Computational statistics, lecture 4

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February 11, 2025

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Markov chain Monte Carlo (MCMC)

(Literature: Givens and Hoeting, 7.1, 7.3; Gentle, 7.3-7.4)

- The algorithms considered so far generate sequences of **independent** observations which follow the target distribution exactly
- We will now consider a method which generates a sequence of **dependent** observations which follow the target distribution **approximately**

- The next observation $(t+1)$ will be generated based on a proposal distribution g which depends on the current observation (t), i.e. $g(\cdot\,|X^{(t)})$
- Since $(X^{(t+1)})$ depends on $(X^{(t)})$ but not on earlier observations, the sequence $(X^{(t)})$ is a Markov chain

MCMC – Metropolis-Hastings algorithm

- A general method to generate the Markov chain is the Metropolis-Hastings (MH) algorithm
- A starting value $x^{(0)}$ is generated from some starting distribution
- Given observation $x^{(t)}$, generate $x^{(t+1)}$ as follows:

1. Sample a candidate x^* from a proposal distribution $g(\cdot|x^{(t)})$
2. Compute the MH ratio $R\left(x^{(t)}, x^*\right) = \dfrac{f(x^*)\, g\left(x^{(t)}|x^*\right)}{f\left(x^{(t)}\right)\, g\left(x^*|x^{(t)}\right)}$
3. Sample $x^{(t+1)}$ according to

$$x^{(t+1)} = \begin{cases} x^*, \text{with probability} \min\{R\left(x^{(t)}, x^*\right), 1\} \\ x^{(t)}, \text{otherwise} \end{cases}$$

4. If more observations needed, set `t <- t+1`; go to 1

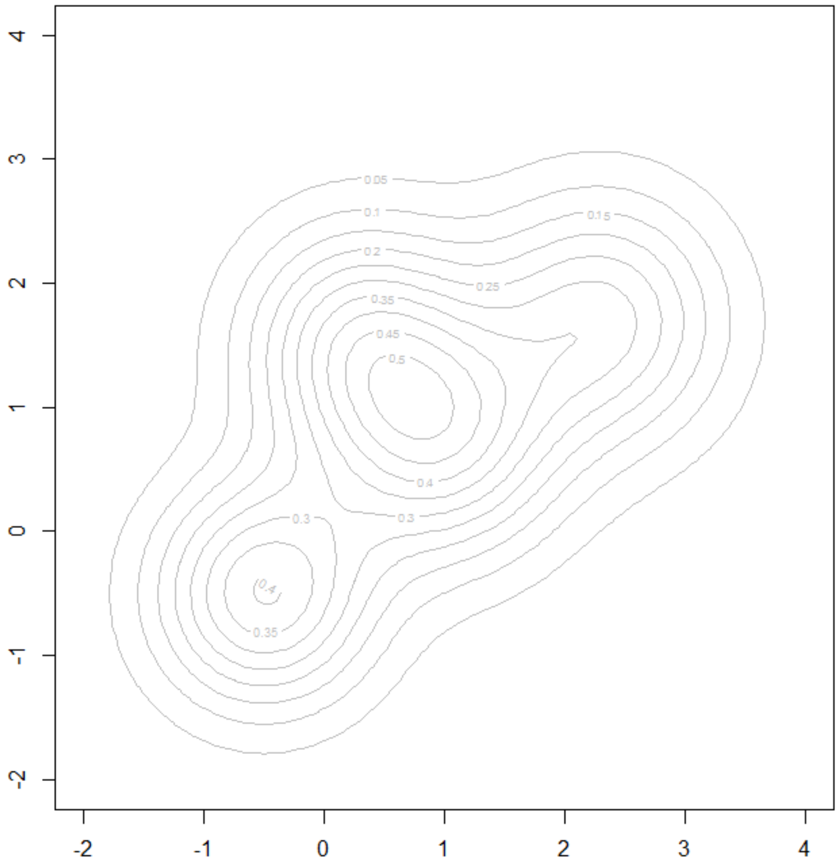
<u>Metropolis algorithm</u>
Special case when g is symmetric:
$g(x^*|x^{(t)}) = g\left(x^{(t)}|x^*\right)$

$= \dfrac{f(x^*)}{f\left(x^{(t)}\right)}$

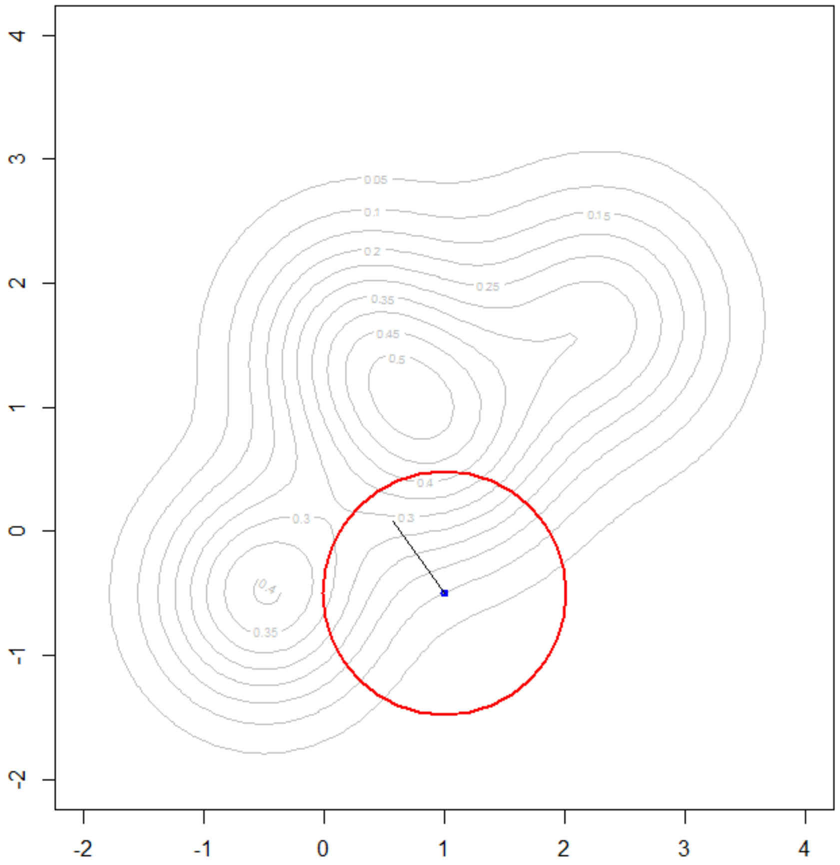
Metropolis alg. – Ex.1

- For illustration, we consider two-dimensional distribution with density f according to contour lines in figure

- Proposal distribution $g(x^*|x^{(t)}) = g(x^{(t)}|x^*)$ $=\frac{1}{\pi r^2}\mathbf{1}\{\|x^{(t)} - x^*\| < r\}$ for some constant r (here=1)

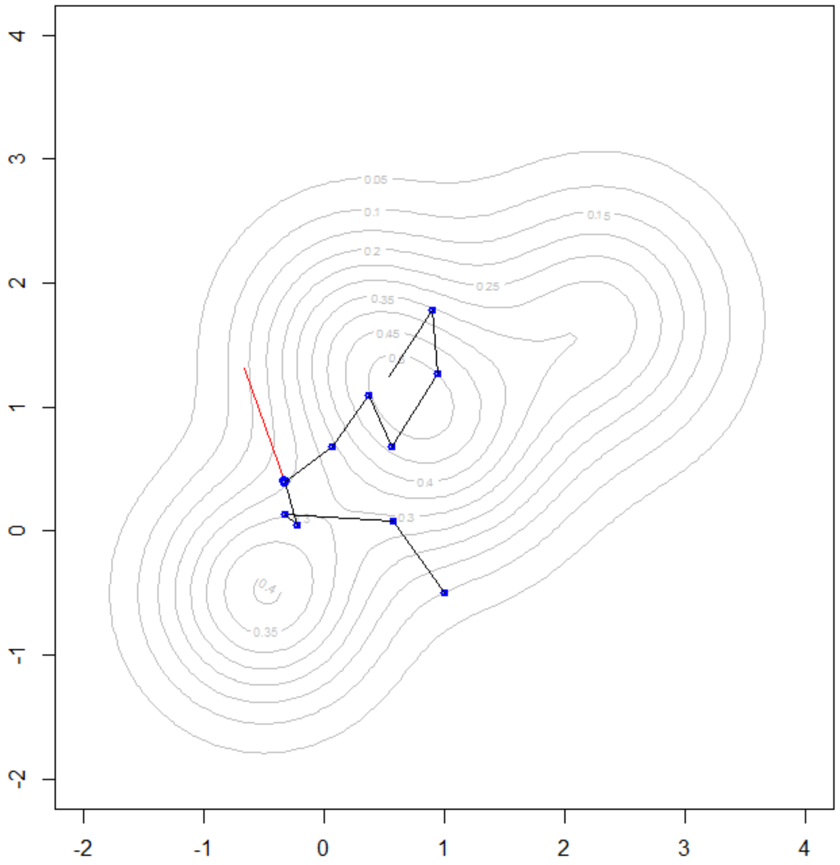


Metropolis alg. – Ex.1



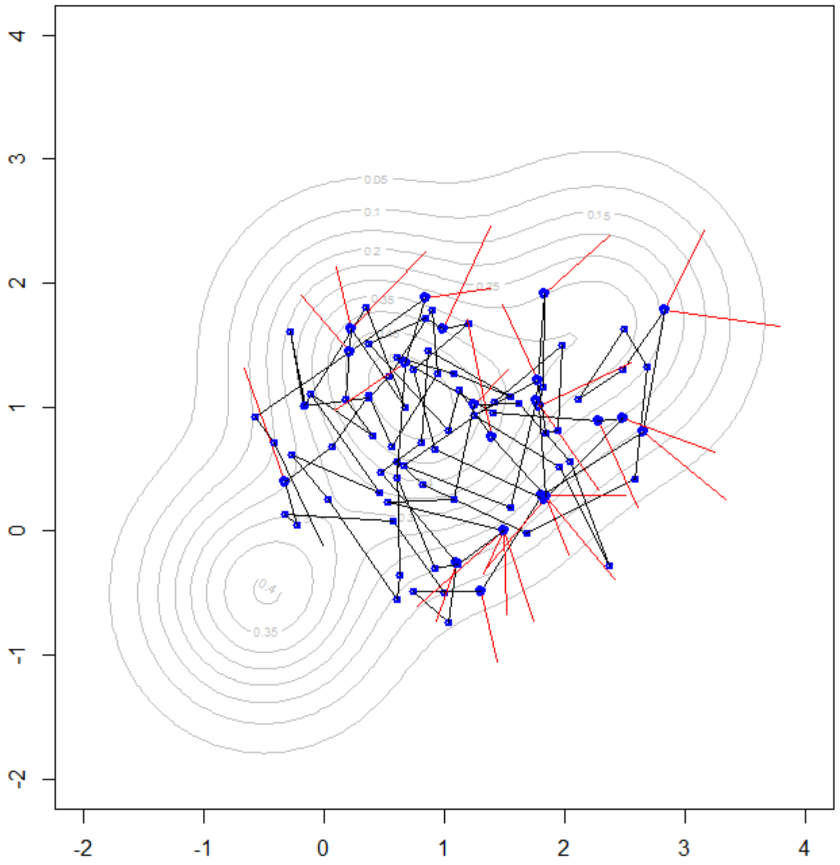
- Proposal distribution $g(x^*|x^{(t)}) = g(x^{(t)}|x^*)$ $= \frac{1}{\pi r^2}\mathbf{1}\{\|x^{(t)} - x^*\| < r\}$ for some constant r (here=1)
- Start here with $x^{(0)} = (1, -0.5)$
- Randomize uniformly on unit circle around $x^{(0)}$ (proposal distribution); result $x^* = (0.58, 0.08)$
- $f(x^*) = 0.296 > f\left(x^{(0)}\right) = 0.098$; so this was an uphill step and is automatically accepted ($R\left(x^{(t)}, x^*\right) = \frac{f(x^*)}{f\left(x^{(t)}\right)} > 1$)

Metropolis alg. – Ex.1



- $x^{(0)} = (1, -0.5)$
- Uphill steps: $x^{(1)} = (0.58, 0.08)$
- $x^{(2)} = (-0.33, 0.13)$
- $x^{(3)} = (-0.23, 0.05)$
- Then downhill step proposed:
  $x^* = (-0.32, 0.4)$,
  $R\left(x^{(t)}, x^*\right) = \dfrac{f(x^*)}{f\left(x^{(t)}\right)} = 0.774$
- Random Unif(0,1) generated: 0.573 and since this is smaller than $R = 0.774$, $x^{(4)} = x^* = (-0.32, 0.4)$ is accepted
- Again downhill step proposed: $x^* = (-0.67, 1.31)$, $R\left(x^{(t)}, x^*\right) = \dfrac{f(x^*)}{f\left(x^{(t)}\right)} = 0.560$; random Unif(0,1): 0.890 and rejection of x^*
- $x^{(5)} = x^{(4)} = (-0.32, 0.4)$

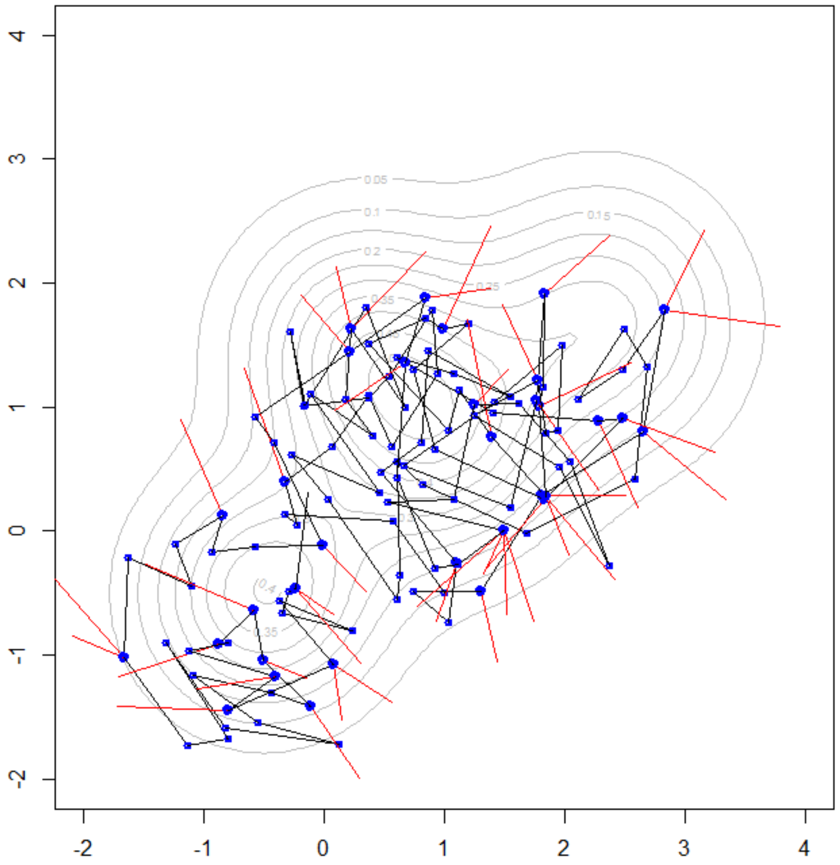
Metropolis alg. – Ex.1



- After several additional iterations (see red lines for rejected proposals), one part of the distribution was explored to a good extend
- Since uphill steps preferred, part of distribution with local maximum at (-0.5,-0.5) is not yet ”detected” at all
- Occasionally, the path will arrive at this part as well

Metropolis alg. – Ex.1

- Now, larger parts of distribution explored



- A couple of animations can be found on: https://chi-feng.github.io/mcmc-demo/app.html#RandomWalkMH,standard (choose Algorithm: RandomWalkMH)

Convergence of Metropolis-Hastings

- If Metropolis-Hastings generated sequence $(X^{(t)})$ is an **irreducible and aperiodic chain** (compare Lecture LM2), the distribution of $(X^{(t)})$ **converges to target distribution**

- For example, if target distribution is uniform distribution on intervals $[0, \frac{1}{2}]$ and $[\frac{3}{2}, 2]$, and proposal distribution is uniform distribution on $[X^{(t)} - \frac{1}{2}, X^{(t)} + \frac{1}{2}]$, the requirements above are violated

Bayesian analysis

- Data y is collected and assumed that it is generated according to a distribution with density $f(y|\theta)$; θ is a parameter(-vector) to be estimated
- The posterior density is proportional to product of likelihood and prior:

$f_{posterior}(\theta|y) = \frac{f(y|\theta) \cdot f_{prior}(\theta)}{f(y)}$, where $f(y) = \int f(y|\theta) f_{prior}(\theta) d\theta$

- We would like to generate the posterior distribution $f_{posterior}$
- We have likelihood $f(y|\theta)$ and an assumption for prior $f_{prior}(\theta)$
- For Metropolis-Hastings, we do not need the denominator $f(y)$; it cancels out in the MH ratio (see algorithm):

$$R\left(x^{(t)}, x^*\right) = \frac{f_{posterior}(x^*)\, g\left(x^{(t)}\middle|x^*\right)}{f_{posterior}(x^{(t)})\, g\left(x^*\middle|x^{(t)}\right)}$$

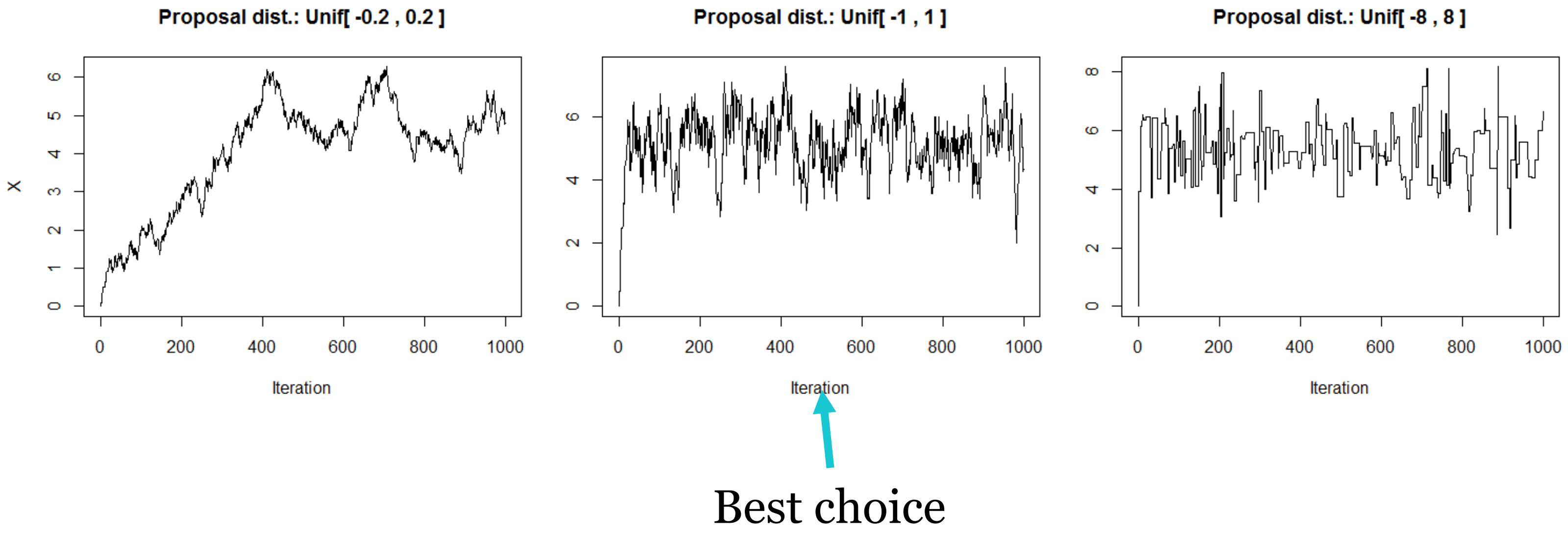
Metropolis algorithm - Example 2

(compare Givens and Hoeting, ex. 5.3)

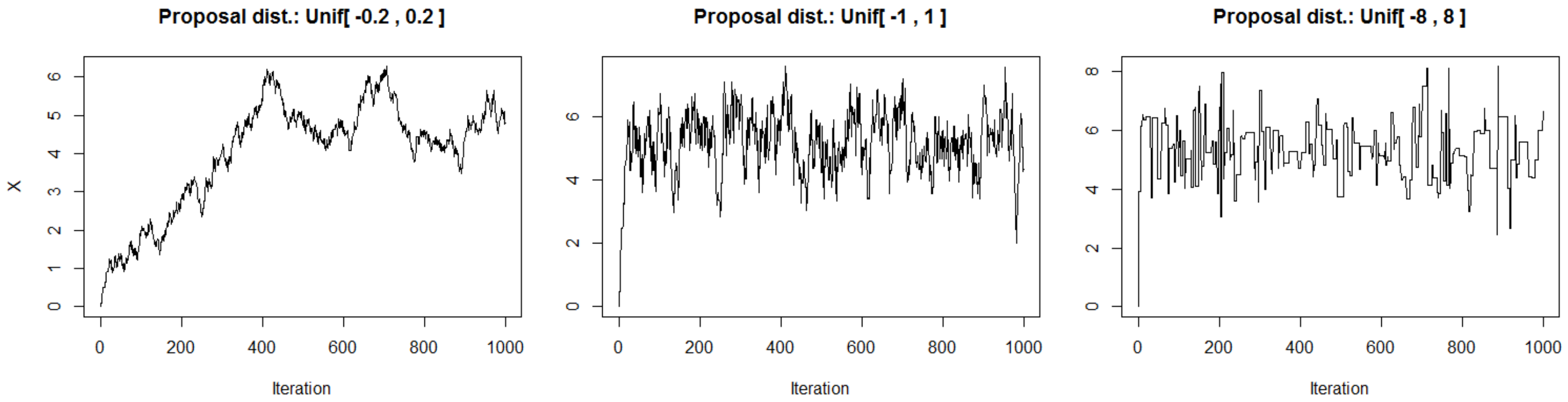
- Consider Bayesian estimation of μ based on $N(\mu, 3^2/7)$ likelihood for μ and Cauchy(5,2) prior; observed mean=5.38
- The posterior density is proportional to product of likelihood and prior
- **Use MCMC to generate random samples following the posterior density**
- Based on these random samples, one can e.g.
  - determine posterior probability that $2 \le \mu \le 8$
  - determine mean and variance of posterior

Metropolis algorithm - Example 2

- We use starting value $x^{(0)} = 0, s = 1000$ iterations and following proposal distributions $g(\cdot\,|x^{(t)})$:
  $x^{(t)}$+Unif[-0.2,0.2], $x^{(t)}$+Unif[-1,1], $x^{(t)}$+Unif[-8,8]
- **Sample path plots** show simulated values $x^{(t)}$ vs. iteration number t



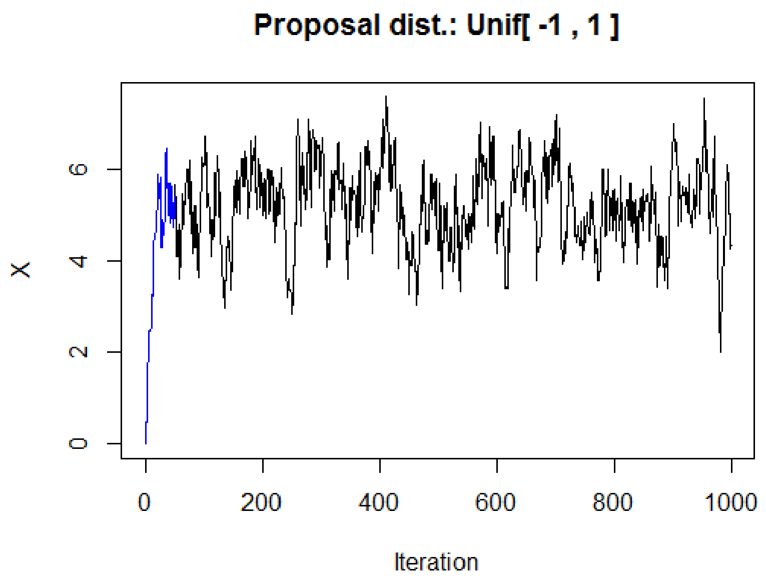
Metropolis algorithm - Example 2

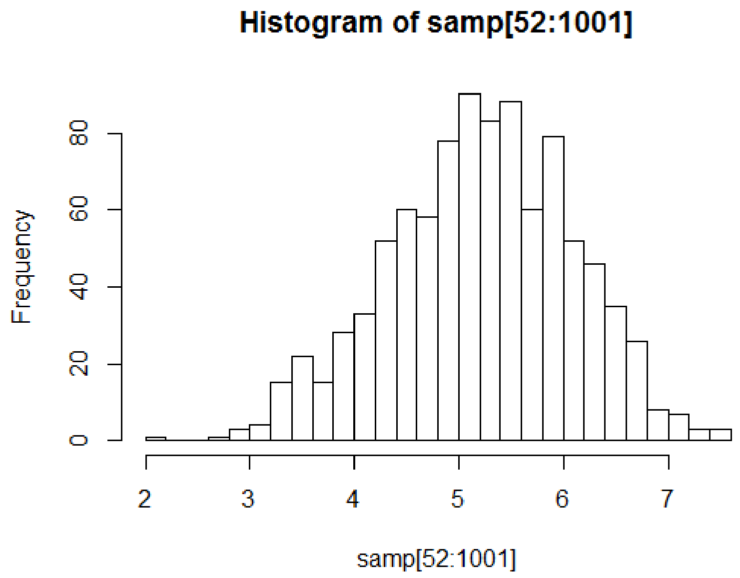


- Count “acceptance rate” (=proportion accepted proposals)
- Here: 98% 78% 18%
- Best results for 44% (uni-dim. case) to 23.4% (high dim. case) acceptance probability (theory based on normal target and proposal functions, see Givens and Hoeting, Chapter 7.3, for references about that)
- For multimodal functions lower acceptance probabilities might be good

Metropolis algorithm - Example 2

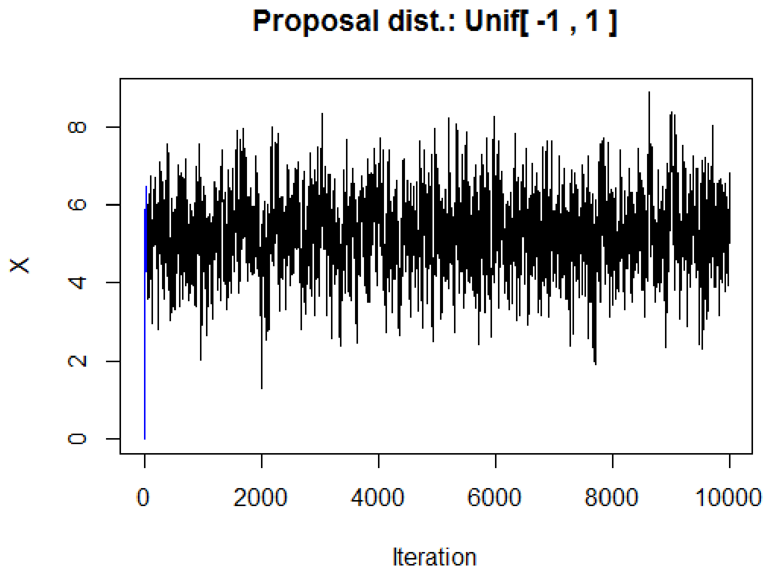
- Based on sample path plots, we might choose $x^{(t)}$+Unif[-1,1] as proposal distribution
- Often, one wants to discard initial samples (**burn-in** period) which highly depend on starting value, e.g. 50 values + $x^{(0)}$

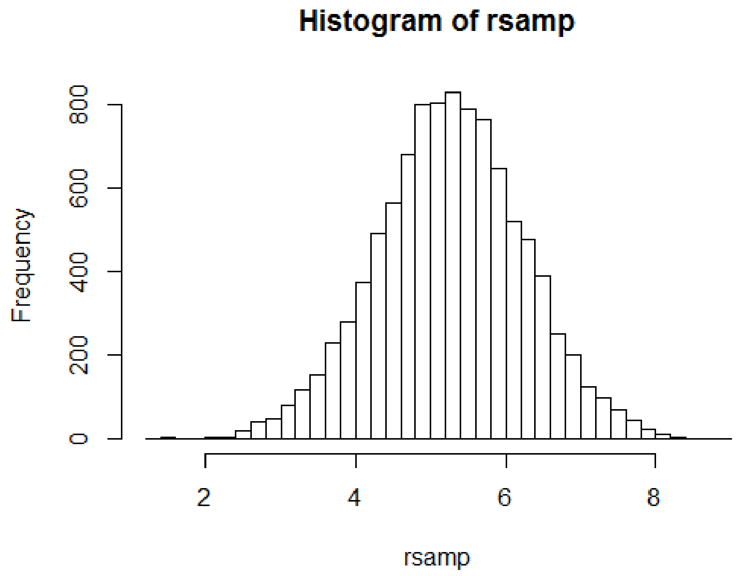




Metropolis algorithm - Example 2

- For $s = 10\,000$ iterations and burn-in of 50, we obtain

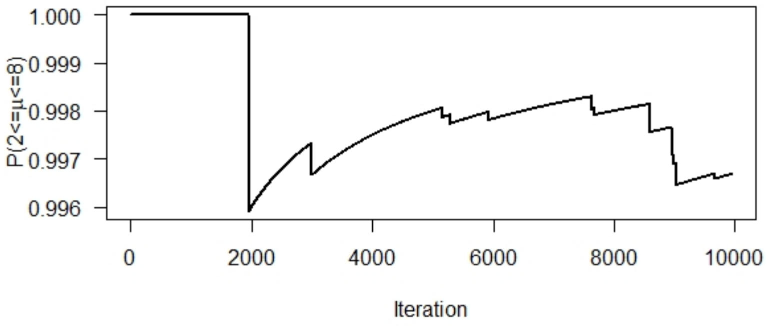




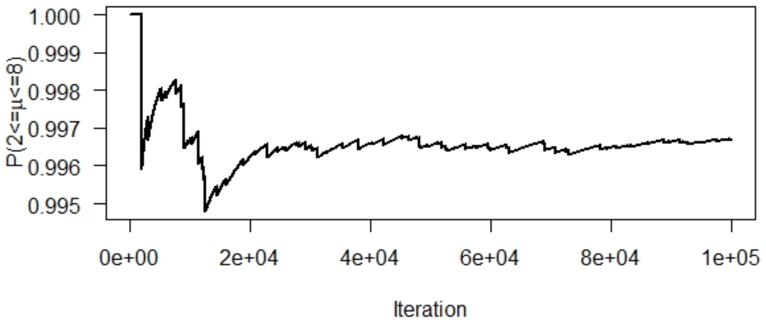
- Monte Carlo estimate for $P(2 \leq \mu \leq 8)$ is 0.9967
  (Monte Carlo standard error=$\sqrt{0.9967 * 0.0033/9950} = 0.0006$)
- Estimated mean = 5.26, standarddeviation =0.99

Metropolis algorithm - Example 2

- Were $s = 10\,000$ iterations enough to ensure convergence?
- Can depend on the purpose …
- E.g. for estimating $P(2 \leq \mu \leq 8)$
- One can monitor cusum/convergence plots showing estimate versus iterations (see Givens and Hoeting, ch.7.3.1.1)
- After 10 000 iterations



After 100 000 iterations



- After 10 000 iterations, we might not be happy with the left graph; we run longer and are happy with 100 000

Metropolis-Hastings with independent proposals

- Other proposal distributions g possible (not necessarily symmetric), e.g. independent proposals
- Proposal distribution depends not on previous value, $g\left(\cdot \,|x^{(t)}\right) = g(\cdot)$
- The MH ratio is $R\left(x^{(t)}, x^*\right) = \frac{f(x^*)\, g\left(x^{(t)}|x^*\right)}{f\left(x^{(t)}\right)\, g\left(x^*|x^{(t)}\right)} = \frac{f(x^*)/g(x^*)}{f\left(x^{(t)}\right)/g(x^{(t)})}$
- A possible application is for Bayesian analysis (f is the posterior) with proposal distribution g being the prior distribution
- f/g is then the likelihood

Gibbs sampling

- Situation:
  - We want to sample a multivariate distribution $f(x_1, \dots, x_d)$ and this density is difficult to sample from
  - The conditional distributions for each single dimension i given fixed values $x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_d$ are easy to sample from
- Gibbs sampling generates a Markov chain converging to distribution f in this situation
- We sample one dimension in turn

Gibbs sampling

- The algorithm:

0. A starting value $\mathrm{x}^{(0)} = (x_1^{(0)}, x_2^{(0)}, \dots, x_d^{(0)})$ is chosen
1. Generate $x_1^{(t+1)}$ following $f(x_1 | x_2^{(t)}, \dots, x_d^{(t)})$
2. Generate $x_2^{(t+1)}$ following $f\left(x_2 \middle| x_1^{(\boldsymbol{t+1})}, x_3^{(t)}, \dots, x_d^{(t)}\right)$

…

i. Generate $x_i^{(t+1)}$ following $f(x_i | x_1^{(\boldsymbol{t+1})}, \dots, x_{i-1}^{(\boldsymbol{t+1})}, x_{i+1}^{(t)}, \dots, x_d^{(t)})$

…

d. Generate $x_i^{(t+1)}$ following $f(x_d | x_1^{(\boldsymbol{t+1})}, \dots, x_{d-1}^{(\boldsymbol{t+1})})$

- Go back to 1. if more points needed

Gibbs sampling

- Example:
  Let $f(x_1, x_2) = c \cdot \mathbf{1}\{x_1^2 + 1.8 \cdot x_1 x_2 + x_2^2 < 1\}$ be the uniform distribution on the ellipse
  $$x_1^2 + 1.8 \cdot x_1 x_2 + x_2^2 < 1$$
- The conditional distribution for x_2 given x_1 is a uniform distribution on the interval $(-0.9x_1 - \sqrt{1 - 0.19x_1^2}, -0.9x_1 + \sqrt{1 - 0.19x_1^2})$ if the term below the root is positive

You can obtain these boundaries by solving $x_1^2 + 1.8 \cdot x_1 x_2 + x_2^2 - 1 = 0$ for x_2

- x_1 given x_2 has a similar distribution with x_2 instead of x_1 in the boundaries