Advanced topics in Markov-chain Monte Carlo

Lecture 5:
Exact sampling approaches in Markov-chain Monte Carlo
Part 2/2: Coupling from the past / hard spheres

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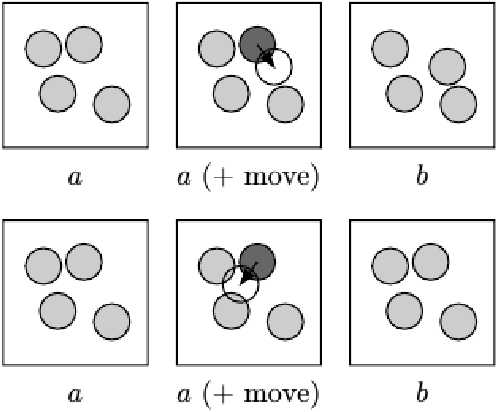
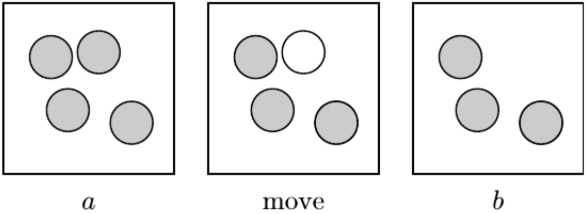
Hard-sphere simulation (traditional)



Hard-sphere simulation (birth-and-death)



$$Z = \sum_{N=0}^{\infty} \lambda^N \int \cdots \int \mathrm{d}x_1 \ldots \mathrm{d}x_N \pi(x_1, \ldots, x_N)$$

- $\pi(a) = \lambda \pi(b)$
- Death probability (per particle, per time interval): $1\mathrm{d}t$
- Birth probability (per unit square): $\lambda \mathrm{d}t$

Poisson distribution

Poisson distribution (number n of events per unit time):

$$\pi_{\Delta t=1}(n) = \frac{\lambda^n \mathrm{e}^{-\lambda}}{n!}$$

Poisson distribution (number n of events per time $\mathrm{d}t$):

$$\pi_{\mathrm{d}t}(n) = \frac{(\lambda \mathrm{d}t)^n \mathrm{e}^{-\lambda \mathrm{d}t}}{n!} \implies \pi_{\mathrm{d}t}(1) = \lambda \mathrm{d}t, \pi_{\mathrm{d}t}(2) = 0$$

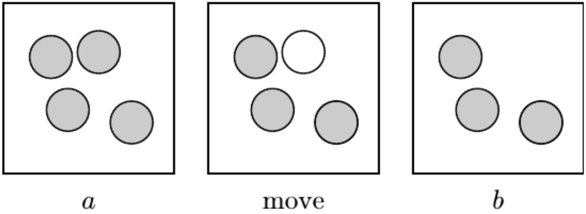
Poisson waiting time: Probability that next event after time t:

$$\mathbb{P}(t) = (1 - \lambda \mathrm{d}t), \ldots, (1 - \lambda \mathrm{d}t)\lambda \mathrm{d}t$$

$$\mathbb{P}(t) = \underbrace{\overbrace{(1 - \lambda \mathrm{d}t) \to (1 - \lambda \mathrm{d}t)}^{\sum \mathrm{d}t = t}}_{\mathrm{e}^{-\lambda t}} \lambda \mathrm{d}t$$

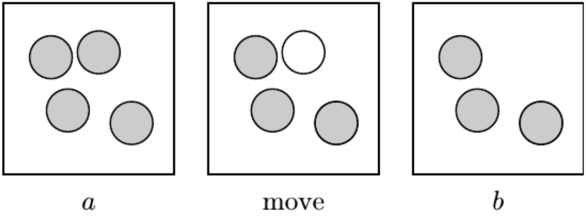
...can be sampled with $t = (-\log \mathrm{ran}[0, 1])/\lambda$

Birth-and-death (principle 1)



- N spheres, each of them may die.
- a new sphere may be born (but there may be problems).
- rate for next event: $N + \lambda$.
- $\mathbb{P}(\text{death}) \propto N$ and $\mathbb{P}(\text{birth}) \propto \lambda$, reject if overlap.

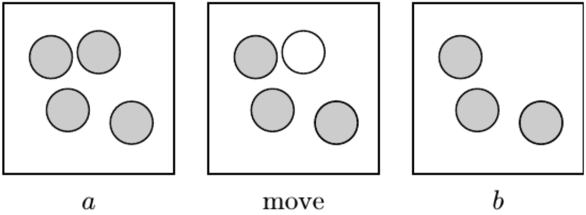
Birth-and-death (implementation 1)



- start with $N = 0$ spheres
- Go to next-event time : $-\log \texttt{ran} / (N + \lambda)$ (in steps of 1)
- sample random number $\texttt{ran}[0, 1]$: if smaller than $\lambda / (\lambda + N)$: add a disk (reject if overlap), otherwise delete a disk.

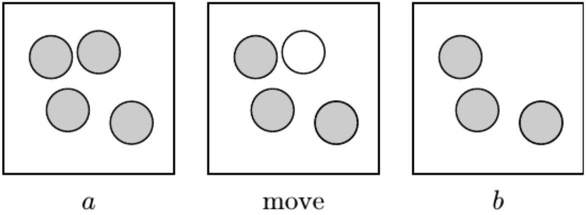
NB: Check configuration at integer time steps, for sampling.

Birth-and-death (principle 2)



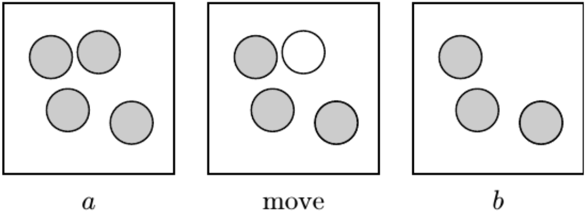
- N spheres, each of them knows when it will die (sad) rate=1.
- a new sphere may be born (but there may be problems) rate $= \lambda$.

Birth-and-death (implementation 2)



- start with $N = 0$ spheres.
- Advance to next birth time : $-\log \text{ran}[0, 1]/\lambda$ (in steps of 1).
- If no rejection, install death time $-\log \text{ran}[0, 1]$

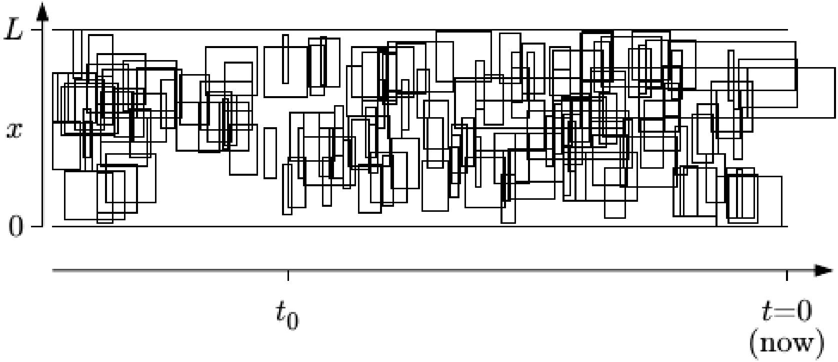
Birth-and-death (principle 3)



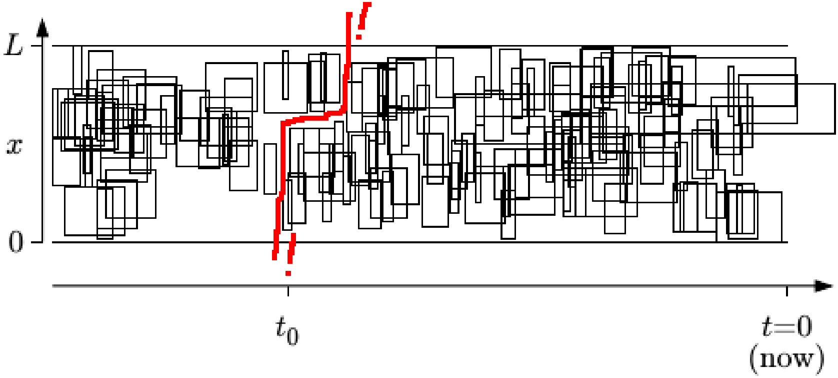
- Hyptothetical spheres are born with rate $= \lambda$, and they die with rate 1.

Check later whether all this pans out correctly.

Birth-and-death (implementation 3)

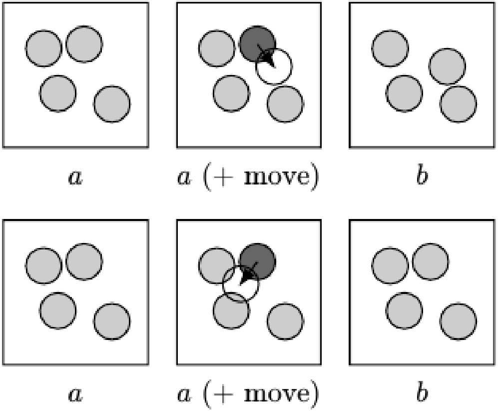


Birth-and-death (implementation 3)



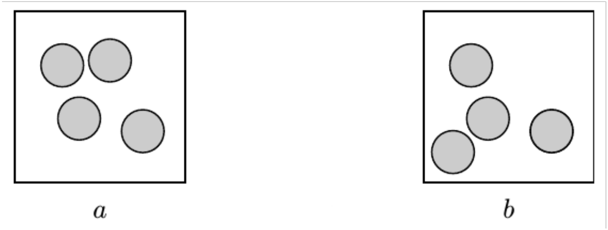
- Can be made into a perfect sampling algorithm

Hard-sphere simulation (traditional)



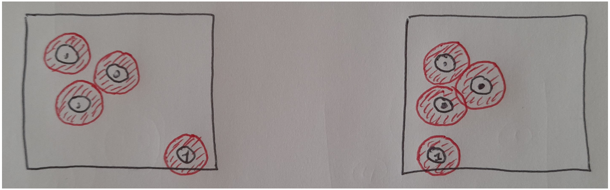
Algorithm remains correct if displacement random in box.

Path coupling 1/2



- At low density, any two configurations of spheres a and z can be connected through a path of length $< 2N$ as follows: $a \to b \to c \to ..... \to z$, where any two neighbors differ only in 1 sphere.
- MC algorithm: Take random sphere, place it at random position anywhere in the box.

Path coupling 2/2



- MC algorithm: Take random sphere, place it at the same random position for both copies.
- $p(1 \to 0)$: Pick 1, move to where it fits in both copies

$$p(1 \to 0) \geq \frac{1}{N}\left[1 - \frac{N-1}{N} 4\eta\right]$$

- $p(1 \to 2)$: Pick $2 \ldots N$ move near to 1_A or 1_B.

$$p(1 \to 2) \leq \frac{N-1}{N}\left[\frac{8}{N}\eta\right]$$

- $\implies$ for $\eta < 1/12$: further coupling likely.