Markov Chain Monte Carlo: innovations and applications in statistical physics

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Content

- Models: Potts and RC
- Introduction: Markov Chain Monte Carlo (MCMC)
- Local algorithms: Metropolis, Sweeny, and Worm
- Collective–mode algorithms: Swendsen-Wang (SW)
- Three pictures for SW method
- Applications: real q>1 RC model, RC model in field, Loop, Anti-Potts, AT, fixed-bond RC, fixed-magnetization Potts, spin-glass
- Some references (incomplete and biased)

Model

- Potts model

Hamiltonian:

$$H = -K \sum_{\langle ij \rangle} \delta(\sigma_i, \sigma_j) \qquad (\sigma = 1, 2, \cdots q)$$

Partition sum:

$$Z = \sum e^{-H/kT}$$

- Random-cluster model

$$Z = \sum_G v^{b(G)} q^{k(G)}$$

Markov Chain Monte Carlo (MCMC)

- desired probability distribution $P(\Gamma)$;
  transition probability matrix $T(\Gamma_{t+1}, \Gamma_t)$
- detailed balancing: $T(\Gamma, \Gamma')P(\Gamma') = T(\Gamma', \Gamma)P(\Gamma)$
- irreducibility (ergodicity)

Efficiency: Critical Slowing-down

$$\tau \propto \xi^z$$

Local algorithms

- Metropolis for Ising

  1), pick up a spin (randomly or sequentially)

  2), calculate the energy cost ΔE if the spin is flipped

  3), flip the spin with probability $\mathrm{Min}(1, e^{-\Delta E/kT})$

  Dynamic exp: $z \approx 2.2$

- Sweeny (two-time scaling): critical speeding-up!

- Worm (three-time scaling)

e_{ij}

Swendsen-Wang (SW) Method

Swendsen-Wang Simulation:

1), for each edge e_{ij}, if $\sigma_i = \sigma_j$, place a bond with $p = 1 - e^{-K}$; otherwise, do nothing.

2), for each connected component (FK cluster), randomly pick up one of the q states.

Three Pictures for SW Method

- Edward-Sokal Picture

1), Exact mapping between the Potts model and the random-cluster (RC) model:

$$Z = \sum_{A \subseteq E} q^{k(A)} (1-p)^{|E|-|A|} p^{|A|}$$

2), Bond-Spin-joint probability measure:

$$P(\vec{n},\sigma) \propto \prod_{e \in E} [(1-p)\delta_{n_e,0} + p\delta_{n_e,1}\delta_e(\sigma)]$$

! SW method passes back and forward between the bond and the spin representation of the Potts model.

- Domany's Picture

1), Hamiltonian: $H = \sum_i H_i$; $H_i(\vec{\sigma}) = E_1$ or E_2 is a two-energy-level system.

2), Probability measure

$$\exp(-H_i) = e^{-E_2}(1 + v_i \delta_{H_i, E_1})$$

with $(v_i = e^{E_2 - E_1} - 1)$

3), for unit i in energy E_1, place bond with $p_i = v_i / (1 + v_i)$.

4), Perform operations that conserve energies of units i with bonds. (do-nothing is surely one valid operation)

- Induced subgraph Picture

1, RC model

$$Z = \sum_{A\subseteq E} \prod_{e\in E} v_e \prod_{i=1}^{k(A)} q = \sum_{A\subseteq E} \prod_{e\in E} v_e \prod_{i=1}^{k(A)} \sum_{\alpha=1}^{m} q_m$$

2, Coloring: Independently for each component, assign it a "color" α with probability q_α / q. Vertex set V is partitioned as $V = \bigcup_{\alpha=1}^{m} V_\alpha$. Conditioning on the color assignment, independently on each induced subgraph $G[V_\alpha]$ is a q_α -state RC model.

3, Choose any MC method to update the induced RC model. Particularly, it is a bond percolation for q=1. Do nothing is also a valid update.

Application

- Chayes-Machta Method for q>1 RC Model

1, RC Model

$$Z = \sum_{A \subseteq E} v^{|A|} q^{k(A)} = \sum_{A \subseteq E} v^{|A|} [q_1 + q_2]^{k(A)} \qquad (q_1 = 1, q_2 = q - 1)$$

2, Independently for each component, color it to be "1" with $p = 1/q$, and color it be "2" with $p = (q-1)/q$.

3, Update subgraph $G[V_1]$ as the bond percolation, and do nothing for $G[V_2]$.

- Potts Model in a field

1, Partition sum

$$Z = \sum_{\sigma} \prod_{e \in E} \exp(K\delta_{\sigma_e}) \prod_{j \in V} h\delta_{\sigma_j,1} = \sum_{A \subseteq E} v^{|A|} \prod_{i=1}^{k(A)} [(q-1) + |V_i|^h]$$

2, Independently for each component, color it to be “1” with $p_1 = |V_i|^h / [(q-1) + |V_i|^h]$; otherwise, color it be “2”.

3, Update subgraph $G[V_1]$ as the bond percolation, and do nothing for $G[V_2]$.

- Loop Model (Honeycomb)

1, Partition sum

$$Z = \sum_{\substack{A \subseteq E: \\ \text{Eulerian}}} x^{|A|} n^{|c(A)|}$$

c(A): Loop (cyclomatic) number

2, Physical relevance:

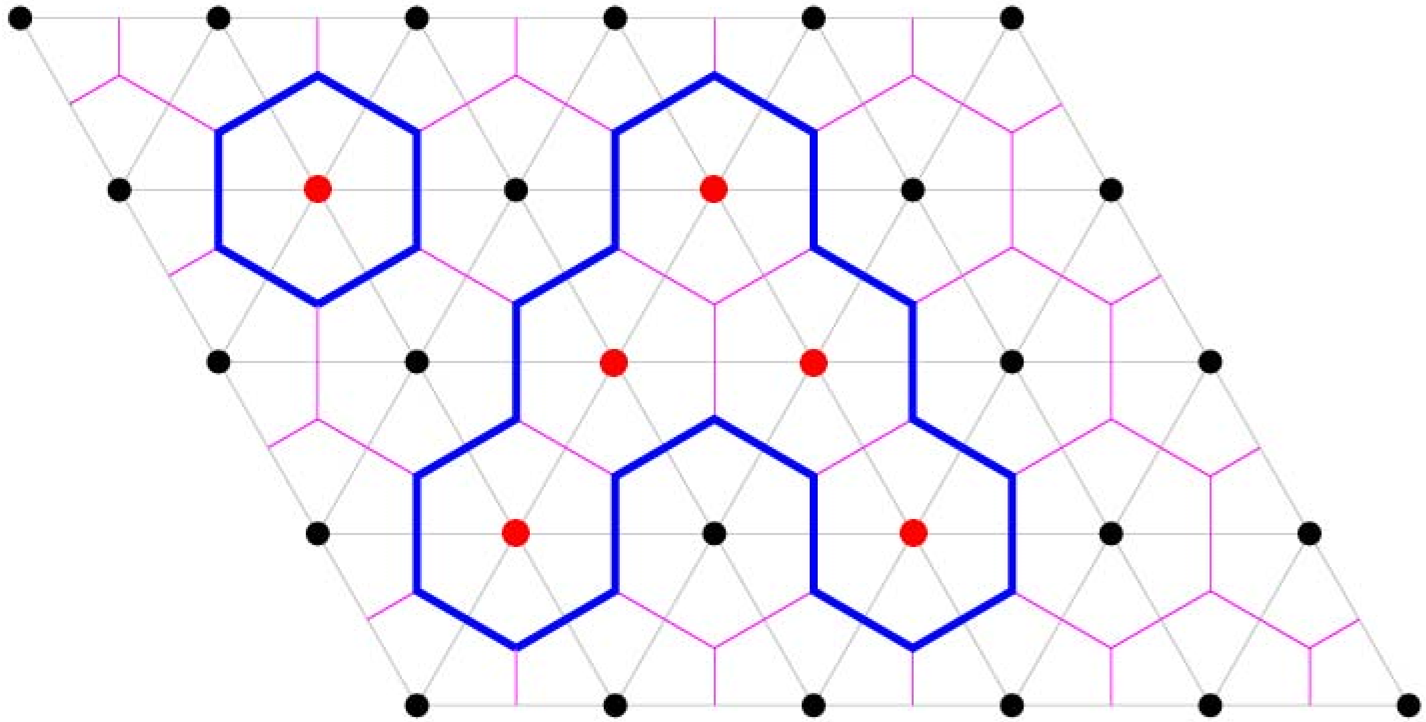
(a), it is the high-T graph of Nienhuis's O(n) spin model.

For q=1, it is a graph representation of Ising model.

(b), for $q \to 0$, it reduces to the self-avoiding random walk (SAW).

(c), it plays an important role in the stochastic Loewner evolution(SLE)

Honeycomb-Triangular Lattice



Honeycomb-Triangular Lattice

- Simulation for n=1 (Honeycomb)

1, Plaque update:

2, Worm algorithm

3, Cluster simulation of the Ising-spin model on triangular lattice with coupling $e^{-2K^*} = x$.

(Duality relation between high-T and Low-T graphs)

- Cluster Simulation for n>1 (Honeycomb)

Start from bond config. on H and spin config. on T .

1, Color each loop (cycle) to be “1” with $p = 1/n$ and to be “2” with $p = 1 - 1/n$. Color isolated sites to be “1”.

2, Place bonds on each edge e^* on triangular lattice T . If the dual e does not entirely lie in V_1, place a bond; otherwise, place a bond with $p = 1 - x$.

3, Form clusters on T . Independently for each component, flip the Ising spins with $p = 1/2$.

4, New bond config. on H is the low-T graph of spins on T

! *Analogous idea applies to face-/corner-cubic model*

- Antiferromagnetic Potts model (Domany picture):

1, Edge weight:

$$\exp(K\delta_{\sigma_i\sigma_j}) = e^K[1+(e^{-K}-1)(1-\delta_{\sigma_i,\sigma_j})]$$

2, Choose two of the q states—say q_1 and q_2. Place bond with $p = 1 - e^K$ on edges connecting states q_1 and q_2.

3, Form clusters. Independently for each cluster, interchange Potts states $q_1 \leftrightarrow q_2$ with $p = 1/2$.

- Antiferromagnetic triangular Ising model:

1, Hamiltonian:

$$H = -\sum_{e_{ij}\in E} K s_i s_j = -\sum_{\Delta_i} H_{\Delta_i}$$

$H_\Delta = K$ (two satisfied and one unsatisfied bond).

$H_\Delta = -3K$ (three unsatisfied bonds).

2, Δ weight: $\exp(-H_\Delta) = e^{3K}[1+(e^{-4K}-1)\delta_{H_\Delta,K}]$

3, For each Δ, place a bond with $p = 1 - e^{4K}$ on one of the two satisfied bonds.

4, For clusters, and update Ising spins.

- Fixed-bond-number RC model

1, Definition:

$$Z = \sum_{A \subseteq E; |A| = \text{const.}} v^{|A|} q^{k(A)}$$

2, For each cluster, color it to be “1” with $p = 1/q$, and color it be “2” with $p = 1 - 1/q$.

3, On subgraph $G[V_1]$, do Kawasaki dynamic for bond percolation, and do nothing for $G[V_2]$.

- Geometric Cluster algorithm (Ising Model)

  Let vertices i, j, k map onto i', j', k' under certain transformation—i.e., the spatial inversion. Under interchanging-spin operation $s_i \leftrightarrow s_{i'}$, the energy associated with edges e_{ij} and $e_{i'j'}$ has two levels:

$$H_e = -K(s_i s_j + s_{i'} s_{j'}) :\equiv E_1 \text{ or}$$

$$H_e = -K(s_i s_{j'} + s_{i'} s_j) :\equiv E_2$$

Say $E_1 < E_2$, weight:

$$\exp[-H_{e_{ij}, e_{i'j'}}] = e^{-E_2}[1 + (e^{E_2 - E_1} - 1)\delta_{H_e, E_1}]$$

- Geometric Cluster algorithm (Ising Model)

  (Single-Cluster version)

  1, randomly chose a site i . Let i and its mapping i' be in the cluster, and do operation $s_i \leftrightarrow s_{i'}$.

  2, for all neighbor sites k of i (not yet in cluster):
  If $\delta_{H_e,E_1} = 1$, place a bond with $p = 1 - e^{E_1 - E_2}$, do $s_k \leftrightarrow s_{k'}$ and include k, k' in the cluster (stack). Otherwise, do nothing.

  3, read a site j from stack, do Step 2. Erase j from stack.

  4, Repeat Steps 2 and 3 until stack is empty.

- Embedding methods for a variety of systems.

  1), O(n) spin model

  2), Ashkin-Teller model

  3), Baxter-Wu model

  ….

- Replica and simulated tempering MC for spin glass
- SW-like MC algorithm for quantum Potts model

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