Advanced topics in Markov-chain Monte Carlo

Lecture 3:
Mixing and autocorrelations in hard spheres
Part 2/2: Reversible and non-reversible hard-sphere Markov chains

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02 February 2022

References

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- T. Chou, K. Mallick, R. K. P. Zia **Non-equilibrium statistical mechanics: from a paradigmatic model to biological transport** Reports on Progress in Physics 74, 116601 (2011)
- Lacoin, H. **The cutoff profile for the simple exclusion process on the circle** The Annals of Probability 44, 3399–3430 (2016)
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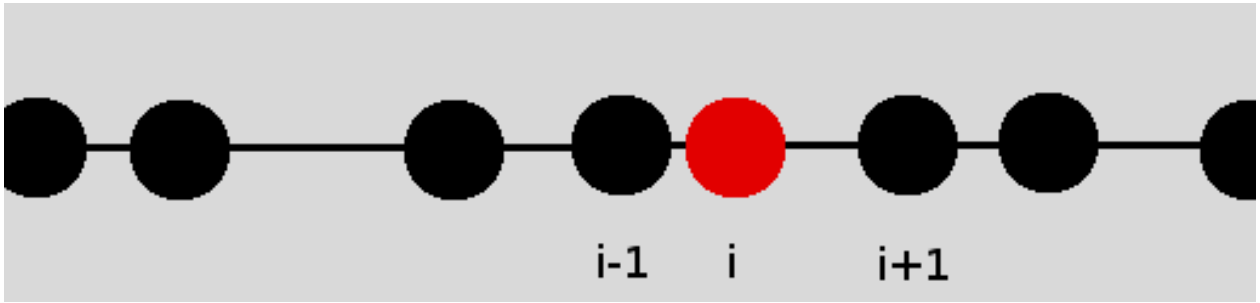
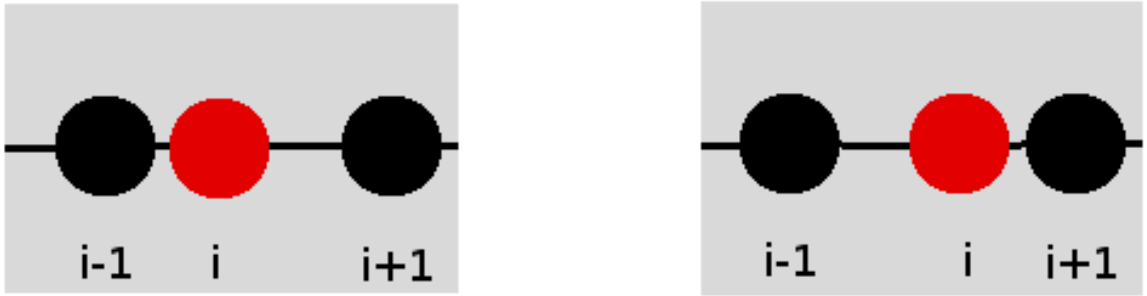
Local Metropolis algorithm 1/5



- Spheres on a $1d$ interval (with or without pbc).
- $\pi(x_1, \ldots, x_N)$ non-trivial (see Krauth (2006)).
- Local Metropolis: $x_i \to x_i \pm \epsilon$ (with pbc).
- $\Omega^{\text{Met}} = \{x_1 < x_2 < \cdots < x_N\}$, $\mathbf{x} = \{x_1, \ldots, x_N\}$.
- $\mathcal{D} = \mathbb{R} \times \{1, \ldots, N\}$ (or some symmetric interval)
- Local Metropolis: Sample element of $\mathcal{D}$, apply to $\mathbf{x}_t$

Local Metropolis algorithm 2/5

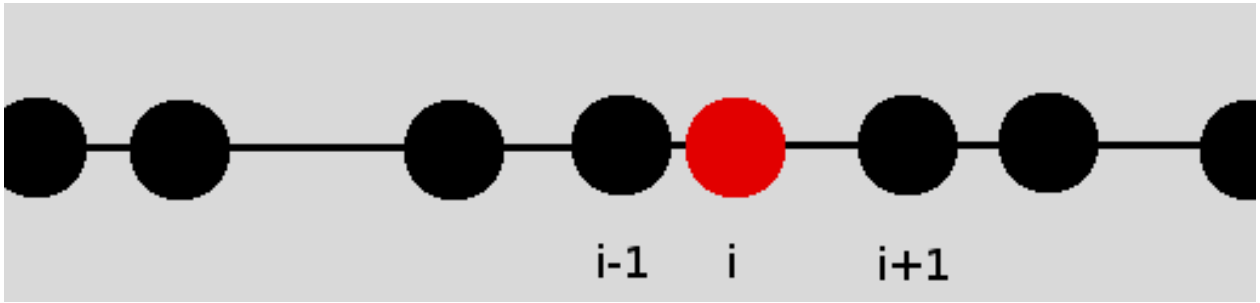


- $\Omega^{\text{Met}} = \{x_1 < x_2 < \cdots < x_N\}$, $\mathbf{x} = \{x_1, \ldots, x_N\}$.
- $\mathcal{D}^{\text{Met}} = \mathbb{R} \times \{1, \ldots, N\}$ (or some symmetric interval)
- Local Metropolis: Sample element of $\mathcal{D}$, apply to $\mathbf{x}_t$
- Detailed balance:

$$\pi_a p(a \to b) = \pi_b p(b \to a)$$

- Probability distribution on $\mathbb{R}$ symmetric
- Almost no condition on sampling of $\mathcal{N} = \{1, \ldots, N\}$.

Local Metropolis algorithm 3/5

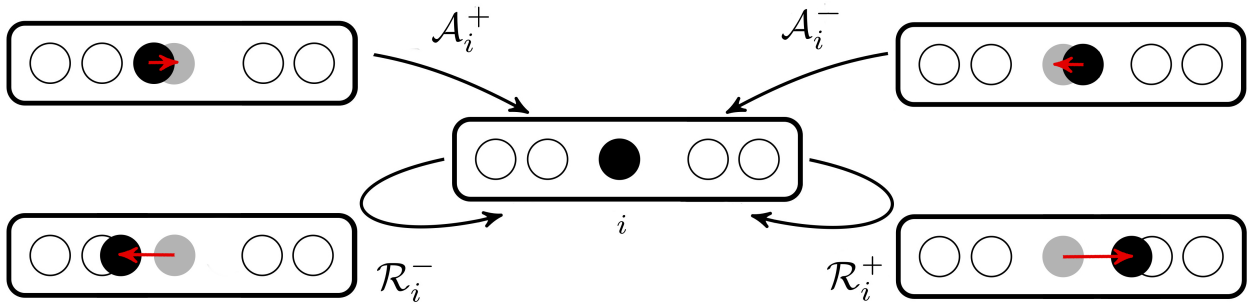


- Reversible Metropolis: $x_i \to x_i \pm \epsilon$ (reject if overlap)
- Global balance:

$$\mathcal{F}_a^{\text{Met}} = \frac{1}{2N} \sum_i \int_0^\infty \mathrm{d}\epsilon \underbrace{\left(\mathcal{A}_i^+ + \mathcal{R}_i^+ + \mathcal{A}_i^- + \mathcal{R}_i^-\right)}_{=2 \text{ for any } \epsilon} = 1.$$

- NB: $\mathcal{A}_i^+(\epsilon) + \mathcal{R}_i^-(\epsilon) = 1$ also $\mathcal{A}_i^-(\epsilon) + \mathcal{R}_i^+(\epsilon) = 1$.

Local Metropolis algorithm 4/5

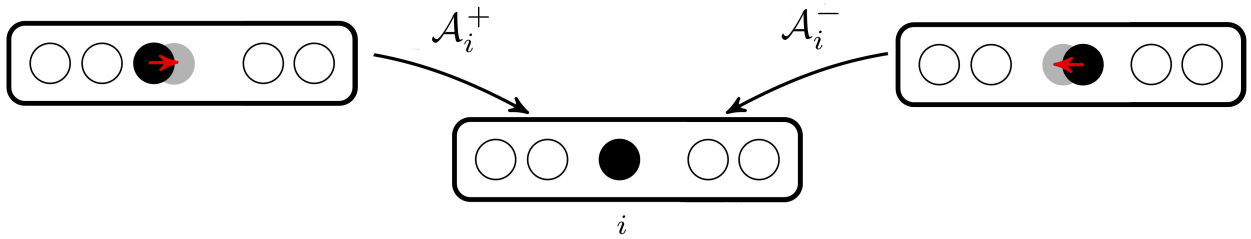


- Reversible Metropolis: $x_i \to x_i \pm \epsilon$ (reject if overlap)
- Global balance:

$$\mathcal{F}_a^{\text{rev}} = \frac{1}{2N} \sum_i \int_0^\infty \mathrm{d}\epsilon \underbrace{\left(\mathcal{A}_i^+ + \mathcal{R}_i^+ + \mathcal{A}_i^- + \mathcal{R}_i^-\right)}_{=2 \text{ for any } \epsilon} = 1.$$

- NB: $\mathcal{A}_i^+(\epsilon) + \mathcal{R}_i^-(\epsilon) = 1$; $\mathcal{A}_i^-(\epsilon) + \mathcal{R}_i^+(\epsilon) = 1$.
- Good exercise.

Local Metropolis algorithm 5/5



Variant:

- Heat bath: $x_i \to \mathrm{ran}(x_{i-1} + 2\sigma, x_{i+1} - 2\sigma)$
- Mixing time $\mathcal{O}\left(N^3 \log N\right)$ with fixed boundary conditions (Randall, Winkler 2005).
- Mixing time $\mathcal{O}\left(N^3\right) \ldots \mathcal{O}\left(N^3 \log N\right)$ with periodic boundary conditions
  (Randall, Winkler 2005).
- Numerically: $\mathcal{O}\left(N^3 \log N\right)$ for Metropolis and heat bath.

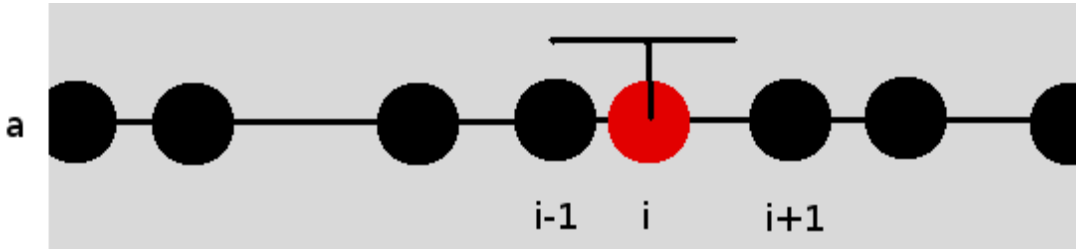
Symmetric simple exclusion process 1/2

- $\Omega^{\text{Met}} = \{x_1 < x_2 < \cdots < x_N\}$, $\mathbf{x} = \{x_1, \ldots, x_N\}$.
- $\mathcal{D}^{\text{Met}} = \mathbb{R} \times \{1, \ldots, N\}$ (or some symmetric interval)
- $\Omega^{\text{SSEP}} = \{x_1 < x_2 < \cdots < x_N\}$, $\mathbf{x} = \{x_1, \ldots, x_N\} \in \mathbb{N}^N$.
- $\mathcal{D}^{\text{SSEP}} = \{-, +\} \times \{1, \ldots, N\}$

Symmetric simple exclusion process 2/2

- Mixing time of SSEP $\mathcal{O}\left(N^3 \log N\right)$ (Lacoin)
- Many studies

Sequential Metropolis algorithm

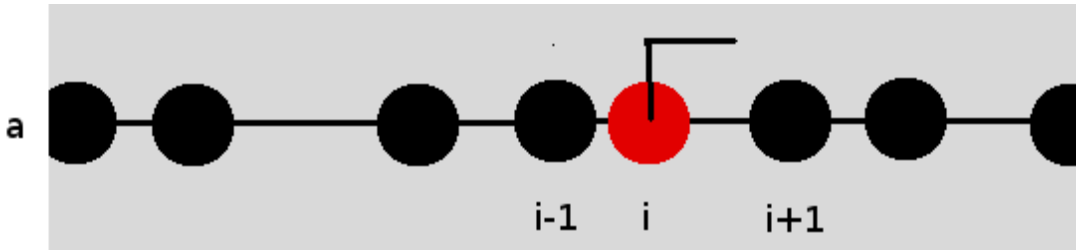


- $\Omega^{\text{Met}} = \{x_1 < x_2 < \cdots < x_N\}$, $\mathbf{x} = \{x_1, \ldots, x_N\}$.
- $\mathcal{D}^{\text{Met}} = \mathbb{R} \times \{1, \ldots, N\}$
- $\hat{\Omega}^{\text{Seq}} = \Omega^{\text{Met}} \times \mathcal{N}$ (particle lifting).
- Sequential Metropolis: Update 0, then 1, then 2, ...
- Global balance:

$$\mathcal{F}_a^{\text{seq}} = \frac{1}{2} \int_0^\infty \mathrm{d}\epsilon \left(\mathcal{A}_i^+ + \mathcal{R}_i^+ + \mathcal{A}_i^- + \mathcal{R}_i^- \right) = 1.$$

- Many sequences of indices are OK.
- Thm: Any sequential version of a reversible Markov chain satisfies global balance (conditions apply).

Forward Metropolis algorithm 1/2

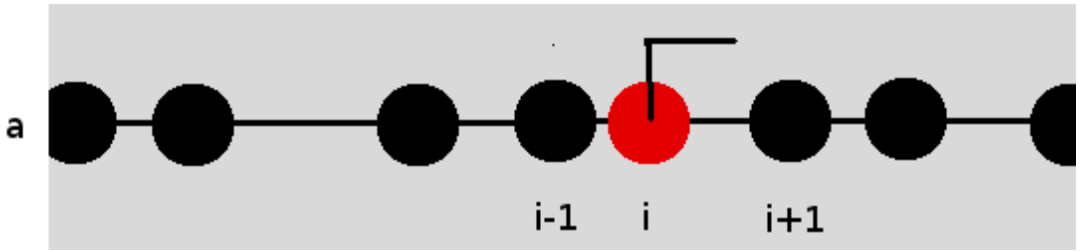


- $\Omega^{\text{Met}} = \{x_1 < x_2 < \cdots < x_N\}$, $\mathbf{x} = \{x_1, \ldots, x_N\}$.
- $\mathcal{D}^{\text{Met}} = \mathbb{R} \times \mathcal{N} = \mathbb{R}^+ \times \{+,-\} \times \mathcal{N}$
- $\hat{\Omega}^{\text{Forw}} = \Omega^{\text{Met}} \times \{+,-\}$ (displacement lifting).
- $\mathcal{D}^{\text{Forw}} = \mathbb{R}^+ \times \mathcal{N}$
- Forward Metropolis: $x_i \to x_i + \epsilon$ (NB: random i)
- Sample-space halving...
-

$$\mathcal{F}_a^{\text{forw}} = \frac{1}{N} \sum_i \underbrace{\left(\mathcal{A}_i^+ + \mathcal{R}_{i-1}^+\right)}_{=1 \text{ for any } \epsilon} = 1,$$

- Lattice version: Totally asymmetric simple exclusion process (TASEP).
- NB: Forward sequential Metropolis is wrong (see TD).

Forward Metropolis algorithm 1/2



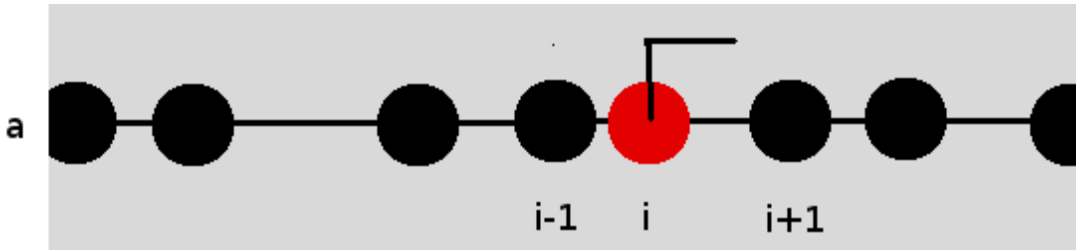
- $\Omega^{\text{Met}} = \{x_1 < x_2 < \cdots < x_N\}$, $\mathbf{x} = \{x_1, \ldots, x_N\}$.
- $\mathcal{D}^{\text{Met}} = \mathbb{R} \times \mathcal{N} = \mathbb{R}^+ \times \{+, -\} \times \mathcal{N}$
- $\hat{\Omega}^{\text{Forw}} = \Omega \times \{+, -\}$ (displacement lifting).
- Forward Metropolis: $x_i \to x_i + \epsilon$ (NB: random i)
- Sample-space halving...
- $$\mathcal{F}_a^{\text{forw}} = \frac{1}{N} \sum_i \underbrace{\left(\mathcal{A}_i^+ + \mathcal{R}_{i-1}^+\right)}_{=1 \text{ for any } \epsilon} = 1,$$
- NB: Forward sequential Metropolis is wrong (see TD).

Forward Metropolis algorithm 2/2

Totally asymmetric simple exclusion process

- $\Omega^{\text{SSEP}} = \{x_1 < x_2 < \cdots < x_N\} \in \mathbb{N}^N$
- $\mathcal{D}^{\text{SSEP}} = \{+, -\} \times \mathcal{N}$
- $\hat{\Omega}^{\text{TASEP}} = \Omega^{\text{SSEP}} \times \{+, (-)\}$ (displacement lifting).
- $\mathcal{D}^{\text{TASEP}} = \mathcal{N}$
- Sample-space halving...
- TASEP mixing times are known analytically.

Lifted Forward Metropolis algorithm



- $\Omega^{\text{Met}} = \{x_1 < x_2 < \cdots < x_N\}$, $\mathbf{x} = \{x_1, \ldots, x_N\}$.
- $\mathcal{D}^{\text{Met}} = \mathbb{R} \times \mathcal{N} = \mathbb{R}^+ \times \{+, -\} \times \mathcal{N}$
- $\hat{\Omega}^{\text{Lift-Forw}} = \Omega \times \{+, -\} \times \mathcal{N}$ (displacement + particle lifting).
- $\mathcal{D}^{\text{Lift-Forw}} = \mathbb{R}^+$
- Move i forward if accepted
- Otherwise: lifting move $i \to i + 1$
- Sample-space halving again.
- $$\mathcal{F}^{\text{lift}}_{(a,i)} = \mathcal{A}^+_i + \mathcal{R}^+_{i-1} = 1.$$
- Analogous to the lifted Metropolis algorithm on the path graph.

Mixing time (operational) 1/2

- Half-system distance (with $\delta_i = x_i - x_{i-1} - d$ with d diameter, L system size, $L_{\text{free}} = L - Nd$):

$$u = \underbrace{\delta_{i+N/2} + \ldots + \delta_{i+1}}_{N/2 \text{ terms}}.$$

- Equilibrium distribution of half-system distance:

$$\pi(u) = \frac{\Gamma(N-1)}{L_{\text{free}}^{N-1}} \frac{(L_{\text{free}} u - u^2)^{N/2-1}}{(N/2-1)!^2}.$$

- Variance of half-system distance:

$$\operatorname{Var} u = \frac{N^2 \ell_{\text{free}}^2}{4(N+1)}.$$

- Compact initial condition:

$$\operatorname{Var}_{\text{compact}}(u) = \langle u^2 \rangle_{\text{compact}} - \langle u \rangle_{\text{compact}}^2 = \frac{N^2 \ell_{\text{free}}^2}{4}.$$

Mixing time (operational) 2/2