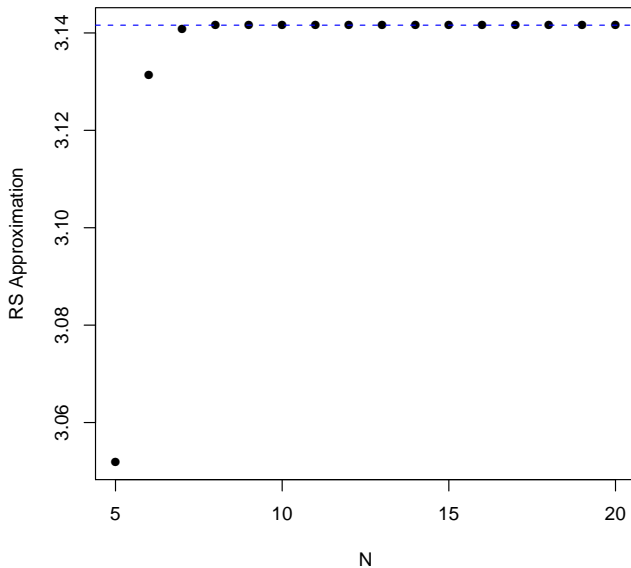
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# Main slide of this tutorial

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MC methods are very powerful computational tools.

Never replace analytical solutions with MC approximations.

When using MC solutions beware of its slow convergence rate.

# Monte Carlo methods

In two lectures we introduce several Monte Carlo (MC) methods for integrating and/or sampling from nontrivial densities.

- MC integration
  - Simple MC integration
  - MC integration via importance sampling (IS)
- MC sampling
  - Rejection method
  - Sampling importance resampling (SIR)
- Iterative MC sampling
  - Metropolis-Hastings algorithms
  - Simulated annealing
  - Gibbs sampler

Lectures based on the book by Gamerman and Lopes (1996).

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- **MC integration** (Geweke, 1989)
- **Rejection methods** (Gilks and Wild, 1992)
- **SIR** (Smith and Gelfand, 1992)
- **Metropolis-Hastings algorithm** (Hastings, 1970)
- **Simulated annealing** (Metropolis *et al.*, 1953)
- **Gibbs sampler** (Gelfand and Smith, 1990)

# Two main tasks

- 1 Compute high dimensional integrals:

$$E_{\pi}[h(\theta)] = \int h(\theta)\pi(\theta)d\theta$$

- 2 Obtain

*a sample  $\{\theta_1, \dots, \theta_n\}$  from  $\pi(\theta)$*

when only

*a sample  $\{\tilde{\theta}_1, \dots, \tilde{\theta}_m\}$  from  $q(\theta)$*

is available.

$q(\theta)$  is known as the *proposal/auxiliary* density.

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## Bayes via MC

MC methods appear frequently, but not exclusively, in modern Bayesian statistics.

Posterior and predictive densities are hard to sample from:

$$\text{Posterior} : \pi(\theta) = \frac{f(x|\theta)p(\theta)}{f(x)}$$

$$\text{Predictive} : f(x) = \int f(x|\theta)p(\theta)d\theta$$

Other important integrals and/or functionals of the posterior and predictive densities are:

- Posterior modes:  $\max_{\theta} \pi(\theta)$ ;
- Posterior moments:  $E_{\pi}[g(\theta)]$ ;
- Density estimation:  $\hat{\pi}(g(\theta))$ ;
- Bayes factors:  $f(x|M_0)/f(x|M_1)$ ;
- Decision:  $\max_d \int U(d, \theta)\pi(\theta)d\theta$ .

# MC integration

The objective here is to compute moments

$$E_{\pi}[h(\theta)] = \int h(\theta)\pi(\theta)d\theta$$

If  $\theta_1, \dots, \theta_n$  is a random sample from  $\pi(\cdot)$  then

$$\bar{h}_{mc} = \frac{1}{n} \sum_{i=1}^n h(\theta_i) \rightarrow E_{\pi}[h(\theta)] \quad \text{as } n \rightarrow \infty.$$

If, additionally,  $E_{\pi}[h^2(\theta)] < \infty$ , then

$$V_{\pi}[\bar{h}_{mc}] = \frac{1}{n} \int \{h(\theta) - E_{\pi}[h(\theta)]\}^2 \pi(\theta) d\theta$$

and

$$v_{mc} = \frac{1}{n^2} \sum_{i=1}^n (h(\theta_i) - \bar{h}_{mc})^2 \rightarrow V_{\pi}[\bar{h}_{mc}] \quad \text{as } n \rightarrow \infty.$$

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## Example i.

The objective here is to compute<sup>1</sup>

$$p = \int_0^1 [\cos(50\theta) + \sin(20\theta)]^2 d\theta$$

by noticing that the above integral can be rewritten as

$$E_{\pi}[h(\theta)] = \int h(\theta)\pi(\theta)d\theta$$

where  $h(\theta) = [\cos(50\theta) + \sin(20\theta)]^2$  and  $\pi(\theta) = 1$  is the density of a  $U(0, 1)$ . Therefore

$$\hat{p} = \frac{1}{n} \sum_{i=1}^n h(\theta_i)$$

where  $\theta_1, \dots, \theta_n$  are i.i.d. from  $U(0, 1)$ .

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<sup>1</sup>True value is 0.965.

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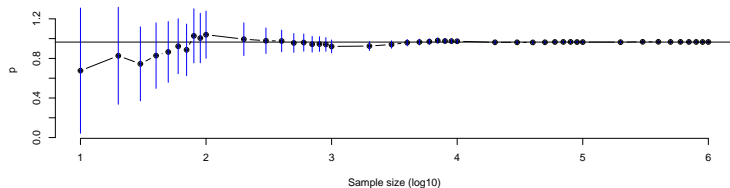
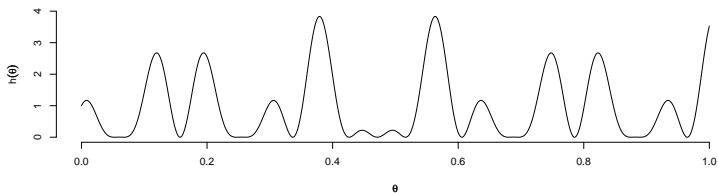
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The objective is still the same, ie to compute

$$E_{\pi}[h(\theta)] = \int h(\theta)\pi(\theta)d\theta$$

by noticing that

$$E_{\pi}[h(\theta)] = \int \frac{h(\theta)\pi(\theta)}{q(\theta)} q(\theta) d\theta$$

where  $q(\cdot)$  is an *importance function*.

If  $\theta_1, \dots, \theta_n$  is a random sample from  $q(\cdot)$  then

$$\Rightarrow \bar{h}_{is} = \frac{1}{n} \sum_{i=1}^n \frac{h(\theta_i) \pi(\theta_i)}{q(\theta_i)} \rightarrow E_{\pi}[h(\theta)]$$

as  $n \rightarrow \infty$ .

Ideally,  $q(\cdot)$  should be

- As close as possible to  $h(\cdot)\pi(\cdot)$ , and
- Easy to sample from.

## Example ii.

The objective here is to estimate

$$p = \Pr(\theta > 2) = \int_2^{\infty} \frac{1}{\pi(1 + \theta^2)} d\theta = 0.1475836$$

where  $\theta$  is a standard Cauchy random variable.

A natural MC estimator of  $p$  is

$$\hat{p}_1 = \frac{1}{n} \sum_{i=1}^n I\{\theta_i \in (2, \infty)\}$$

where  $\theta_1, \dots, \theta_n \sim \text{Cauchy}(0,1)$ .

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A more elaborated estimator based on a change of variables from  $\theta$  to  $u = 1/\theta$  is

$$\hat{p}_2 = \frac{1}{n} \sum_{i=1}^n \frac{u_i^{-2}}{2\pi[1 + u_i^{-2}]}$$

where  $u_1, \dots, u_n \sim U(0, 1/2)$ .

The true value is  $p = 0.147584$ .

$n$	$\hat{p}_1$	$\hat{p}_2$	$v_1^{1/2}$	$v_2^{1/2}$
100	0.100000	0.1467304	0.030000	0.001004
1000	0.137000	0.1475540	0.010873	0.000305
10000	0.148500	0.1477151	0.003556	0.000098
100000	0.149100	0.1475591	0.001126	0.000031
1000000	0.147711	0.1475870	0.000355	0.000010

With only  $n = 1000$  draws,  $\hat{p}_2$  has roughly the same precision that  $\hat{p}_1$ , which is based on  $1000n$  draws, ie. three orders of magnitude.

# Rejection method

The objective is to draw from a target density

$$\pi(\theta) = c_\pi \tilde{\pi}(\theta)$$

when only draws from an auxiliary density

$$q(\theta) = c_q \tilde{q}(\theta)$$

is available, for normalizing constants  $c_\pi$  and  $c_q$ .

If there exist a constant  $A < \infty$  such that

$$0 \leq \frac{\tilde{\pi}(\theta)}{A\tilde{q}(\theta)} \leq 1 \quad \text{for all } \theta$$

then  $q(\theta)$  becomes a *blanketing density* or an *envelope* and  $A$  the *envelope constant*.

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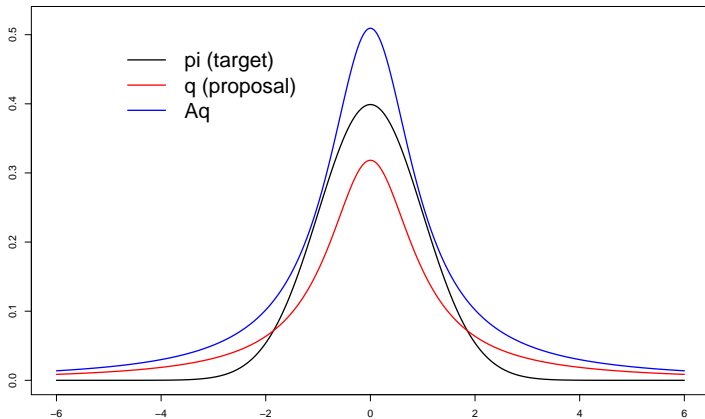
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# Blanket distribution



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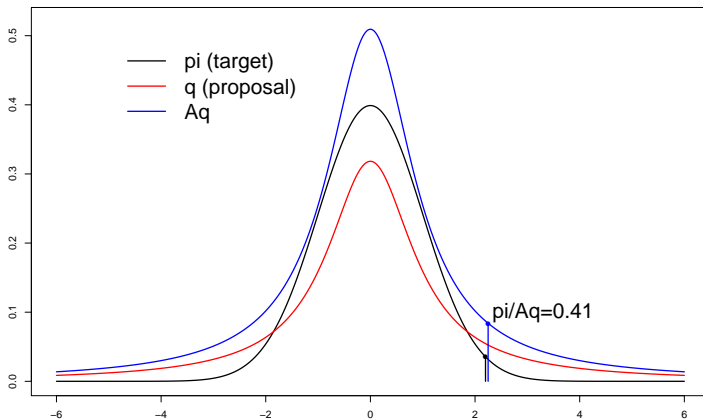
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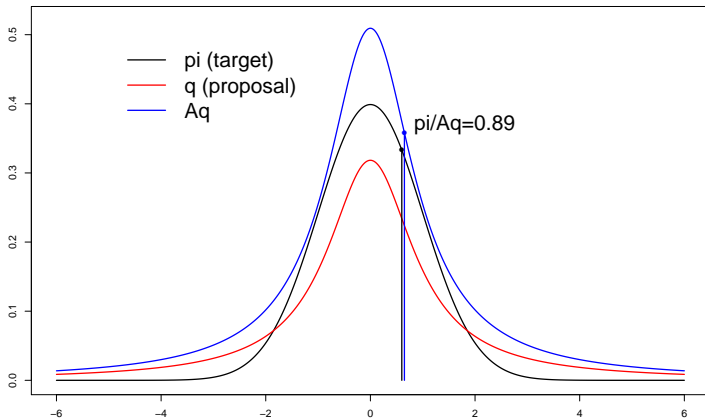
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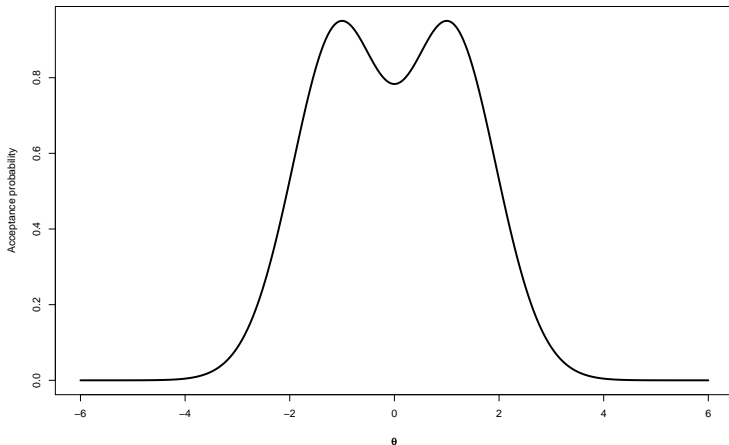
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# Acceptance probability



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Drawing from  $\pi(\theta)$ .

- 1 Draw  $\theta^*$  from  $q(\cdot)$ ;
- 2 Draw  $u$  from  $U(0, 1)$ ;
- 3 Accept  $\theta^*$  if  $u \leq \frac{\tilde{\pi}(\theta^*)}{A\tilde{q}(\theta^*)}$ ;
- 4 Repeat 1, 2 and 3 until  $n$  draws are accepted.

Normalizing constants  $c_\pi$  and  $c_q$  are not needed.

The **theoretical acceptance rate** is  $\frac{c_q}{Ac_\pi}$ .

The smaller the  $A$ , the larger the acceptance rate.

## Example iii.

### Enveloping the standard normal density

$$\pi(\theta) = \frac{1}{\sqrt{2\pi}} \exp\{-0.5\theta^2\}$$

by a Cauchy density  $q_C(\theta) = 1/(\pi(1 + \theta^2))$ , or a uniform density  $q_U(\theta) = 0.05$  for  $\theta \in (-10, 10)$ .

**Bad proposal:** The maximum of  $\pi(\theta)/q_U(\theta)$  is roughly  $A_U = 7.98$  for  $\theta \in (-10, 10)$ . The theoretical acceptance rate is 12.53%.

**Good proposal:** The max of  $\pi(\theta)/q_C(\theta)$  is equal to  $A_C = \sqrt{2\pi/e} \approx 1.53$ . The theoretical acceptance rate is 65.35%.

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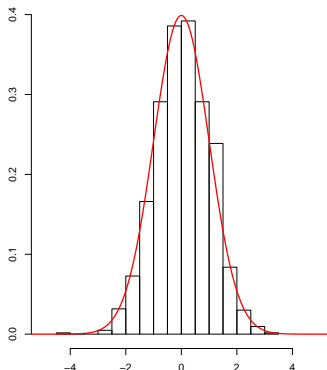
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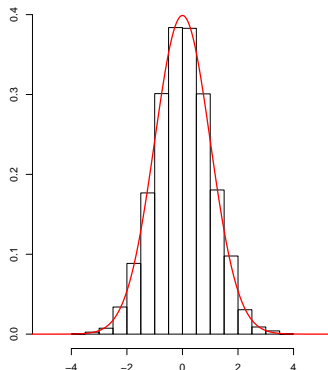
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UNIFORM PROPOSAL



CAUCHY PROPOSAL



Empirical rates: 0.1265 (Uniform) and 0.6483 (Cauchy)  
Theoretical rates: 0.1253 (Uniform) and 0.6535 (Cauchy)

# SIR method

No need to rely on the existence of  $A!$

## Algorithm

- 1 Draw  $\theta_1^*, \dots, \theta_n^*$  from  $q(\cdot)$
- 2 Compute (unnormalized) weights

$$\omega_i = \pi(\theta_i^*)/q(\theta_i^*) \quad i = 1, \dots, n$$

- 3 Sample  $\theta$  from  $\{\theta_1^*, \dots, \theta_n^*\}$  such that

$$\Pr(\theta = \theta_i^*) \propto \omega_i \quad i = 1, \dots, n.$$

- 4 Repeat  $m$  times step 3.

Rule of thumb:  $n/m = 20$ .

Ideally,  $\omega_i = 1/n$  and  $\text{Var}(\omega) = 0$ .

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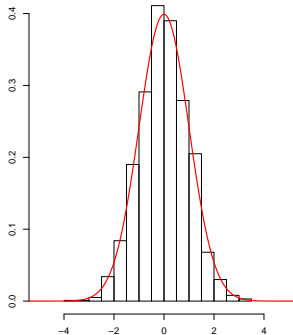
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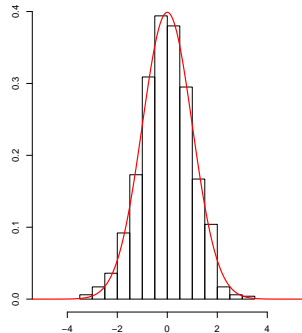
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UNIFORM PROPOSAL



CAUCHY PROPOSAL



Fraction of redraws: 0.391 (Uniform) and 0.1335 (Cauchy)  
Variance of weights: 4.675 (Uniform) and 0.332 (Cauchy)

## Example iv. 3-component mixture

Assume that we are interested in sampling from

$$\pi(\theta) = \alpha_1 p_N(\theta; \mu_1, \Sigma_1) + \alpha_2 p_N(\theta; \mu_2, \Sigma_2) + \alpha_3 p_N(\theta; \mu_3, \Sigma_3)$$

where  $p_N(\cdot; \mu, \Sigma)$  is the density of a bivariate normal distribution with mean vector  $\mu$  and covariance matrix  $\Sigma$ . The mean vectors are

$$\mu_1 = (1, 4)' \quad \mu_2 = (4, 2)' \quad \mu_3 = (6.5, 2),$$

the covariance matrices are

$$\Sigma_1 = \begin{pmatrix} 1.0 & -0.9 \\ -0.9 & 1.0 \end{pmatrix} \quad \text{and} \quad \Sigma_2 = \Sigma_3 = \begin{pmatrix} 1.0 & -0.5 \\ -0.5 & 1.0 \end{pmatrix},$$

and weights  $\alpha_1 = \alpha_2 = \alpha_3 = 1/3$ .

A bit of history

Monte Carlo methods

Two main tasks  
Bayes via MC

MC integration

MC via IS

Rejection method

SIR method

Examples

3-component mixture  
2-component mixture

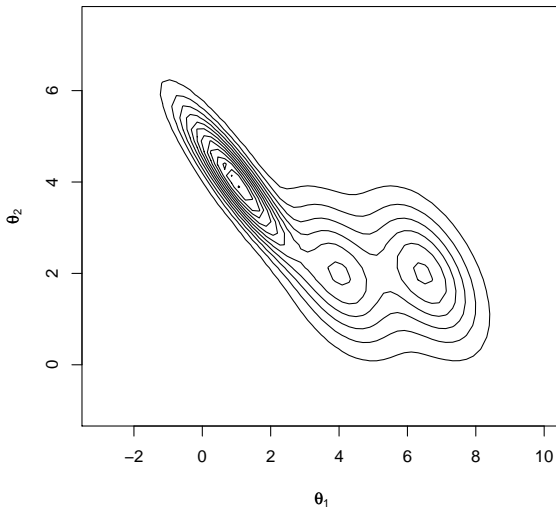
MCMC methods

MH algorithms  
Simulated annealing  
Gibbs sampler

Books on MC methods

References

# Target $\pi(\theta)$



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history

Monte Carlo  
methods

Two main tasks  
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MC  
integration

MC via IS

Rejection  
method

SIR method

Examples

**3-component  
mixture**

2-component  
mixture

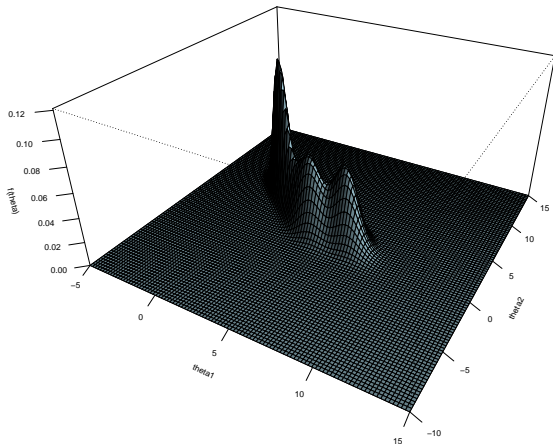
MCMC  
methods

MH algorithms  
Simulated  
annealing  
Gibbs sampler

Books on MC  
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# Target $\pi(\theta)$



A bit of history

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Examples

**3-component mixture**

2-component mixture

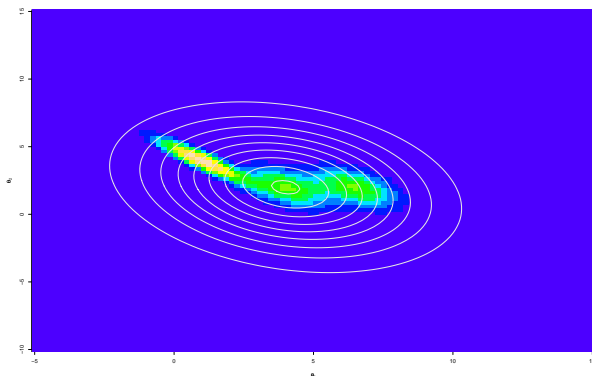
MCMC methods

MH algorithms  
Simulated annealing  
Gibbs sampler

Books on MC methods

References

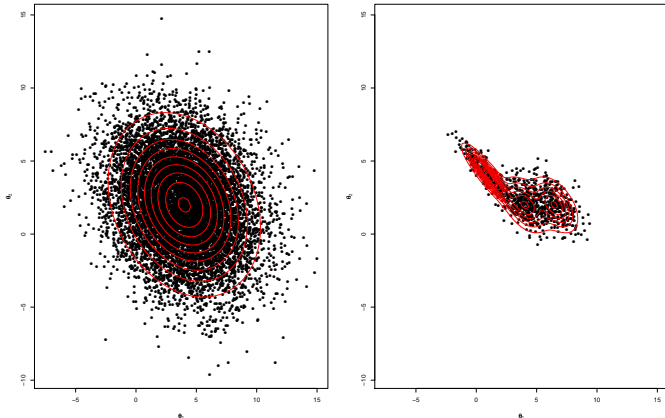
# Proposal $q(\theta)$



$q(\theta) \sim N(\mu, \Sigma)$  where

$$\mu_2 = (4, 2)' \quad \text{and} \quad \Sigma = 9 \begin{pmatrix} 1.0 & -0.25 \\ -0.25 & 1.0 \end{pmatrix}$$

# Rejection method



Acceptance rate: 9.91% of  $n = 10,000$  draws.

# SIR method

A bit of history

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Examples

3-component mixture

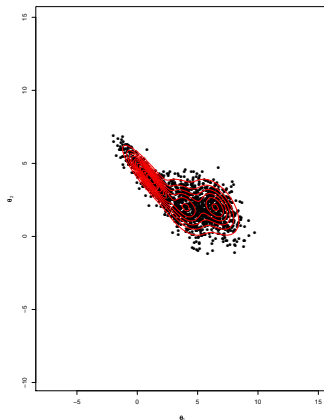
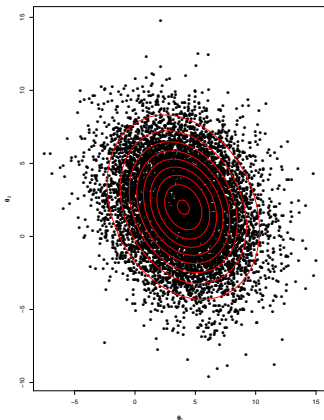
2-component mixture

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Fraction of redraws: 29.45% of ( $n = 10,000, m = 2,000$ ).

# Rejection & SIR

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**3-component  
mixture**

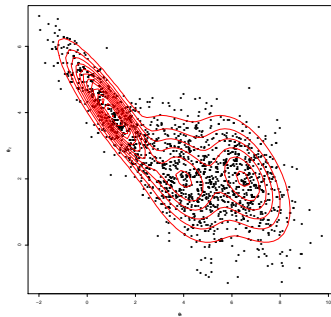
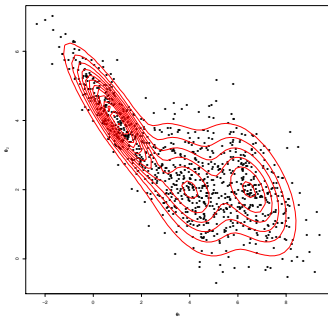
2-component  
mixture

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References



## Example v. 2-component mixture

Let us now assume that

$$\pi(\theta) = \alpha_1 p_N(\theta; \mu_1, \Sigma_1) + \alpha_3 p_N(\theta; \mu_3, \Sigma_3)$$

where mean vectors are

$$\mu_1 = (1, 4)' \quad \mu_3 = (6.5, 2),$$

the covariance matrices are

$$\Sigma_1 = \begin{pmatrix} 1.0 & -0.9 \\ -0.9 & 1.0 \end{pmatrix} \quad \text{and} \quad \Sigma_3 = \begin{pmatrix} 1.0 & -0.5 \\ -0.5 & 1.0 \end{pmatrix},$$

and weights  $\alpha_1 = 1/3$  and  $\alpha_3 = 2/3$ .

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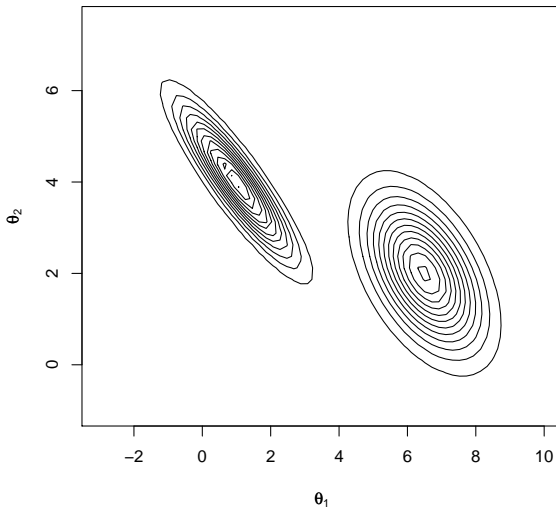
MCMC  
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# Target $\pi(\theta)$



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**2-component mixture**

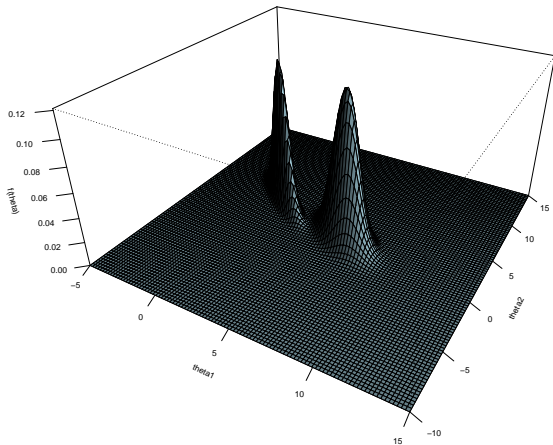
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# Target $\pi(\theta)$



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**2-component mixture**

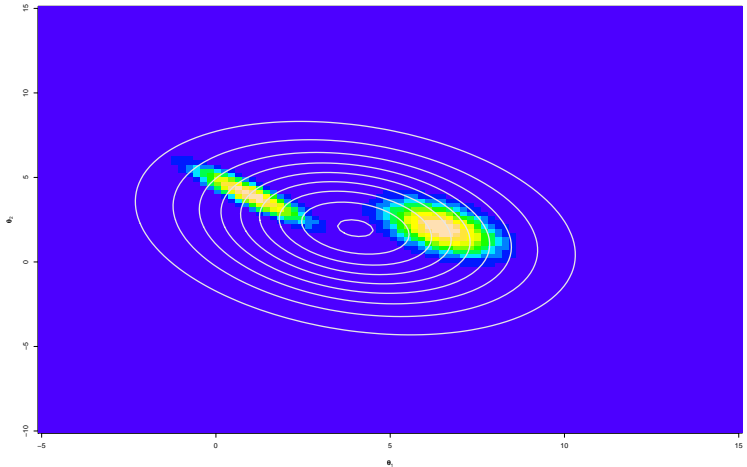
MCMC methods

MH algorithms  
Simulated annealing  
Gibbs sampler

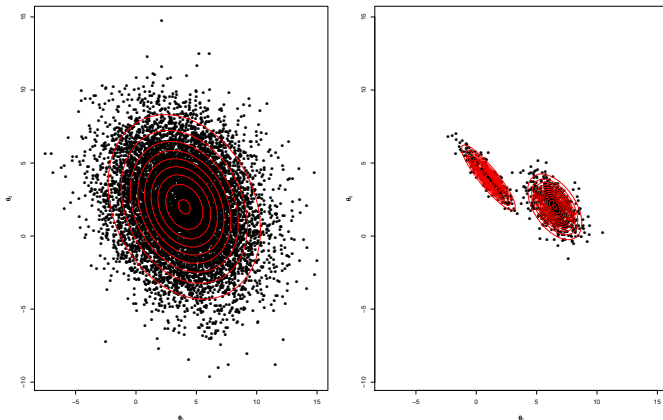
Books on MC methods

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# Proposal $q(\theta)$



# Rejection method



Acceptance rate: 10.1% of  $n = 10,000$  draws.

# SIR method

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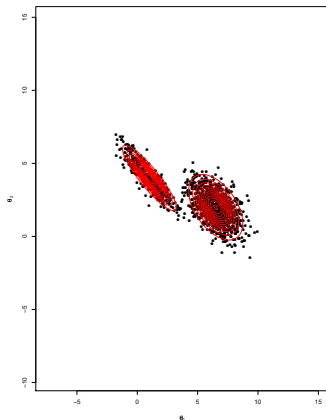
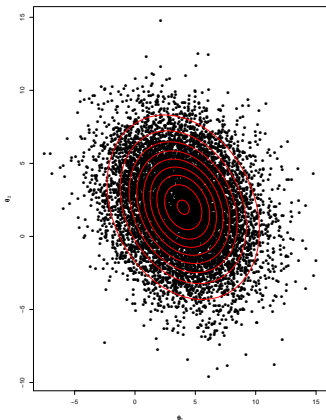
2-component mixture

MCMC methods

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Fraction of redraws: 37.15% of  $(n = 10,000, m = 2,000)$ .

# Rejection & SIR

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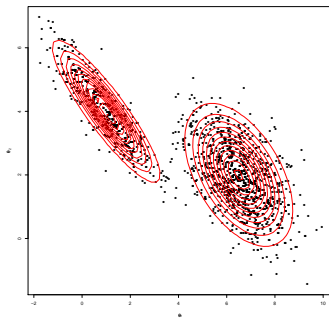
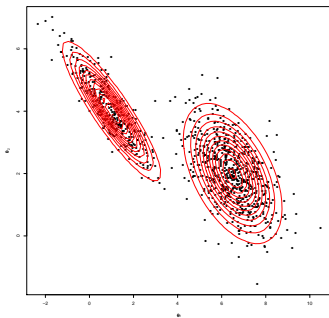
**2-component mixture**

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## Rao-Blackwellization

Suppose one wants to compute

$$I = E\{h(x)\} = \int_{\mathcal{Y}} \int_{\mathcal{X}} h(x) p(x, y) dx dy.$$

A simple MC integration based on draws  $(x_1, y_1), \dots, (x_n, y_n)$  is

$$I_1 = \frac{1}{n} \sum_{i=1}^n h(x_i)$$

In some cases the integral can be partially solved analytically

$$\int_{\mathcal{Y}} \left\{ \int_{\mathcal{X}} h(x) p(x|y) dx \right\} p(y) dy = \int_{\mathcal{Y}} E(h(x)|y) p(y) dy$$

leading to a better MC approximation

$$I_2 = \frac{1}{n} \sum_{i=1}^n E(h(x_i)|y_i)$$

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The basic probability results used are

$$E(h(X)) = E\{E(h(X)|Y)\}$$

and

$$V(h(X)) = E\{V(h(X)|Y)\} + V\{E(h(X)|Y)\}$$

such that

$$V(h(X)) > E\{V(h(X)|Y)\}$$

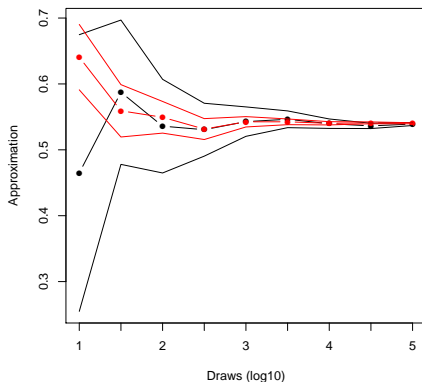
commonly known as *Rao-Blackwell* results.

Never replace analytical solutions with MC approximations.

## Example.

$X|Y \sim N(0, 1/Y)$ ,  $Y \sim G(2.5, 2.5)$  and  $h(x) = \exp\{-x^2\}$ . The two MC approximations are

$$I_1 = \frac{1}{n} \sum_{i=1}^n \exp\{-x_i^2\} \quad \text{and} \quad I_2 = \frac{1}{n} \sum_{i=1}^n \frac{1}{\sqrt{2/y_i + 1}}.$$



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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

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## 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  $\{\theta^{(0)}, \theta^{(1)}, \theta^{(2)}, \dots\}$  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

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

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# Special cases

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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

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

## Example iv. RW Metropolis

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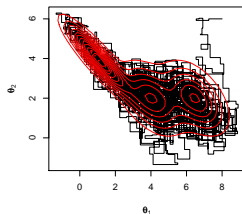
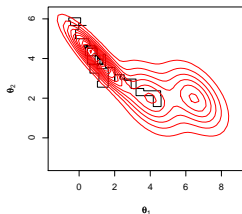
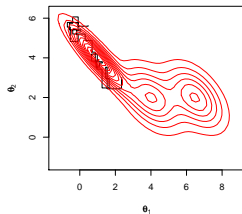
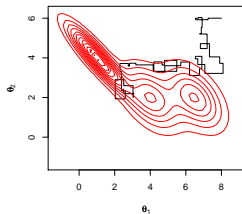
3-component mixture  
2-component mixture

MCMC methods

MH algorithms  
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Gibbs sampler

Books on MC methods

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

## Example iv. Ind. Metropolis

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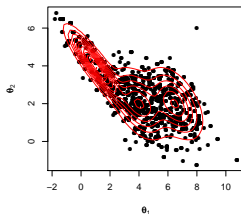
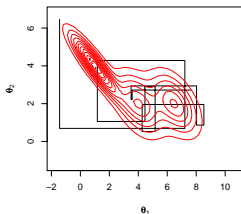
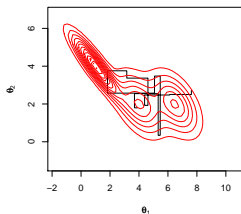
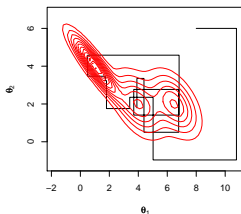
3-component mixture  
2-component mixture

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

# Example iv. Autocorrelations

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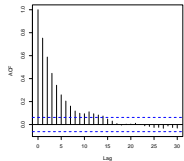
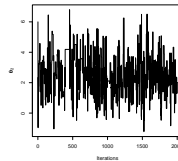
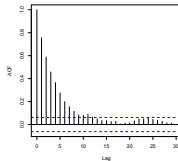
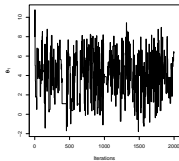
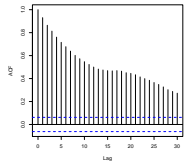
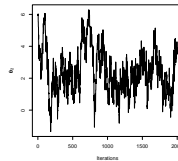
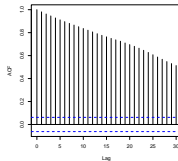
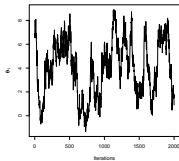
3-component  
mixture  
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# Example v. RW Metropolis

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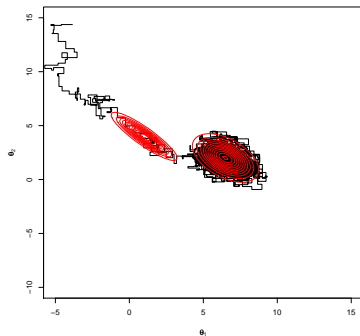
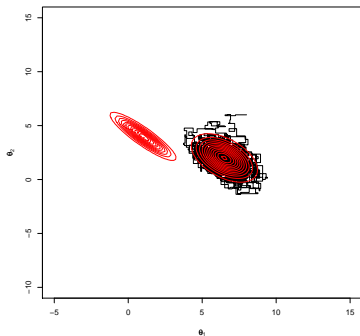
3-component mixture  
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# Example v. Ind. Metropolis

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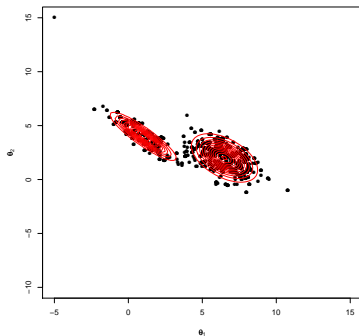
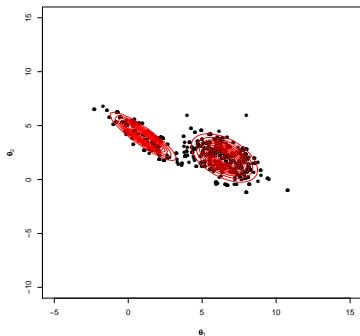
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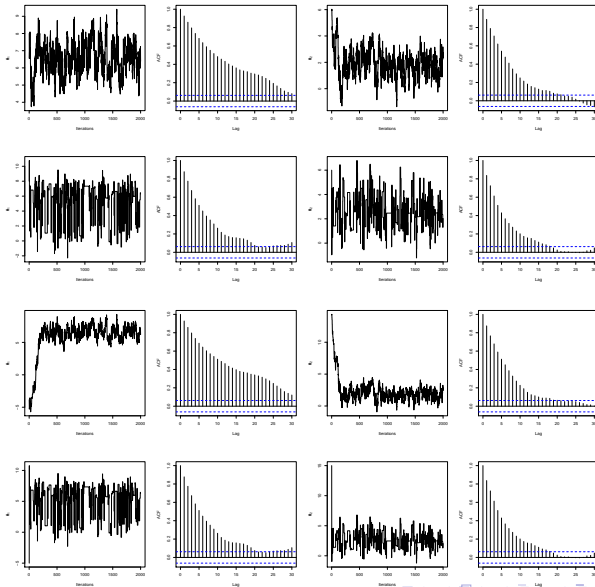
3-component mixture  
2-component mixture

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## Example vi. tuning selection

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

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

where

$$\mu'_1 = (4.0, 5.0)$$

$$\mu'_2 = (0.7, 3.5)$$

$$\Sigma_1 = \begin{pmatrix} 1.0 & 0.7 \\ 0.7 & 1.0 \end{pmatrix}$$

$$\Sigma_2 = \begin{pmatrix} 1.0 & -0.7 \\ -0.7 & 1.0 \end{pmatrix}.$$

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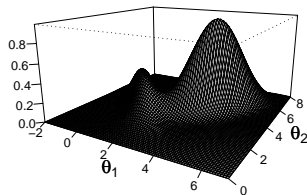
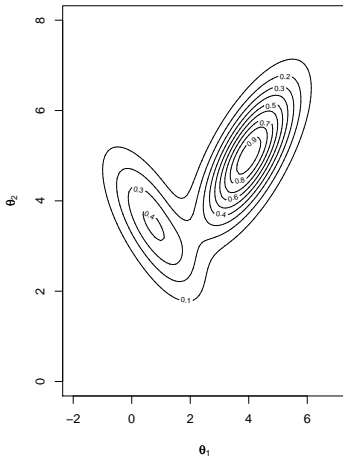
3-component mixture  
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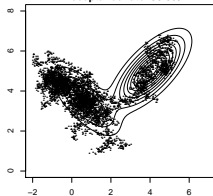
References



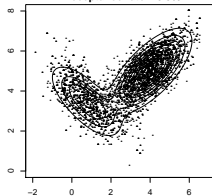
# RW Metropolis

$$q(\theta, \phi) = f_N(\phi; \theta, \nu l_2) \text{ and } \nu = \text{tuning.}$$

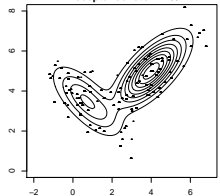
tuning=0.01  
Initial value=(4,5)  
Acceptance rate=93.8%



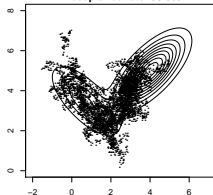
tuning=1  
Initial value=(4,5)  
Acceptance rate=48.5%



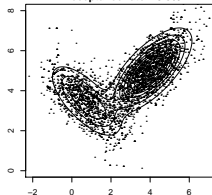
tuning=100  
Initial value=(4,5)  
Acceptance rate=2.4%



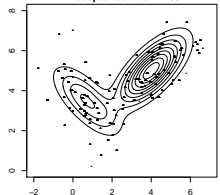
tuning=0.01  
Initial value=(0,7)  
Acceptance rate=93.3%



tuning=1  
Initial value=(0,7)  
Acceptance rate=49.3%



tuning=100  
Initial value=(0,7)  
Acceptance rate=2.4%



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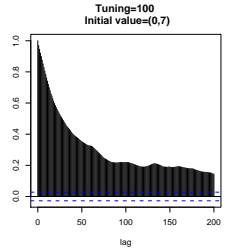
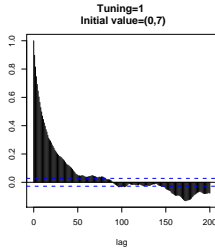
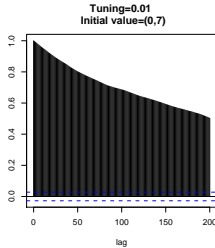
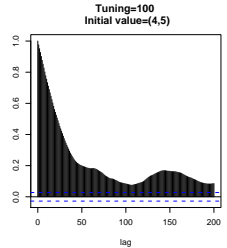
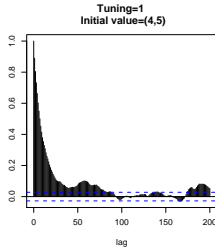
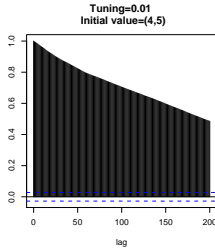
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# Independent Metropolis

$q(\theta, \phi) = f_N(\phi; \mu_3, \nu l_2)$  and  $\mu_3 = (3.01, 4.55)'$ .

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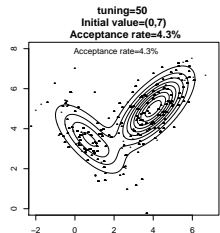
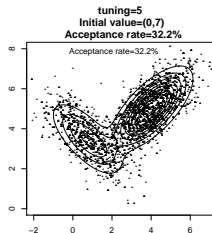
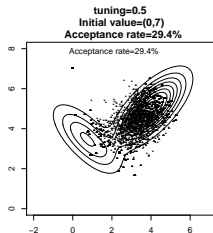
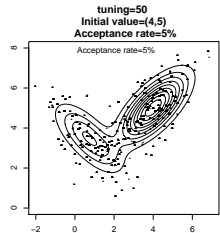
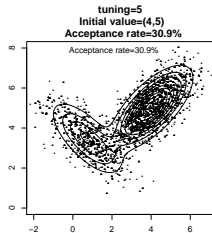
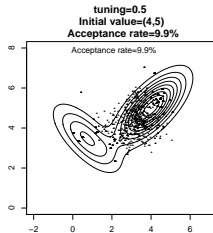
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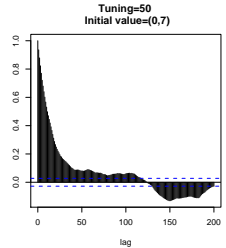
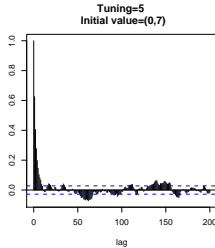
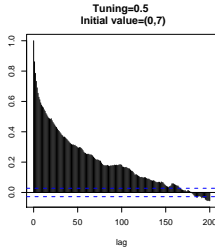
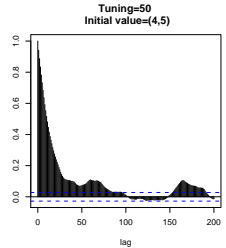
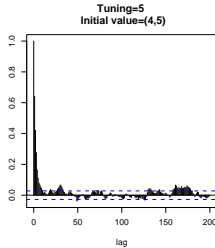
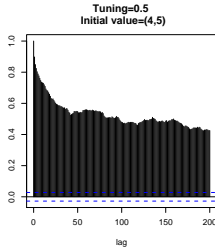
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# Simulated annealing

Simulated annealing<sup>2</sup> is an optimization technique designed to find maxima of functions.

It can be seen as a M-H algorithm that *tempers* with the target distribution:

$$q(\theta) \propto \pi(\theta)^{1/T}$$

where the constant  $T > 1$  receives the physical interpretation of system temperature, hence the nomenclature used (Jennison, 1993).

The *heated* distribution  $q$  is flattened with respect to  $\pi$  and its density gets closer to the uniform distribution, which is particularly relevant for the case of a distribution with distant modes.

By flattening the modes, the moves required to cover adequately the parameter space become more likely.

<sup>2</sup>Kirkpatrick, Gelatt and Vecchi (1983)

## Example vii: Nonlinear surface

Assume that the goal is to find the mode/maximum of

$$\pi(\beta_1, \beta_2) \propto \prod_{i=1}^4 \frac{e^{(\beta_1 + \beta_2 x_i) y_i}}{(1 + e^{\beta_1 + \beta_2 x_i})^5},$$

with  $x = (-0.863, -0.296, -0.053, 0.727)$  and  $y = (0, 1, 3, 5)$ .

The simulated annealing algorithm is implemented for four initial values:

$$(5, 30) \quad (-2, 40) \quad (-4, -10) \quad (6, 0)$$

and two cooling schedules:

$$T_i = 1/i \quad \text{and} \quad T_i = 1/[10 \log(1 + i)].$$

The proposal distribution is  $q(\beta|\beta^{(i)}) = f_N(\beta; \beta^{(i)}, 0.05^2 I_2)$ .

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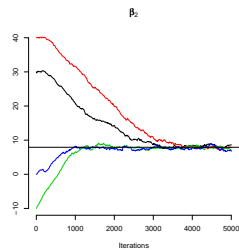
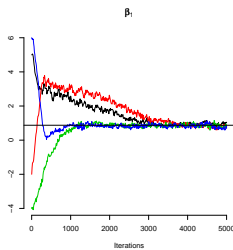
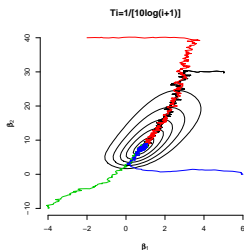
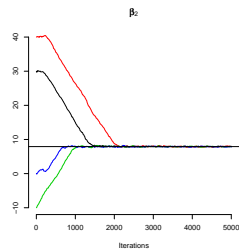
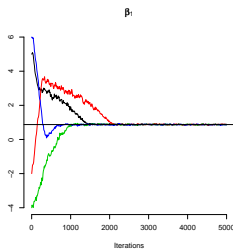
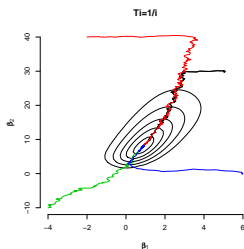
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Newton-Raphson mode: (0.87, 7.91).

$T_i = 1/i$ : mode is (0.88, 7.99) when  $(\beta_1^{(0)}, \beta_2^{(0)}) = (5, 30)$ .

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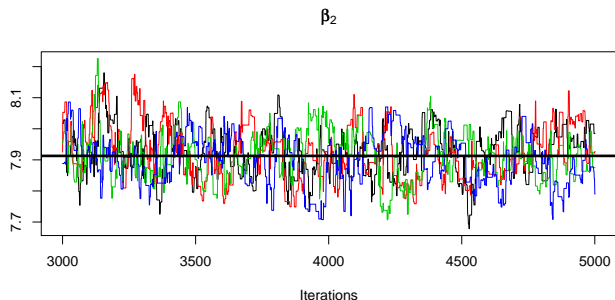
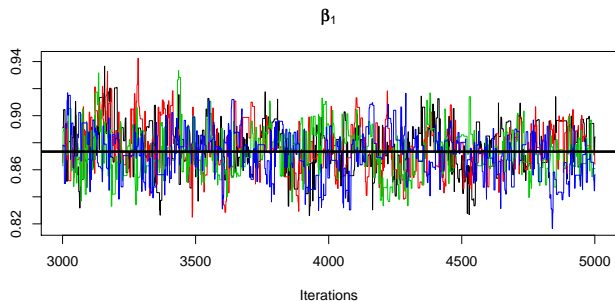
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# Gibbs sampler

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

## Algorithm

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

$$\theta_1^{(j)} \sim \pi(\theta_1 | \theta_2^{(j-1)}, \theta_3^{(j-1)}, \dots)$$

$$\theta_2^{(j)} \sim \pi(\theta_2 | \theta_1^{(j)}, \theta_3^{(j-1)}, \dots)$$

$$\theta_3^{(j)} \sim \pi(\theta_3 | \theta_1^{(j)}, \theta_2^{(j)}, \dots)$$

$$\vdots$$

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 viii: 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

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

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

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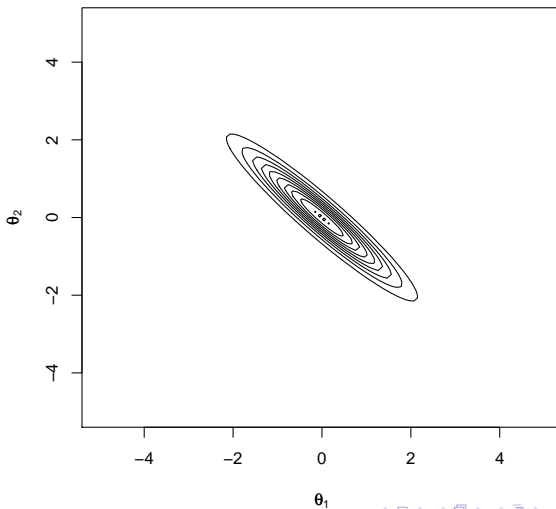
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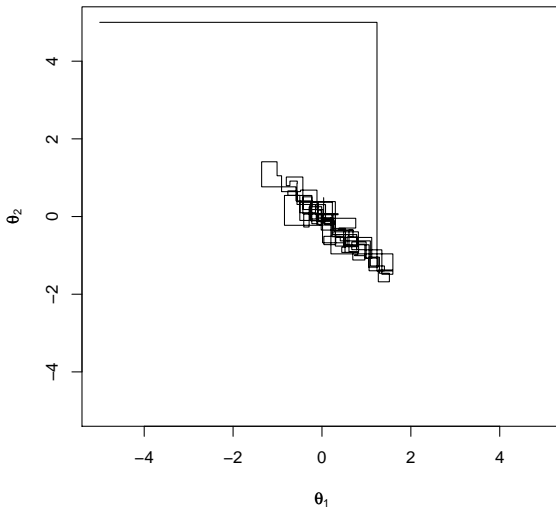
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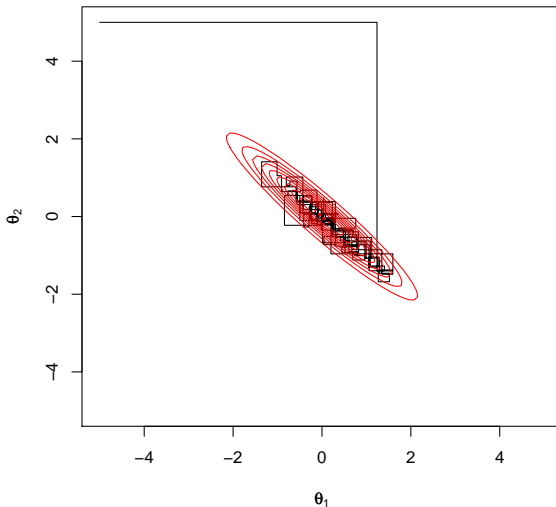
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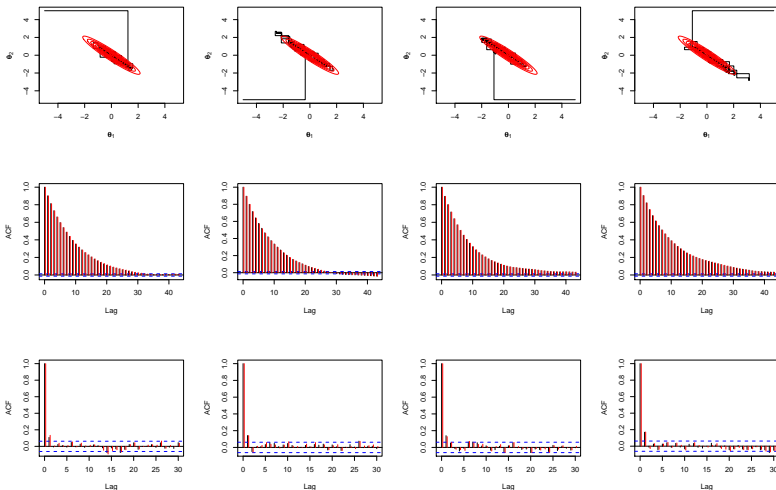
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Middle frame: Based on  $M = 21,000$  consecutive draws.  
Bottom frame: Based on  $M = 1000$  draws, after initial  $M_0 = 1000$  draws and saving every 20th draws.

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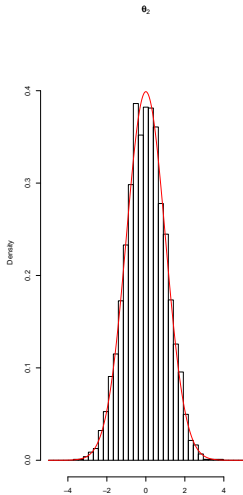
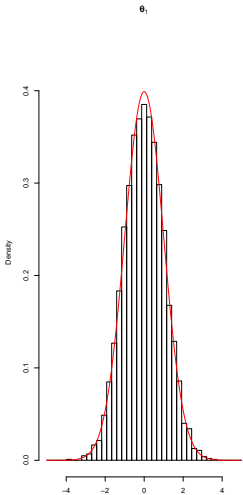
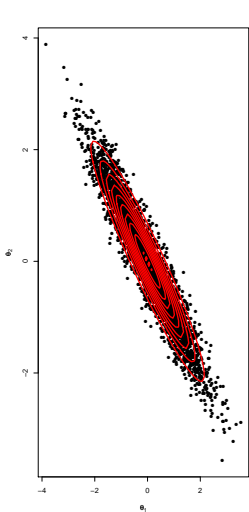
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