

Markov-chain Monte Carlo: A modern primer

Lecture 3: Advances Part 3.2: Consensus sampling

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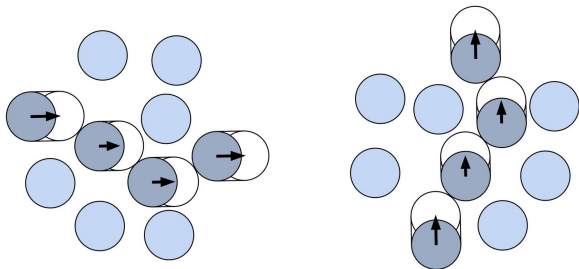
E. P. Bernard, W. Krauth, D. B. Wilson, PRE (2009)

M. Michel, S. C. Kapfer, W. Krauth, JCP (2014)

S. C. Kapfer, W. Krauth, PRL (2015, 2017)

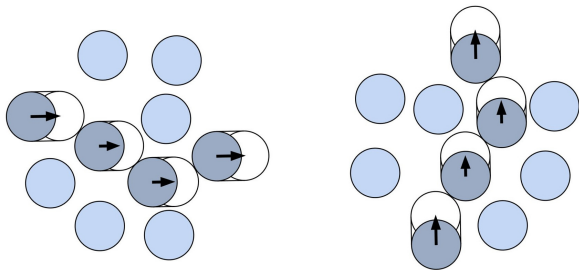
M. F. Faulkner, L. Qin, A. C. Maggs, W. Krauth, JCP (2018)

Lifted MCMC in higher dimensions (1/5)



- Infinitesimal moves (avoid overlaps).
- Particle lifting + direction lifting.
- This algorithm is correct without return moves.

Lifted MCMC in higher dimensions (2/5)



- Consensus sampling (trivial case)

- Metropolis filter

$$p^{\text{Met}}(a \rightarrow b) = \min \left[1, \prod_{i < j} \exp(-\beta \Delta U_{i,j}) \right]$$

- Factorized Metropolis filter (Michel, Kapfer, Krauth 2014)

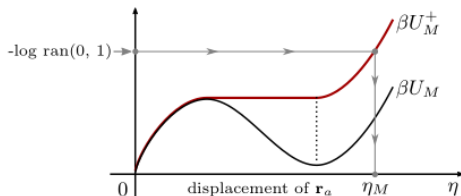
$$p^{\text{Fact.}}(a \rightarrow b) = \prod_{i < j} \min [1, \exp(-\beta \Delta U_{i,j})] .$$

satisfies detailed-balance condition, with a symmetric choice of a priori probabilities.

- Interpretation in terms of Boolean random variables.

$$X^{\text{Fact.}}(a \rightarrow b) = X_{1,2} \wedge X_{1,3} \wedge \cdots \wedge X_{N-1,N}$$

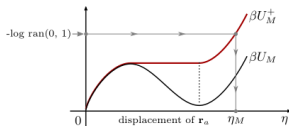
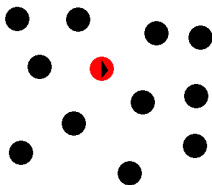
Lifted MCMC in higher dimensions (4/5)



$$p_M(m) = \underbrace{\prod_{l=1}^{m-1} e^{-\beta \Delta U_M^+(l)}}_{\text{accepted}} \overbrace{\left[1 - e^{-\beta \Delta U_M^+(m)} \right]}^{\text{move } m \text{ rejected}}, \quad (1)$$

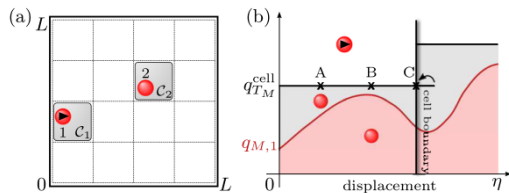
- Peters, de With (2012)

Lifted MCMC in higher dimensions (5/5)



- Compute event-times for all factors.
- Select smallest one.
- Complexity $\mathcal{O}(N)$ unless short-range.

Thinning and sampling (1/1)



- Time-dependent Poisson process $q(x)dx$

$$\underbrace{q(x)dx}_{\text{variable}} = \underbrace{q^{\max}dx}_{\text{constant}} \underbrace{\frac{q(x)}{q^{\max}}}_{\text{rejection}}$$

- This is called “Thinning”, many generalizations.
- ... reduces ECMC to the sampling from a vector of probabilities, one for each cell.

Sampling from a discrete distribution (1/3)

- Rejection sampling (see book)

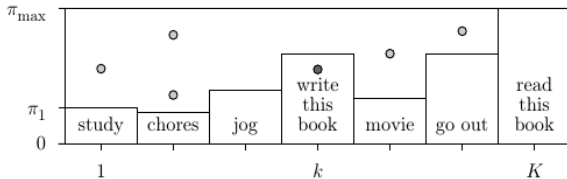


Fig. 1.28 Saturday night problem solved by Alg. 1.13 (reject-finite).

Sampling from a discrete distribution (2/3)

- Tower sampling (see book)

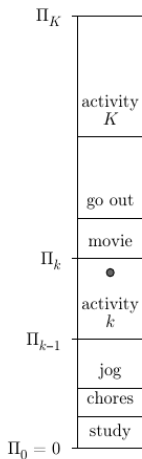
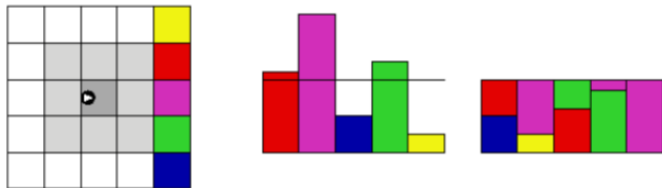


Fig. 1.29 Saturday night problem solved by tower sampling.

Sampling from a discrete distribution (3/3)

- Walker's method of aliases



... Cell-veto sampling using Walker's method.

- Complexity $\mathcal{O}(1)$

Conclusion of masterclass

- **Day 1** Fundamentals: From Balance conditions to non-reversibility and to lifting. Single particle on a path graph.
- **Day 2** Surprises: reversible and non-reversible Markov chains for hard spheres. Perfect sampling.
- **Day 3** Advances: Meta algorithms. Consensus sampling.

A quote contributed by Prof. MJ Bhaseen

- “Mrs Thatcher, do you believe in consensus?” To our surprise, we heard her saying, “Yes, I do believe in consensus; there should be a consensus behind my convictions.” (Malcolm Rifkind)