Stochastic Simulation
Markov Chain Monte Carlo

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MCMC: What we aim to achieve

We have a variable X with a "complicated" distribution.

We cannot sample X directly.

We aim to generate a sequence of X_i's

- which each has the same distribution as X
- but we (have to) allow them to be dependent.

This is an **inverse problem** relative to what we just discussed and to the queueing exercise:
We start with the distribution of X, and aim to design a state machine which has this steady-state distribution.

MCMC example from Bayesian statistics

Prior distribution of parameter

$$P \sim U(0,1) \qquad : \qquad f_P(p) = \mathbf{1} \quad (0 \leq p \leq 1)$$

Distribution of data, conditional on parameter

$$X \text{ for given } P = p \text{ is } \mathrm{Binomial}(n,p)$$

i.e. the data has the conditional probabilities

$$\mathsf{P}(X = i | P = p) = \begin{pmatrix} n \\ i \end{pmatrix} p^i (1-p)^{n-i}$$

The posterior distribution of P

Conditional density of parameter, given observed data $X = i$ (the posterior distribution):

$$f_{P|X=i}(p) = f_P(p) \frac{\mathsf{P}(X = i | P = p)}{\mathsf{P}(X = i)} = c f_P(p) \mathsf{P}(X = i | P = p)$$

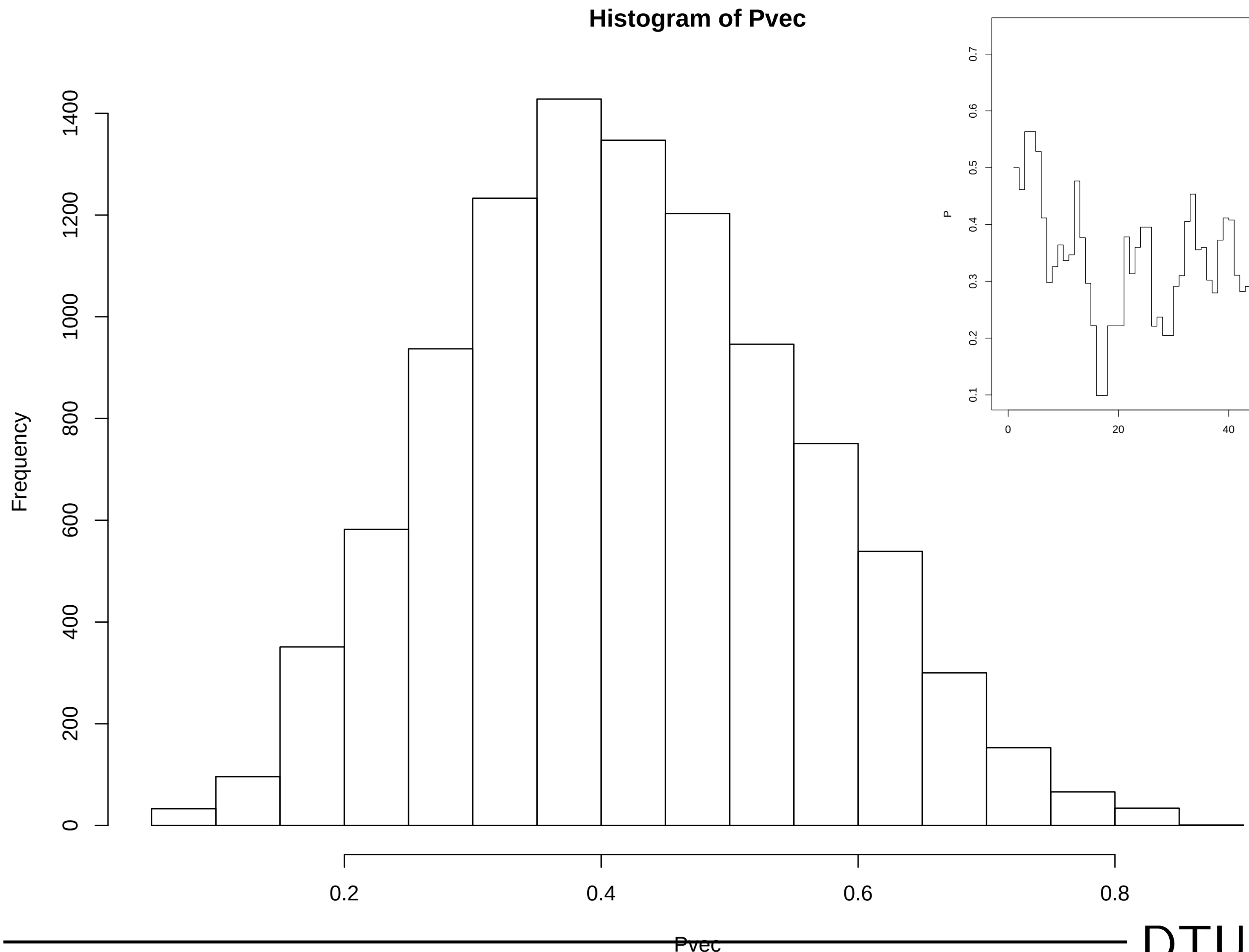
We need the unconditional probability of the observation:

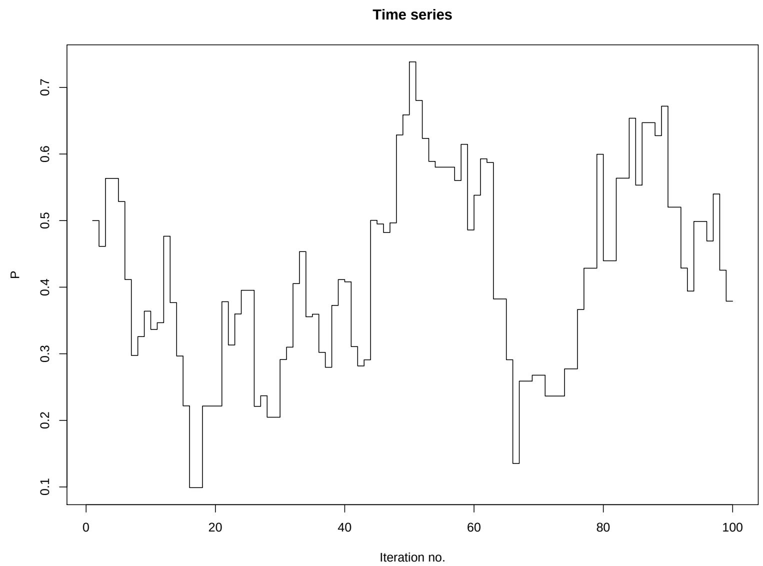
$$\mathsf{P}(X = i) = \int_0^1 f_P(p) \binom{n}{i} p^i (1-p)^{n-i} \, dp$$

We *can* evaluate this; but in more complex models we might not.

AIM: To sample from $f_{P|X=i}$, without evaluating $c = 1/\mathsf{P}(X = i)$.

The posterior distribution





When to apply MCMC?

The distribution is given by

$$f(x) = c \cdot g(x)$$

where the *unnormalized density* g can be evaluated, *but* the normalising constant c cannot be evaluated (easily).

$$c = \frac{1}{\int_{\mathbf{X}} g(x)\, dx}$$

This is frequently the case in Bayesian statistics - the posterior density is proportional to the likelihood function

Note (again) the similarity between simulation and evaluation of integrals

When to apply MCMC? - continued

We want to sample from a distribution is given by

$$f(x) = c \cdot g(x)$$

where the *unnormalized density* g can be evaluated, *but* the normalising constant c cannot be evaluated (easily).

$$c = \frac{1}{\int_{\mathbf{X}} g(x)\, dx}$$

We generate samples from a Markov chain, where we can prove, that the limiting (invariant) distribution is our target distribution ($f(x)$)

Metropolis-Hastings algorithm

- Proposal distribution $h(\boldsymbol{x}, \boldsymbol{y})$
- Acceptance of solution? The solution will be accepted with probability

$$\min\left(1, \frac{f(\boldsymbol{y})h(\boldsymbol{y},\boldsymbol{x})}{f(\boldsymbol{x})h(\boldsymbol{x},\boldsymbol{y})}\right) = \min\left(1, \frac{g(\boldsymbol{y})h(\boldsymbol{y},\boldsymbol{x})}{g(\boldsymbol{x})h(\boldsymbol{x},\boldsymbol{y})}\right)$$

- Avoiding the troublesome constant c!
- Frequently we apply a symmetric proposal distribution $h(\boldsymbol{y}, \boldsymbol{x}) = h(\boldsymbol{x}, \boldsymbol{y})$ Metropolis algorithm to get

$$\left(= \min\left(1, \frac{g(\boldsymbol{y})}{g(\boldsymbol{x})}\right) \text{ for } h(\boldsymbol{y},\boldsymbol{x}) = h(\boldsymbol{x},\boldsymbol{y})\right)$$

Metropolis Hastigs algorithm and local balance

The transition rate $q(\boldsymbol{x},\boldsymbol{y})$ from $\boldsymbol{x}$ to $\boldsymbol{y}$ and vice versa is

$$q(\boldsymbol{x},\boldsymbol{y}) = h(\boldsymbol{x},\boldsymbol{y})\min\left(1, \frac{g(\boldsymbol{y})h(\boldsymbol{y},\boldsymbol{x})}{g(\boldsymbol{x})h(\boldsymbol{x},\boldsymbol{y})}\right)$$

and

$$q(\boldsymbol{y},\boldsymbol{x}) = h(\boldsymbol{y},\boldsymbol{x})\min\left(1, \frac{g(\boldsymbol{x})h(\boldsymbol{x},\boldsymbol{y})}{g(\boldsymbol{y})h(\boldsymbol{y},\boldsymbol{x})}\right)$$

Suppose $g(\boldsymbol{y})h(\boldsymbol{y},\boldsymbol{x}) < g(\boldsymbol{x})h(\boldsymbol{x},\boldsymbol{y})$ then

$$f(\boldsymbol{x})q(\boldsymbol{x},\boldsymbol{y}) = cg(\boldsymbol{x})h(\boldsymbol{x},\boldsymbol{y})\frac{g(\boldsymbol{y})h(\boldsymbol{y},\boldsymbol{x})}{g(\boldsymbol{x})h(\boldsymbol{x},\boldsymbol{y})} = cg(\boldsymbol{y})h(\boldsymbol{y},\boldsymbol{x}) = f(\boldsymbol{y})q(\boldsymbol{y},\boldsymbol{x})$$

Random Walk Metropolis-Hastings

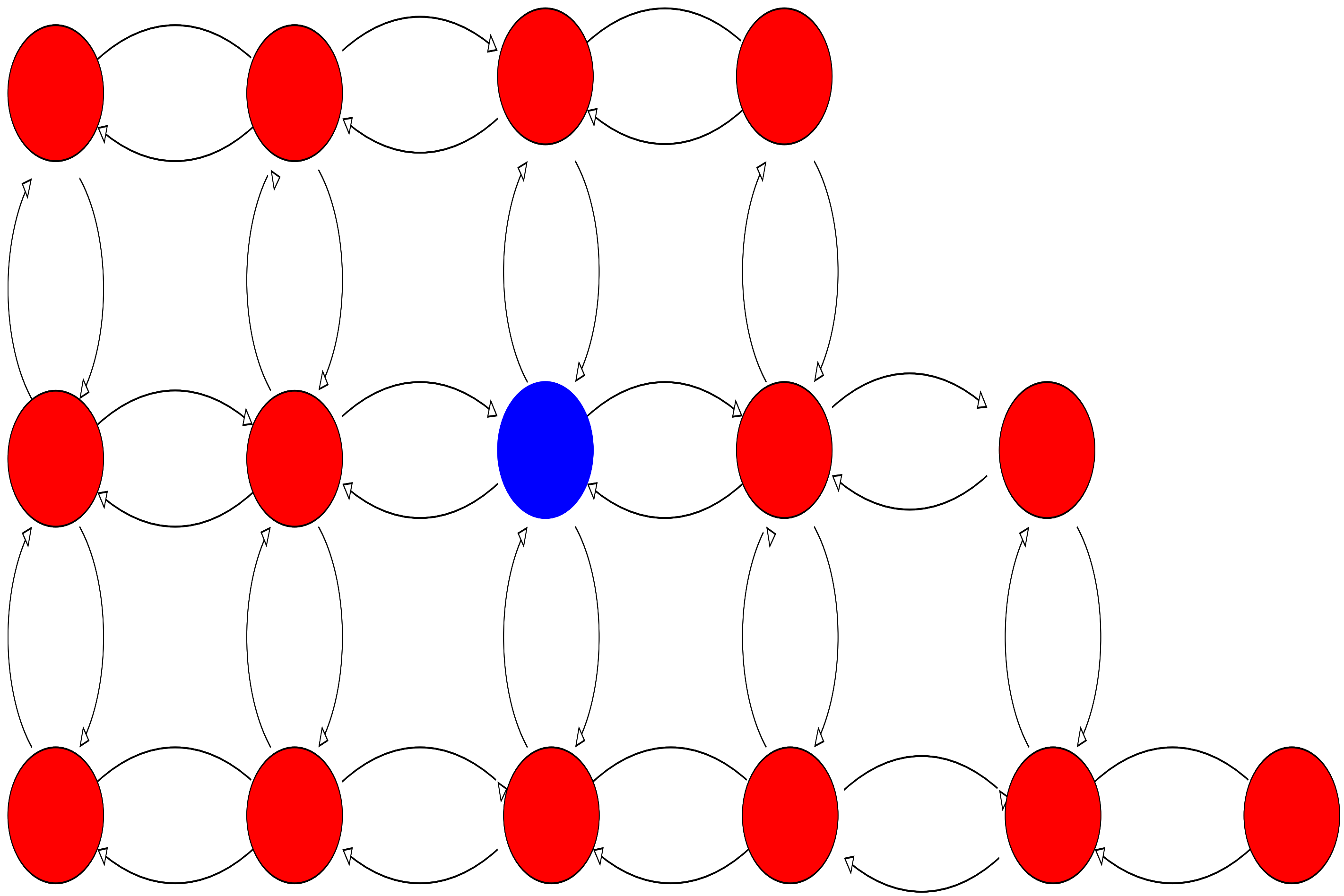
A simple *symmetric* proposal distribution is the random walk

1. At iteration i, the state is X_i
2. *Propose* to jump from X_i to $Y_i = X_i + \Delta X_i$ where ΔX_i is sampled indepedently from a symmetric distribution
   - If $g(Y) \geq g(X_i)$, accept
   - If $g(Y) \leq g(X_i)$, accept w.p. $g(Y)/g(X_i)$
3. On accept: Set $X_{i+1} = Y_i$ and goto 1.
4. On reject: Set $X_{i+1} = X_i$ and goto 1.

Proposal distribution (Gelman 1998)

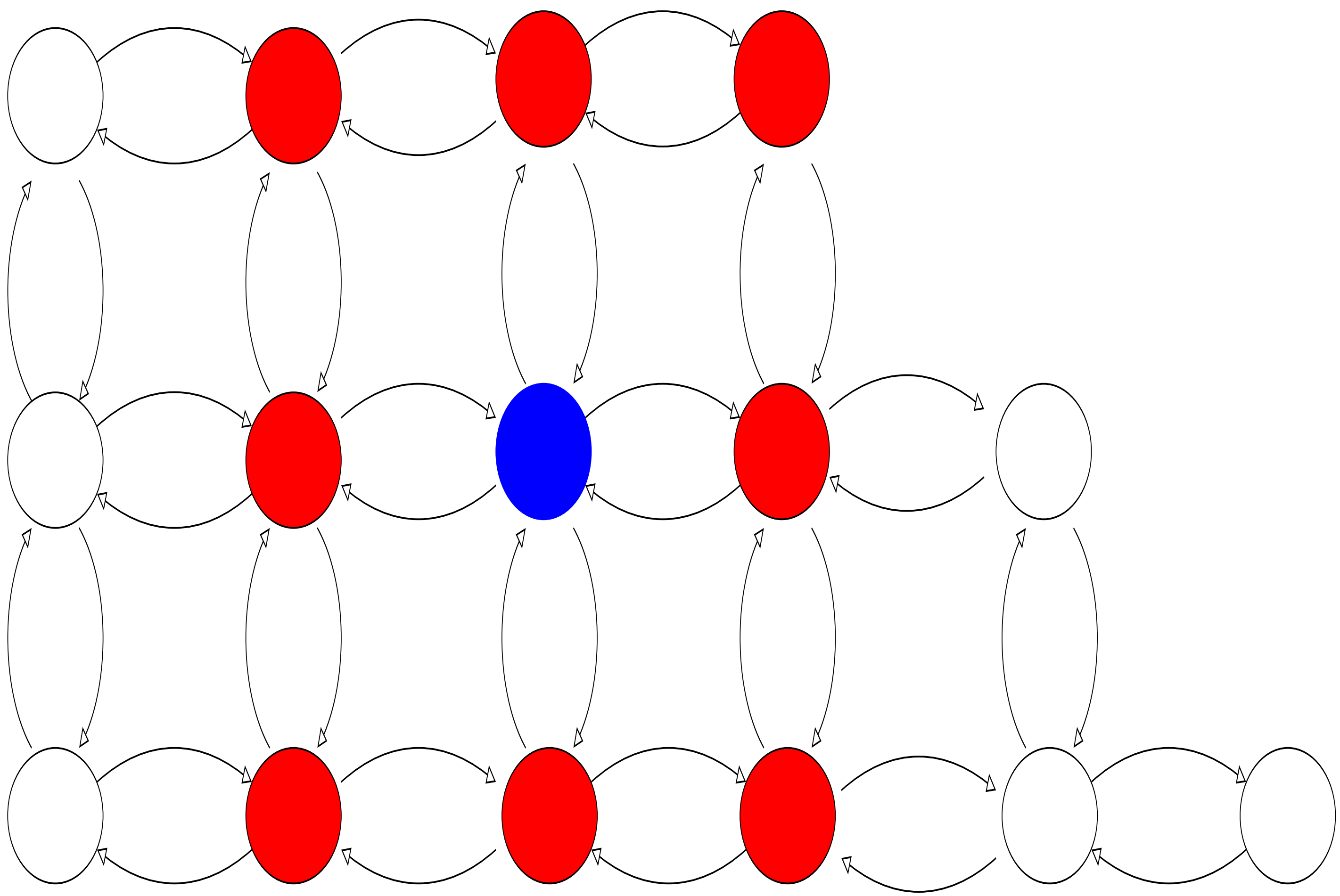
- A good proposal distribution has the following properties
  - For any $\boldsymbol{x}$, it is easy to sample from $h(\boldsymbol{x}, \boldsymbol{y})$
  - It is easy to compute the accpetance probability
  - Each jump goes a reasonable distance in the parameter space
  - The proposals are not rejected too frequently

Illustration of ordinary MCMC sampling



A new proposal can be anywhere in the full region

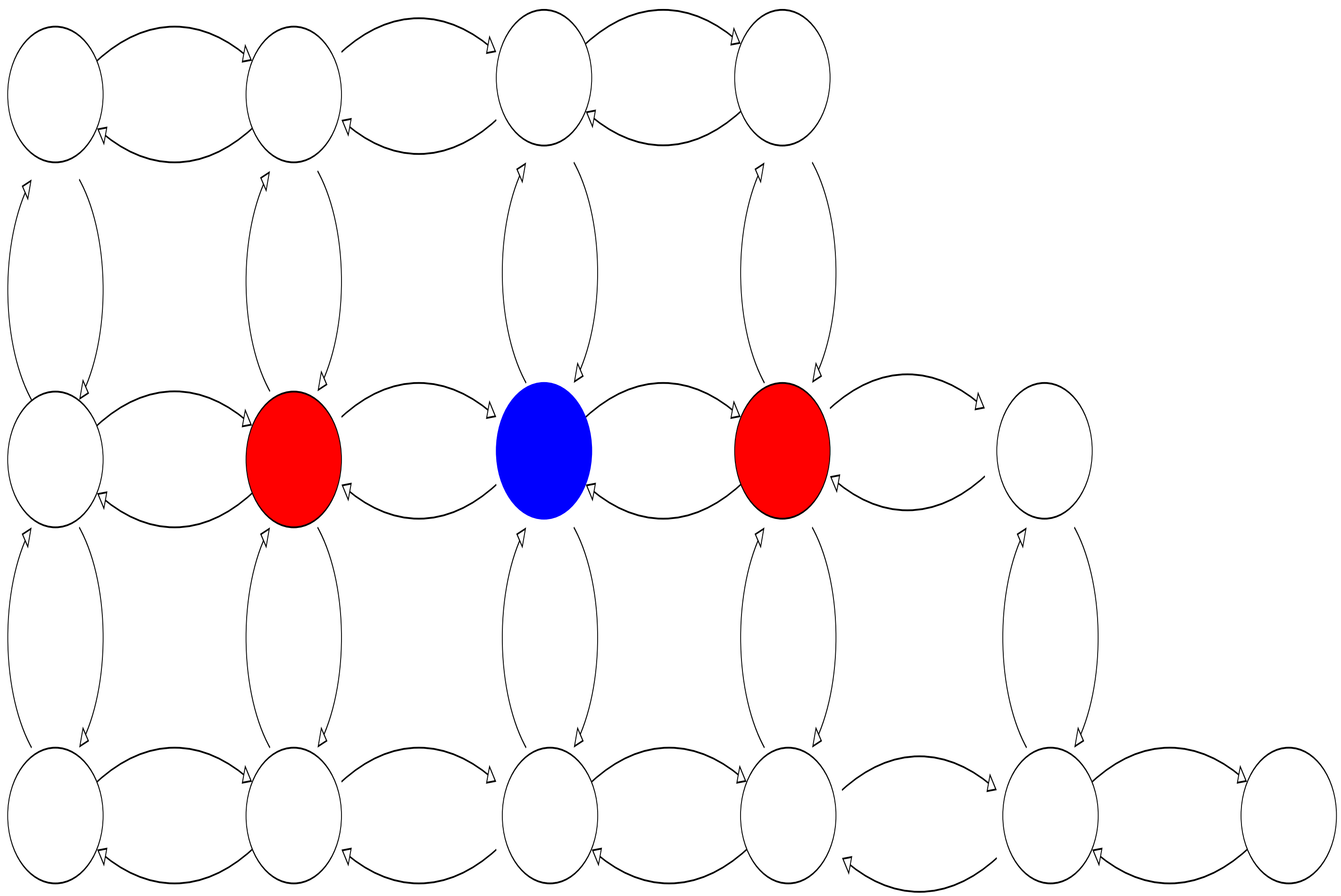
Illustration of ordinary MCMC sampling



A new proposal can be anywhere in the full region. However, typically it will be in the vicinity of the current

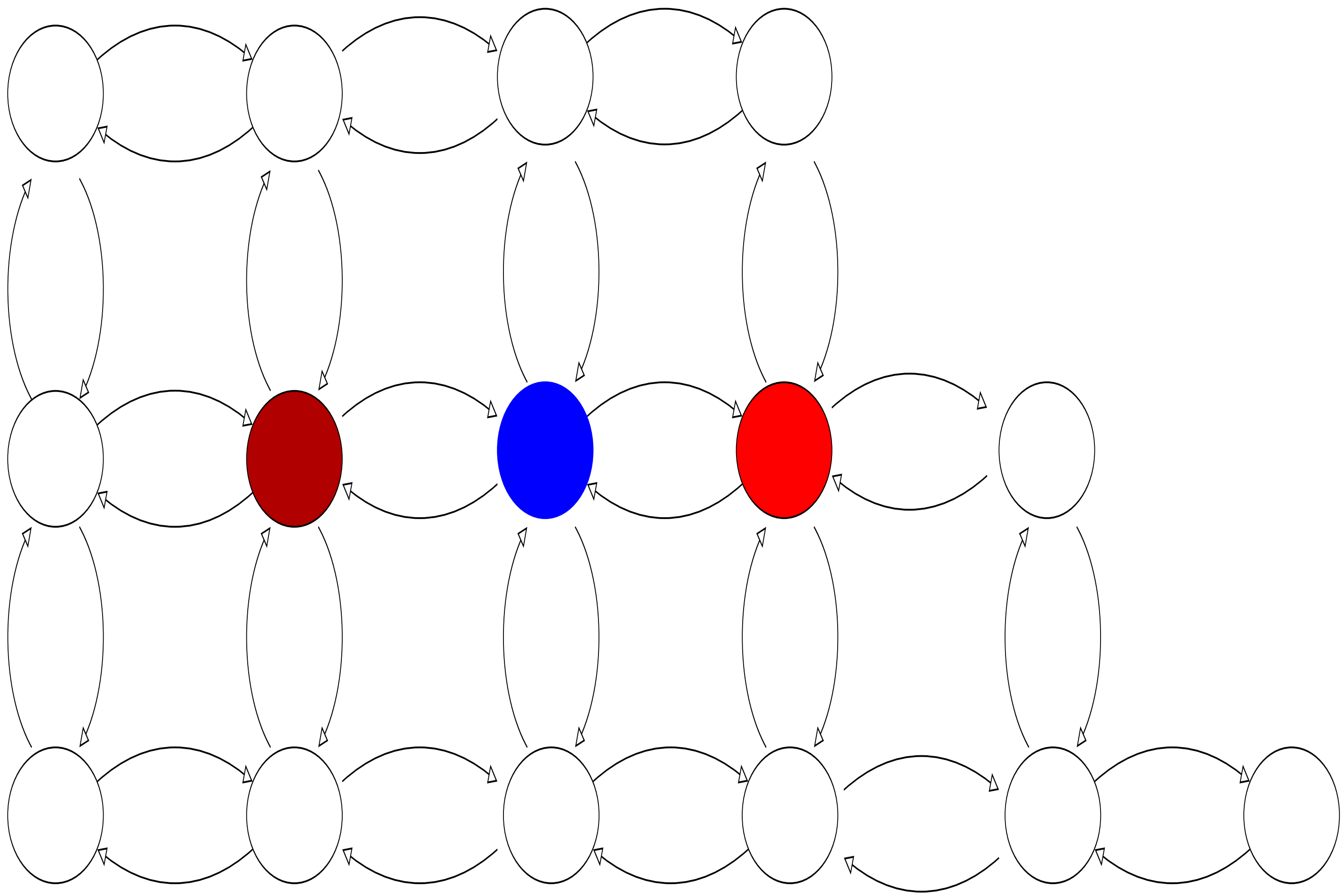
Coordinatewise MCMC sampling

We generate proposal and do acceptance/rejection for one dimension at a time. It can be done systematically or random.



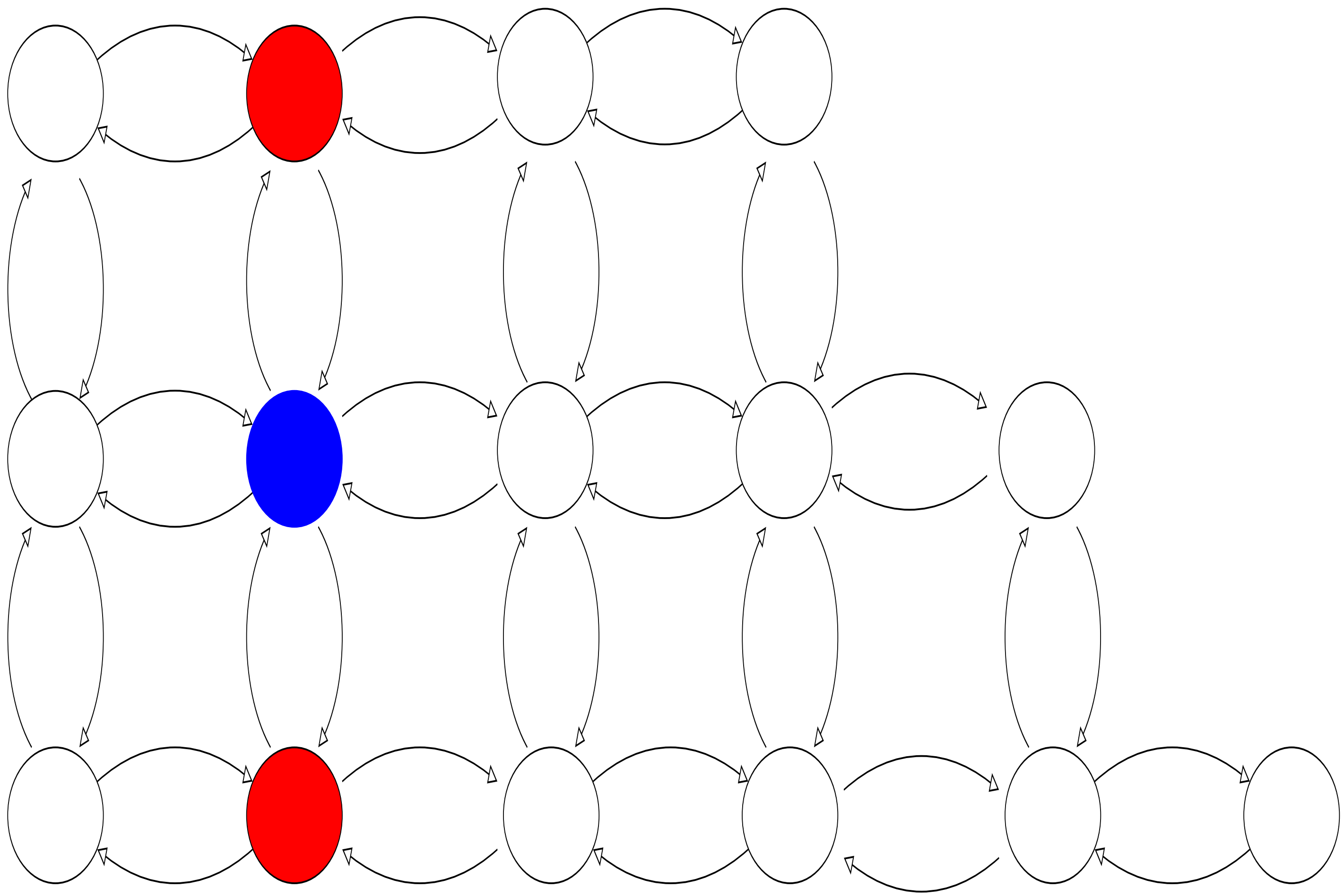
Possibilities in x-direction

Coordinatewise MCMC sampling



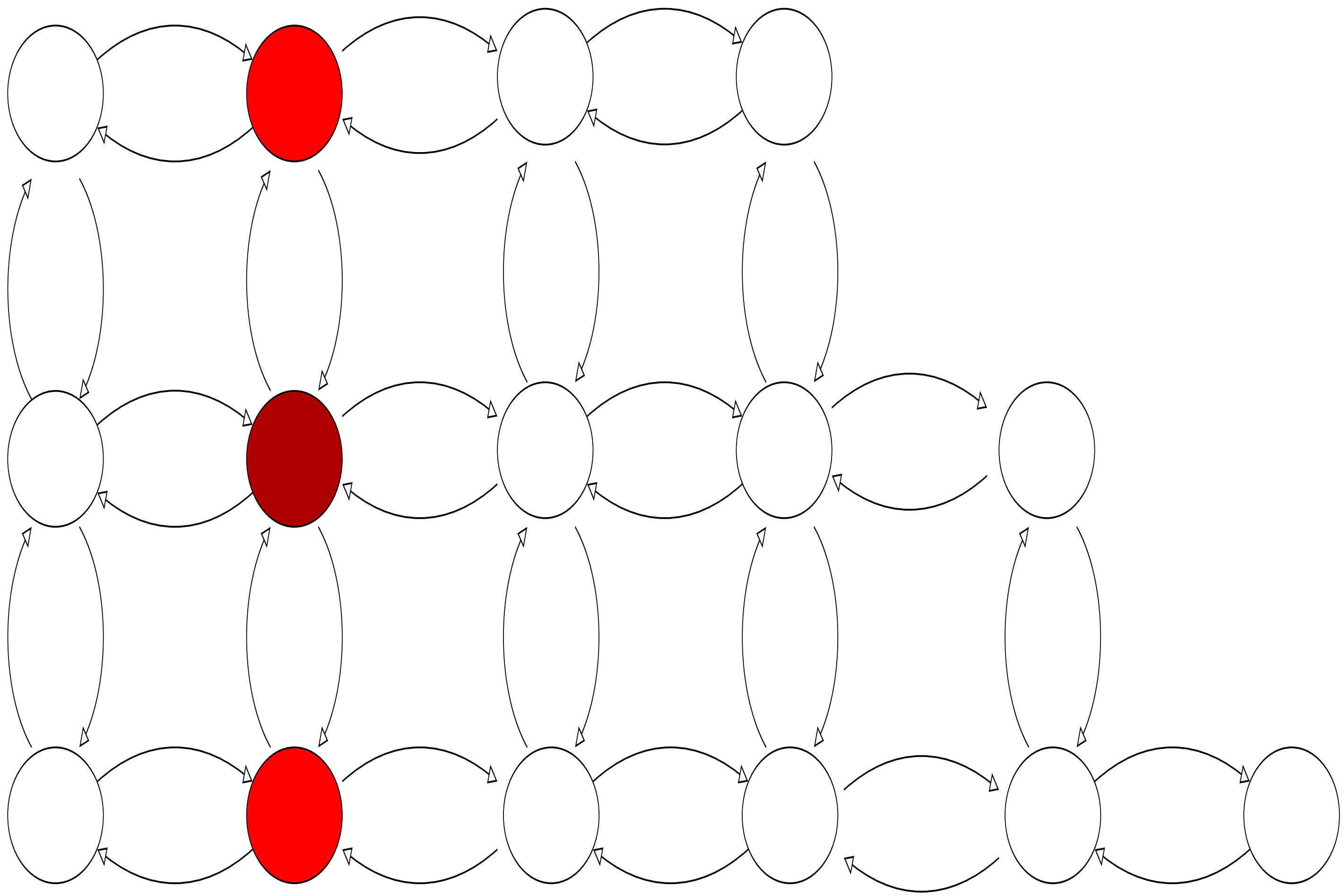
Accepted candidate in x-direction

Coordinatewise MCMC sampling



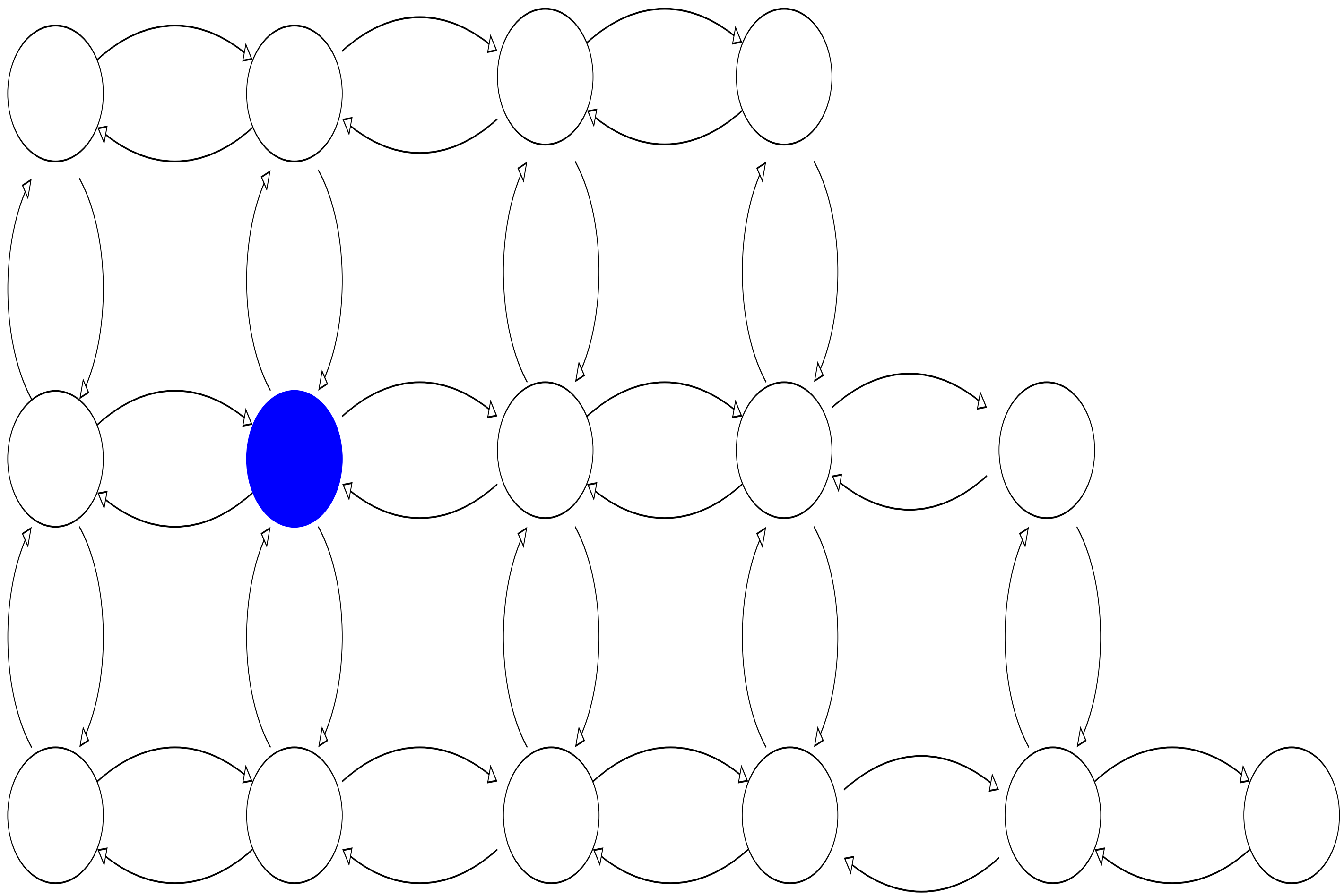
Possibilities in y-direction

Coordinatewise MCMC sampling



Accepted candidate in y-direction

Coordinatewise MCMC sampling

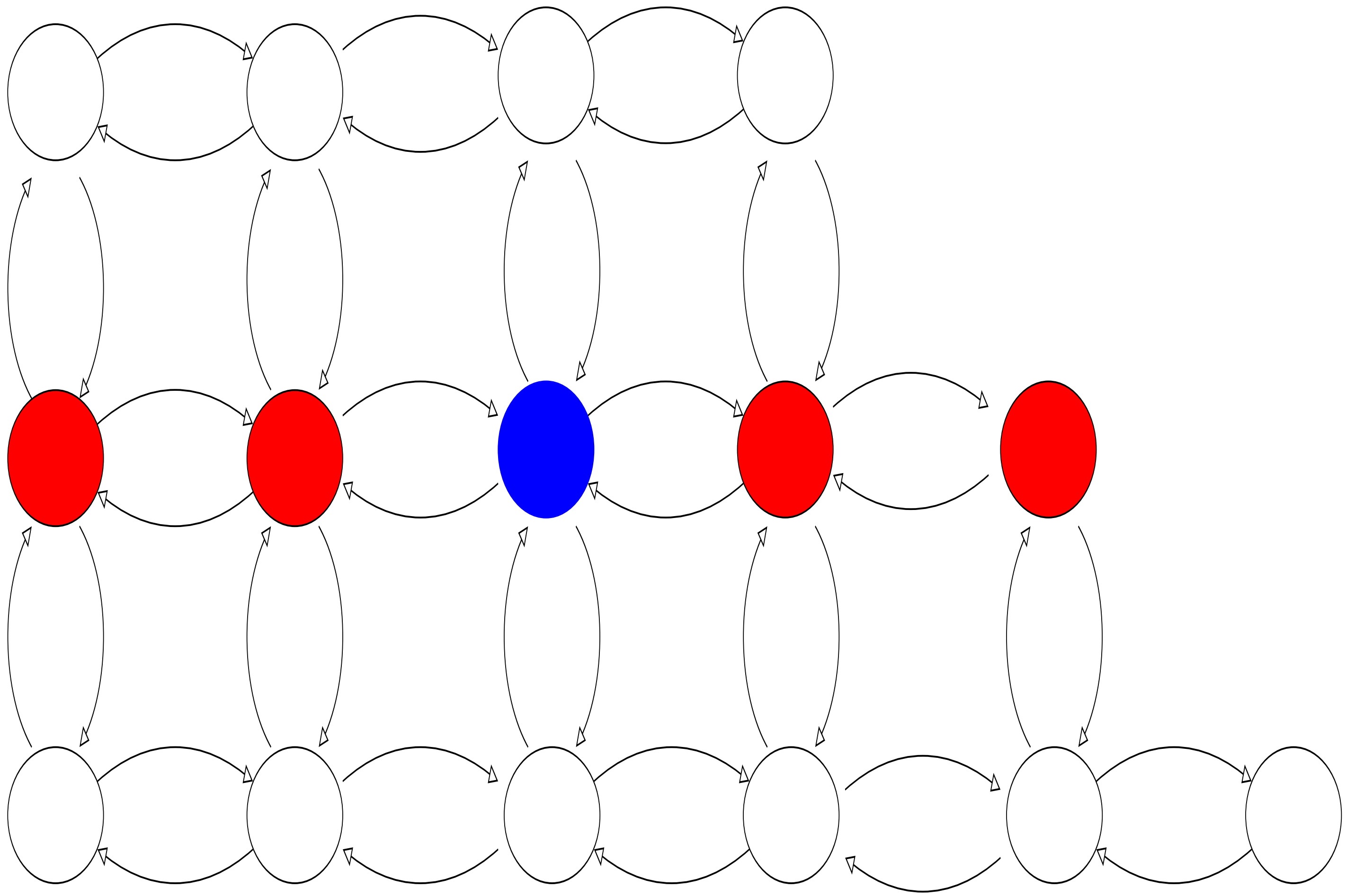


Final update

Gibss sampling

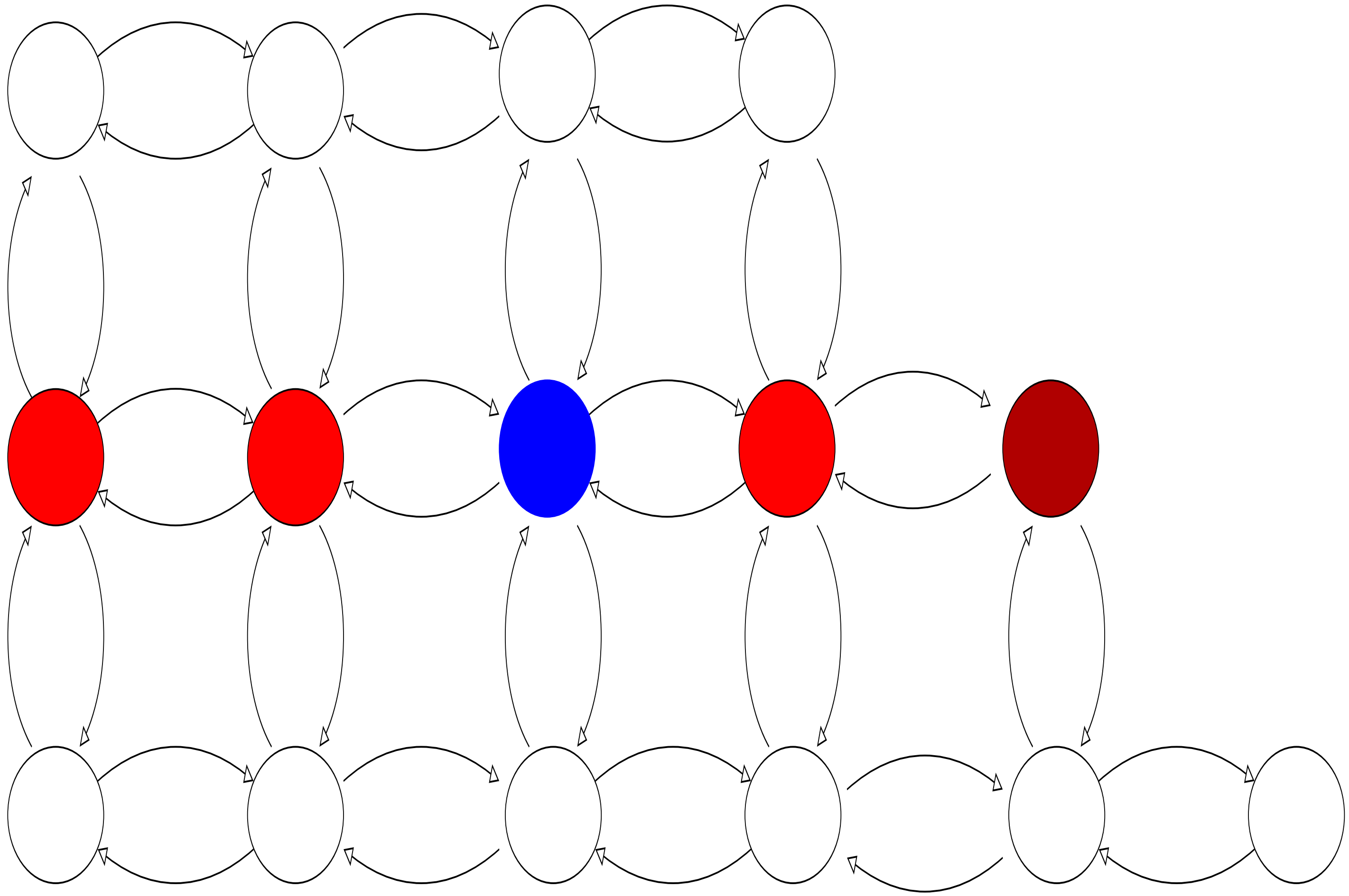
- Applies in multivariate cases where the conditional distribution among the coordinates are known.
- For a multidimensional distribution $\boldsymbol{x}$ the Gibss sampler will modify only one coordinate at a time.
- Typically d-steps in each iteration, where d is the dimension of the parameter space , that is of $\boldsymbol{x}$

Gibbs sampling - first dimension



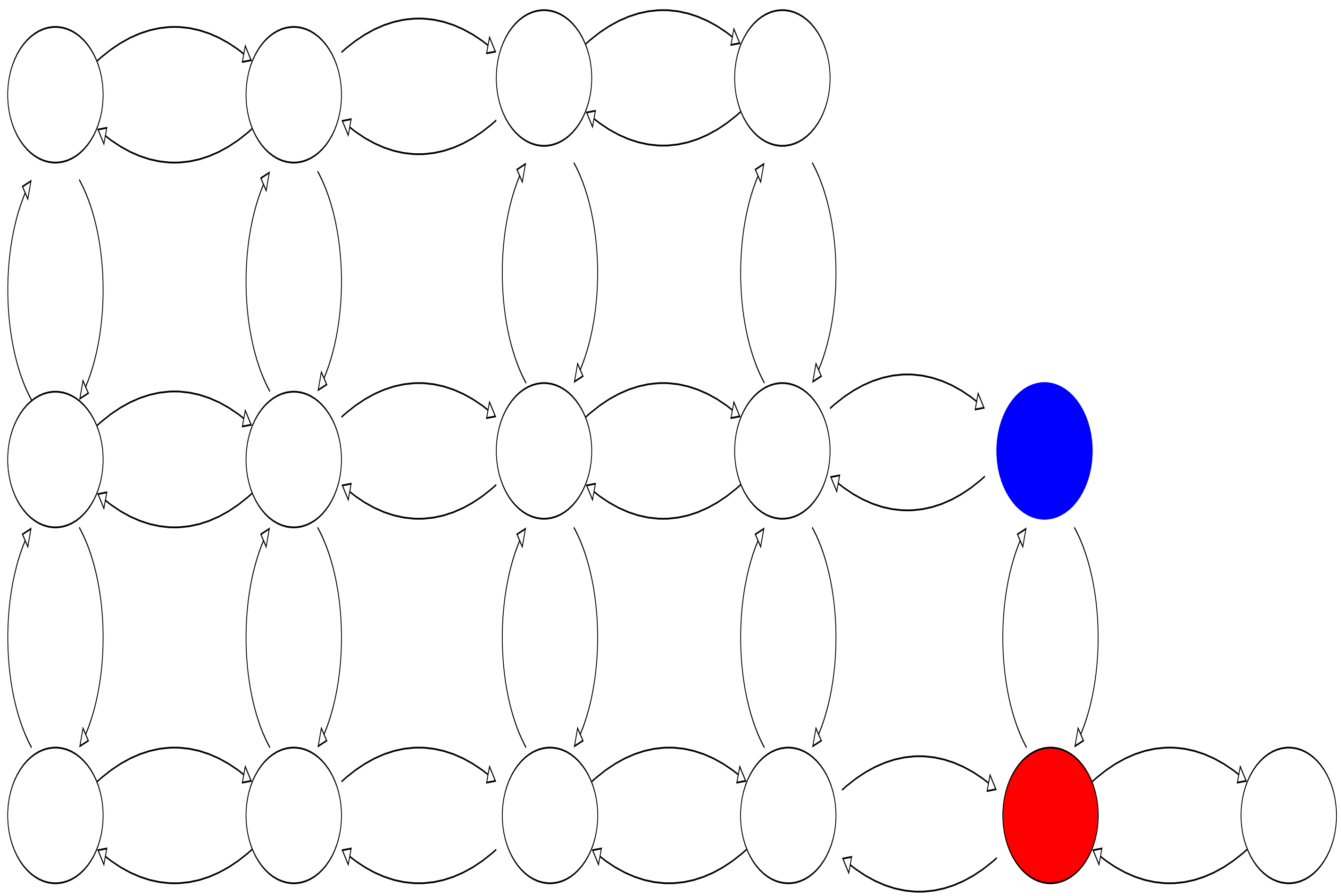
- Each dimension is updated at a time. According to the conditional distribution. Here the first dimension

Gibbs sampling - first dimension



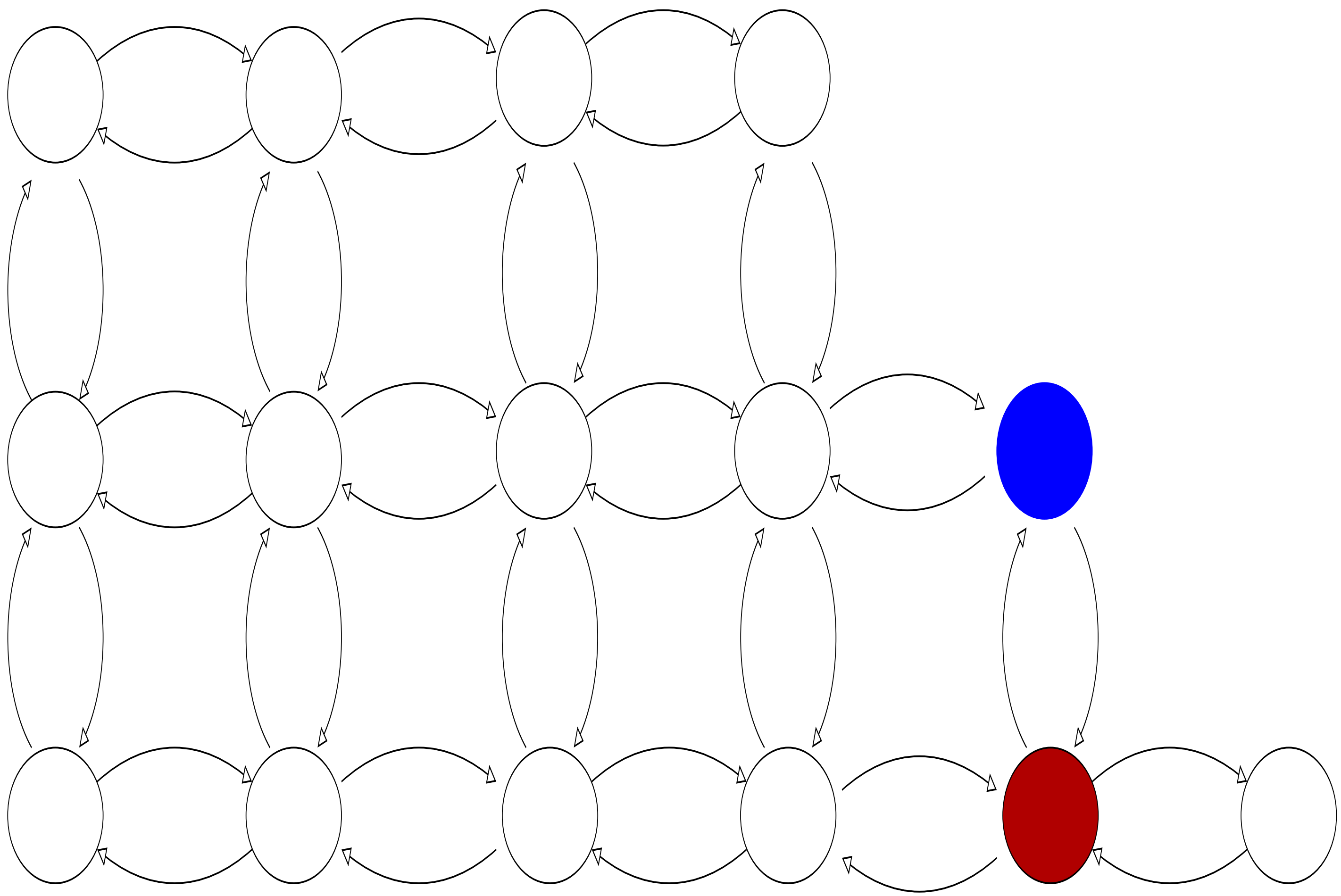
Draw from conditional distribution (no acceptance test).

Gibbs sampling - second dimension



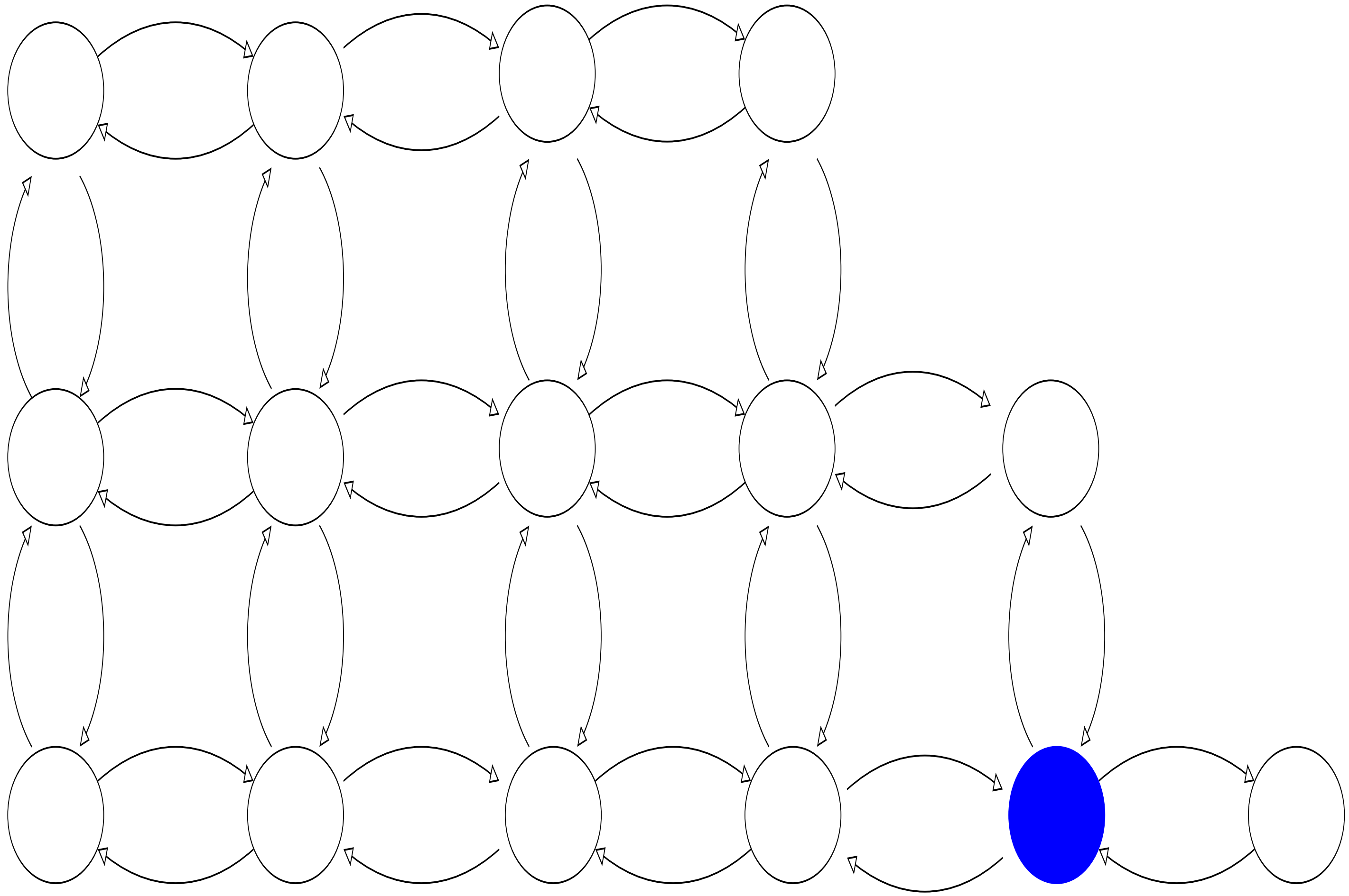
Possibilities in y-direction

Gibbs sampling - second dimension



Pick in y-direction (no acceptance test)

Gibbs sampling - second dimension



Final state after updates in both directions.

Different perspective modelling with Markov chains as oppposed to MCMC sampling

- For an ordinary Markov chain we know $\boldsymbol{P}$ and find $\boldsymbol{\pi}$ - analytically or by simulation
- When we apply MCMC
  - ◇ For a discrete distribution we have $\boldsymbol{\pi} = c\boldsymbol{\alpha}$ construct $\boldsymbol{P}$ which has no physical interpretation in general and obtain samples from $\boldsymbol{\pi}$ by simulation
  - ◇ For a continuous distribution we have the density $f(\boldsymbol{x}) = cg(\boldsymbol{x})$, construct a transition kernel $\boldsymbol{P}(\boldsymbol{x}, \boldsymbol{y})$ and get samples from $f(\boldsymbol{x})$ by simulation.

Remarks

- The method is computer intensive
- It is hard to verify the assumptions (Read: impossible)
- Warmup period strongly recommended (necessary indeed!)
- The samples are dependent (typically correlated)
- Should be run several times with different starting conditions
  - ◇ Comparing within run variance with between run variance
- Check the BUGS site: http://www.mrc-bsu.cam.ac.uk/bugs/and/or links given at the BUGS site

Further reading

- A. Gelman, J.B. Carlin, H.S. Stern, D.B. Rubin: Bayesian Data Analysis, Chapmann & Hall 1998, ISBN 0 412 03991 5
- W.R. Gilks, S. Richarson, D.J. Spiegelhalter: Markov chain Mone Carlo in practice, Chapmann & Hall 1996, ISBN 0 412 05551 1

Beyond Random Walk Metropolis-Hastings

- Proposed points Y_i can be generated with other schemes - this would change the acceptance probabilities.
- In mulitvariate situations, we can process one co-ordinate at a time
- If we know conditional distributions in the mulitvariate setting, then we can apply Gibbs sampling
- This is well suited for *graphical models* with many variables, which each interact only with a few others
- (Decision support systems is a big area of application)
- Many hybrids and specialized versions exist
- Very active research area, both theory and applications

Exercise 6: Markov Chain Monte Carlo

1. The number of busy lines in a trunk group (Erlang system) is given by a truncated Poisson distribution

$$P(i) = c \cdot \frac{A^i}{i!}, \quad i = 0, \ldots m$$

   Generate values from this distribution by applying the Metropolis-Hastings algorithm, verify with a χ^2-test. You can use the parameter values from exercise 4.

2. For two different call types the joint number of occupied lines is given by

$$P(i,j) = c \cdot \frac{A_1^i}{i!} \frac{A_2^j}{j!} \qquad 0 \leq i+j \leq m$$

   You can use $A_1, A_2 = 4$ and $m = 10$.

   (a) Use Metropolis-Hastings, directly to generate variates from this distribution.

(b) Use Metropolis-Hastings, coordinate wise to generate variates from this distribution.

(c) Use Gibbs sampling to sample from the distribution. This is (also) coordinate-wise but here we use the exact conditional distributions. You will need to find the conditional distributions analytically.

In all three cases test the distribution fit with a χ^2 test

The system can be extended to an arbitrary dimension, and we can add restrictions on the different call types.

3. We consider a Bayesian statistical problem. The observations are $X_i \sim \mathsf{N}(\Theta, \Psi)$, where the prior distribution of the pair $(\Xi, \Gamma) = (\log(\Theta), \log(\Psi))$ is standard normal with correlation

$\rho = \frac{1}{2}$. The joint density $f(x,y)$ of (Θ, Ψ) is

$$f(x,y) = \frac{1}{2\pi xy\sqrt{1-\rho^2}} e^{-\frac{\log(x)^2 - 2\rho\log(x)\log(y) + \log(y)^2}{2(1-\rho^2)}}$$

which can be derived using a standard change of variable technique. The task of this exercise is now to sample from the posterior distribution of (Θ, Ψ) using Markov Chain Monte Carlo.

(a) Generate a pair (θ, ψ) from the prior distribution, i.e. the distribution for the pair (Θ, Ψ), by first generating a sample (ξ, γ) of (Ξ, Γ).

(b) Generate $X_i = 1, \ldots, n$ with the values of (θ, ψ) you obtained in item 3a. Use $n = 10$.

(c) Derive the posterior distribution of (Θ, Ψ) given the sample. **Hint** Apply Bayes theorem in the density version.

Remark The sample mean and sample variance are independent. The sample mean follows a normal distribution, while a scaled version of the sample variance follows a χ^2 distribution. This can be used to simplify the expression. This will reduce the computation slightly at the price of using theoretical insight and some analysis.

(d) Generate MCMC samples from the posterior distribution of (Θ, Ψ) using the Metropolis Hastings method.

(e) Repeat item 3d with $n = 100$ and $n = 1000$, still using the values of (θ, ψ) from item 3a. Discuss the results.