Non-reversible Monte Carlo simulation of spin models

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Outline

Simple Mathematical Approach

Definitions

Let $\Omega = \{1, ..., n\}$ finite state space,

P transition matrix, $P(x \to y) = P(x, y)$ and

π invariant distribution such that $\pi P = \pi$.

Detailed Balance Equation

$\pi(x)P(x, y) = \pi(y)P(y, x)$ for all $x, y \in \Omega$.

Simple Mathematical Approach

Convergence Theorem

Let P be the transition matrix of an irreducible and aperiodic Markov chain on finite state space Ω. Then:

(1) There exists a unique invariant distribution π (See [3], p. 14)

(2) For all $x, y \in \Omega$ and $\delta > 0$:

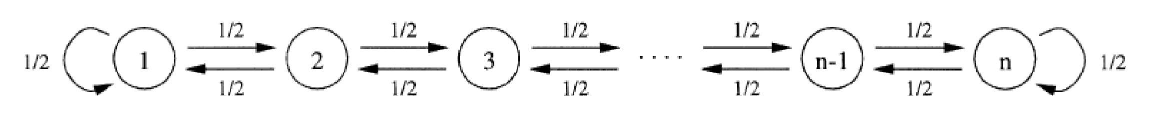
$$|P^t(x, y) - \pi(y)| \leq (1 - \delta)^t$$

(See extra material).

Simple Mathematical Approach

Simple Random Walk

Nearest neighbor random walk with transition probabilities $1/2$.

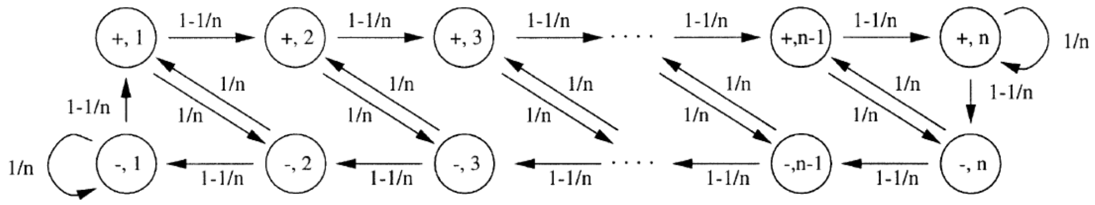


Invariant Distribution

$\pi(x) = 1/n$ for all $x \in \Omega$.

Directed Random Walk

Duplicate state space and introduce an extra label for direction.



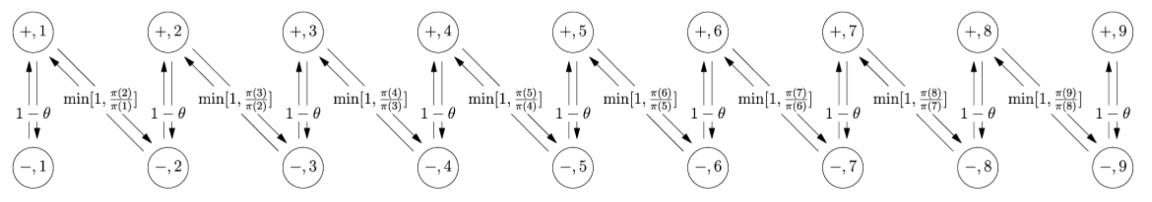
Invariant Distribution

$\pi(\pm, x) = 1/2n$ for all $x \in \Omega$, because P is double-stochastic.

$\pi(x) = 1/n$ for all $x \in \Omega$, marginal distribution (See [2], Chapter 2).

Non-reversible Algorithm

θ is the probability to change direction.



Step A Metropolis update $(\pm, x) \rightarrow (\mp, x \pm 1)$ with acceptance probability:

$$p_{acc} = \min\left[1\,,\ \frac{\pi(\mp, x \pm 1)}{\pi(\pm, x)}\right]\,,$$

Step B Flip label to keep direction $(\pm, x) \rightarrow (\mp, x)$ with fixed probability $1 - \theta$.

(See [1], Chapter 1)

Non-reversible Algorithm

Properties

- No need to consider normalization like in Metropolis algorithm.
- With θ we can control the probability to change direction.
- Convergences because the chain is irreducible and aperiodic.

Invariant Distribution

Both steps leave π invariant.
Step A follows the construction of a Metropolis algorithm.
Step B because $\pi(+, x) = \pi(-, x)$.

Easily derive (See [2], Chapter 5.1):

$\pi(\pm, x) = \pi(x)/2$ for all $x \in \Omega$.

Application Ising-Model

Mean Field Ising Model over Magnetization

State space: $\Omega = \{-1, 1\}^{N^d}$

Spin: $\sigma(v) = \{-1, 1\}$ for all $v \in \Omega$

Magnetization: $M = \sum_{v \in \Omega} \sigma(v)$

Energy Level: $\mathcal{H} = -\frac{J}{2N} \sum_{v,w} \sigma(v)\sigma(w) = -\frac{J}{2N} M^2$

Application Ising-Model

Invariant Distribution (Gibbs distribution)

$$\pi(M) = \frac{N!}{(\frac{N+M}{2})!(\frac{N-M}{2})!} \exp\left(\frac{\beta J M^2}{2N}\right),$$

with inverse temperatur β and exchange matrix J (here $J = 1$).

Acceptance Probability

$$p_{acc} = \min\left[1\,,\ \frac{N \mp M}{N \pm M + 2} \exp\left(\frac{2\beta J}{N}(\pm M + 1)\right)\right]$$

(See [1], Chapter 2)

Application Ising-Model

Nearest Neighbor Ising Model over Energy Level

Energy Level: $\mathcal{H} = -J \sum_{\langle v,w \rangle} \sigma(v)\sigma(w)\,,$ where $\langle v, w \rangle$ are direct neighbors.

Acceptance Probability

In 2-D case a single spin flip can lead to energy changes $\Delta\mathcal{H} = 0$, $\Delta\mathcal{H} = \pm 4$ and $\Delta\mathcal{H} = \pm 8$.

Use Fiber-Algorithm with acceptance probability (See [1], Chapter 3):

$$p_{acc} = \min\left[1\,,\ \frac{K_{\pm|\Delta\mathcal{H}|}}{K'_{\mp|\Delta\mathcal{H}|}} \exp^{-\beta\Delta\mathcal{H}}\right]$$

where K is the number of possible moves before and K' after spin flip.

Fiber-Algorithm

Step A Randomly select stepsize s from a given set.

Step B Metropolis update $(\pm, x) \to (\mp, x \pm s)$ with acceptance probability:

$$p_{acc} = \min\left[1, \frac{\pi(\mp, x \pm s)}{\pi(\pm, x)}\right]$$

Step C Flip label to keep direction $(\pm, x) \to (\mp, x)$ with fixed probability $1 - \theta$.

(See [2] Chapter 5.2 for general approach)

Implementation

Example (Non-reversible 1D-Ising-Model over M)

```
nonrevMFI1D(theta,plotRun,calcIndicators,samples)
>> nonrevMFI1D(0.001,1,0,10000)
```

Example (Non-reversible 2D-Ising-Model over M)

```
nonrevMFI2DM(theta,plotRun,calcIndicators,samples)
>> nonrevMFI2DM(0.001,1,0,10000)
```

Example (Non-reversible 2D-Ising-Model over E)

```
nonrevNNI2DE(theta,plotRun,calcIndicators,samples)
>> nonrevNNI2DE(0.001,1,0,10000)
```

References

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   Non-reversible Monte Carlo simulations of spin models

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Material for this presentation: **http://tinyurl.com/kzmthcq**