Course 11/1

Metropolis algorithm

- Detailed balance
- Metropolis algorithm
- Choice of trial step
- Choice of starting configuration

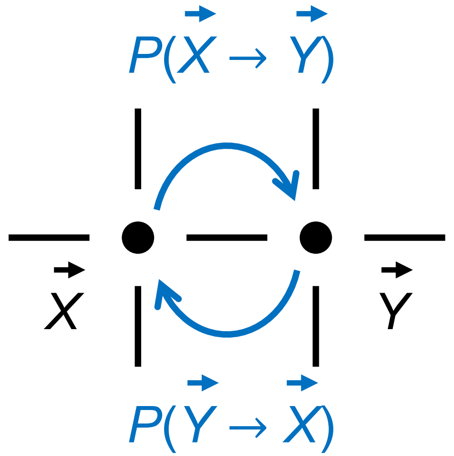
Detailed balance

The invariant distribution satisfies the following master equation:

$$N(\vec{X}, n+1) - N(\vec{X}, n) = -\sum_{\vec{Y}} P(\vec{X} \to \vec{Y})\, N(\vec{X}, n) + \sum_{\vec{Y}} P(\vec{Y} \to \vec{X})\, N(\vec{Y}, n)$$

Where $N(\vec{X}, n)$ is the number of walkers in configuration $\vec{X}$ at step n of the Markovian chain.

A particular solution of this equation can be found by imposing the condition of detailed balance:

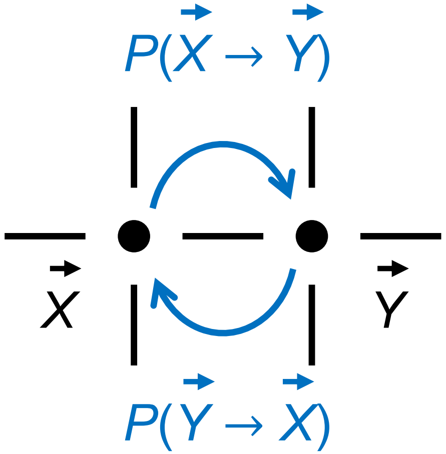


No net flux of walkers across one “connection”

$$N(\vec{X}\to\vec{Y}, n) = N(\vec{X},n)\, P(\vec{X}\to\vec{Y})$$

$$N(\vec{Y}\to\vec{X}, n) = N(\vec{Y},n)\, P(\vec{Y}\to\vec{X})$$

Detailed balance



$$N(\vec{X}\rightarrow\vec{Y},\, n) \;=\; N(\vec{X},n)\; P(\vec{X}\rightarrow\vec{Y})$$

$$N(\vec{Y}\rightarrow\vec{X},\, n) \;=\; N(\vec{Y},n)\; P(\vec{Y}\rightarrow\vec{X})$$

Net flux from $\vec{Y}$ to $\vec{X}$:

$$\Delta N(\vec{Y}\rightarrow\vec{X},\, n) \;=\; N(\vec{Y}\rightarrow\vec{X},\, n) \;-\; N(\vec{X}\rightarrow\vec{Y},\, n)$$

$$= \; N(\vec{Y},n)\; P(\vec{X}\rightarrow\vec{Y}) \left[\frac{P(\vec{Y}\rightarrow\vec{X})}{P(\vec{X}\rightarrow\vec{Y})} - \frac{N(\vec{X},n)}{N(\vec{Y},n)} \right]$$

At equilibrium $\Delta N = 0$

$$\frac{N(\vec{X},\, \mathrm{eq})}{N(\vec{Y},\, \mathrm{eq})} \;=\; \frac{P(\vec{Y}\rightarrow\vec{X})}{P(\vec{X}\rightarrow\vec{Y})}$$

Restoration of equilibrium

Net flux from $\vec{Y}$ to $\vec{X}$:

$$\Delta N(\vec{Y}\to\vec{X}, n) = N(\vec{Y}\to\vec{X}, n) - N(\vec{X}\to\vec{Y}, n)$$

$$= N(\vec{Y},n)\, P(\vec{X}\to\vec{Y}) \left[\frac{P(\vec{Y}\to\vec{X})}{P(\vec{X}\to\vec{Y})} - \frac{N(\vec{X},n)}{N(\vec{Y},n)} \right]$$

At equilibrium $\Delta N = 0$

$$\frac{N(\vec{X},\mathrm{eq})}{N(\vec{Y},\mathrm{eq})} = \frac{P(\vec{Y}\to\vec{X})}{P(\vec{X}\to\vec{Y})}$$

Suppose there are too many walkers in $\vec{X}$ at step n :

$$N(\vec{X},n) > N(\vec{X},\mathrm{eq}) \quad \Rightarrow \quad \Delta N(\vec{Y}\to\vec{X}, n) < 0$$

$$\Rightarrow \quad N(\vec{X}\to\vec{Y}, n) > N(\vec{Y}\to\vec{X}, n)$$

….then there is a net flux of walkers towards $\vec{Y}$

Transition probabilities & weight function: Relation

At equilibrium

$$\frac{N(\vec{X}, \mathrm{eq})}{N(\vec{Y}, \mathrm{eq})} = \frac{P(\vec{Y} \rightarrow \vec{X})}{P(\vec{X} \rightarrow \vec{Y})}$$

Our goal

$$N(\vec{X}, \mathrm{eq}) \propto \omega(\vec{X})$$

Condition to be set for the transition probabilities

$$\boxed{\frac{P(\vec{Y} \rightarrow \vec{X})}{P(\vec{X} \rightarrow \vec{Y})} = \frac{\omega(\vec{X})}{\omega(\vec{Y})}}$$

Metropolis algorithm

Metropolis, Rosenbluth, Rosenbluth, Teller, and Teller, *J. Chem. Phys*. **21**, 1087 (1953)

Two-step procedure

1. Trial step For a walker at $\vec{X}_n$, a trial step towards $\vec{X}_t$ is proposed.

The weight function $\omega(\vec{X}_t)$ is evaluated and compared to $\omega(\vec{X}_n)$:

$$r = \frac{\omega(\vec{X}_t)}{\omega(\vec{X}_n)}$$

Note that this only requires the ratio of the weight functions and not the normalization over the full configuration space!

Metropolis algorithm

$$r = \frac{\omega(\vec{X}_t)}{\omega(\vec{X}_n)}$$

2. Decision step

1

$r \geq 1$ The trial configuration is more probable than the current one.

Accepted $\vec{X}_{n+1} = \vec{X}_t$

$r < 1$ The trial configuration is less probable than the current one.

The step is accepted with probability r .

A random number $\eta \in (0,1)$ is extracted.

2

$\eta \leq r$ Accepted $\vec{X}_{n+1} = \vec{X}_t$

$\eta > r$ Rejected $\vec{X}_{n+1} = \vec{X}_n$

Does this lead to the correct invariant distribution?

In the Metropolis algorithm, the transition probability $P(\vec{X} \to \vec{Y})$ is defined in two steps:

$$P(\vec{X} \to \vec{Y}) = T(\vec{X} \to \vec{Y})\ A(\vec{X} \to \vec{Y})$$

where $T(\vec{X} \to \vec{Y})$ is the probability of selecting the $\vec{X} \to \vec{Y}$ transition and $A(\vec{X} \to \vec{Y})$ is the probability of accepting the $\vec{X} \to \vec{Y}$ transition.

At equilibrium

$$\frac{N(\vec{X}, \mathrm{eq})}{N(\vec{Y}, \mathrm{eq})} = \frac{P(\vec{Y} \to \vec{X})}{P(\vec{X} \to \vec{Y})} = \frac{T(\vec{Y} \to \vec{X})\, A(\vec{Y} \to \vec{X})}{T(\vec{X} \to \vec{Y})\, A(\vec{X} \to \vec{Y})} \overset{?}{=} \frac{\omega(\vec{X})}{\omega(\vec{Y})}$$

Does this lead to the correct invariant distribution?

$$\frac{T(\vec{Y} \rightarrow \vec{X})\, A(\vec{Y} \rightarrow \vec{X})}{T(\vec{X} \rightarrow \vec{Y})\, A(\vec{X} \rightarrow \vec{Y})} \stackrel{?}{=} \frac{\omega(\vec{X})}{\omega(\vec{Y})} \quad \Rightarrow \quad \frac{A(\vec{Y} \rightarrow \vec{X})}{A(\vec{X} \rightarrow \vec{Y})} \stackrel{?}{=} \frac{\omega(\vec{X})}{\omega(\vec{Y})}$$

For simplicity, we assume $T(\vec{X}\rightarrow\vec{Y}) = T(\vec{Y}\rightarrow\vec{X})$, i.e. the probability of selecting the forward transition is the same as that of selecting the backward one.

Let us check for the Metropolis algorithm:

	$\vec{Y}\rightarrow\vec{X}$	$\vec{X}\rightarrow\vec{Y}$
$\frac{\omega(\vec{X})}{\omega(\vec{Y})} > 1$	$A(\vec{Y}\rightarrow\vec{X}) = 1$	$A(\vec{X}\rightarrow\vec{Y}) = \frac{\omega(\vec{Y})}{\omega(\vec{X})}$
$\frac{\omega(\vec{X})}{\omega(\vec{Y})} < 1$	$A(\vec{Y}\rightarrow\vec{X}) = \frac{\omega(\vec{X})}{\omega(\vec{Y})}$	$A(\vec{X}\rightarrow\vec{Y}) = 1$

The Metropolis algorithm yields the correct weight function!

Barker's algorithm

$$\frac{A(\vec{Y} \rightarrow \vec{X})}{A(\vec{X} \rightarrow \vec{Y})} \stackrel{?}{=} \frac{\omega(\vec{X})}{\omega(\vec{Y})}$$

	$\vec{Y}\rightarrow\vec{X}$	$\vec{X}\rightarrow\vec{Y}$
Barker	$A(\vec{Y}\rightarrow\vec{X}) = \dfrac{\omega(\vec{X})}{\omega(\vec{X})+\omega(\vec{Y})}$	$A(\vec{X}\rightarrow\vec{Y}) = \dfrac{\omega(\vec{Y})}{\omega(\vec{X})+\omega(\vec{Y})}$

Barker's algorithm also yields the correct weight function!

The Metropolis algorithm has proven to be very effective in many cases!

Choice of trial step

- Too hazardous steps lead to a high rejection rate, thus the sampling becomes inefficient.

- Too safe steps lead to slow sampling (long and inefficient).

Practical recommended rule

$$\boxed{\#\ \text{rejected moves} \;\cong\; \#\ \text{accepted moves}}$$

Choice of starting configuration

- It is better to choose a probable configuration as initial configuration.
- The result is independent of the starting point, but we have to wait that the system reaches equilibrium.

Integral

$$I = \int A(\vec{X})\, \omega(\vec{X})\, d\vec{X}$$

Metropolis estimate

$$I \cong \frac{1}{N - N_0} \sum_{i > N_0}^{N} A(\vec{X}_i)$$

N_0 configurations are left out of the average on the way to equilibrium

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