ACCEPTANCE RATIOS OF MONTE CARLO SIMULATIONS WITH LOCAL UPDATES

VENIAMIN BLINOV[B], EVGENI BUROVSKI[A;B], WOLFHARD JANKE[C],
MARIA GUSKOVA[A;B], LEV SHCHUR[A;B]

A NATIONAL RESEARCH UNIVERSITY HIGHER SCHOOL OF ECONOMICS, 101000 MOSCOW, RUSSIA
B SCIENCE CENTER IN CHERNOGOLOVKA, 142432 CHERNOGOLOVKA, RUSSIA
C INSTITUT FÜR THEORETISCHE PHYSIK, UNIVERSIT ÄT LEIPZIG, POSTFACH 100 920, 04009 LEIPZIG, GERMANY

We study acceptance ratios of local updates in Monte Carlo simulations of classical spin models. We derive analytic expressions for the expected value of the acceptance ratios of Metropolis and heat bath updates for a one-dimensional Ising model, and find that for the Metropolis updates, the mean value of the acceptance ratio is a linear function of the energy; for the heat bath algorithm, the dependence is close to linear outside of the low temperature range. These analytic expressions are corroborated by numeric simulations. We also report results of numeric simulations of related classical spin models: the two-dimensional Ising model, one- and two-dimensional three- and four-state Potts models, and one- and two-dimensional XY model.

POTTS MODEL

One-dimensional q-state Potts model defined by the Hamiltonian function

$$H_{Potts} = -J\sum_{i=1}^{L}\delta(S_i, S_{i+1})$$

Where the coupling constant $J > 0$ and $S_i \in \{1, \dots, q\}$, $\delta(S_i, S_{i+1})$ is the Kronecker delta, which equals one whenever $S_i = S_{i+1}$ and zero otherwise.

ACCEPTANCE RATIO

We take L to be even throughout, so that $\sum_i Q_i$ is even. The partition function corresponding to Eq. (3) then reads:

$$Z = x^{-\frac{L}{2}}\sum_{l=0}^{L/2} C_L^{2l} x^{2l}, \qquad (4)$$

where $x = e^{2\beta J}$ and β is inverse temperature. Performing the summation we obtain

$$Z = \frac{1}{2}x^{-\frac{L}{2}}[(x+1)^L + (x-1)^L] \qquad (5)$$

Note that flipping a spin S_j flips the values of two bond charges, Q_j and Q_{j-1}. The acceptance probabilities are defined by the sum $q \equiv Q_j + Q_{j-1}$.
Denoting the expected value of the acceptance probability by R, the expected value of the rejection probability is then

$$1 - R = \sum_{l=0}^{\frac{L}{2}}(1 - x^{-2})\frac{2l}{N}\frac{2l-1}{N-1}\frac{C_L^{2l}x^{2l}x^{-\frac{L}{2}}}{Z} \qquad (6)$$

Here the factor $2l(2l-1)/N(N-1)$ counts the probability that, in a configuration with
$\sum_i Q_i = 2l$, for a randomly chosen site j we have $Q_j = Q_{j-1} = 1$.
The sum entering Eq. (6) is readily computed by differentiating the binomial formula twice. The result is

$$1 - R = \frac{x^2-1}{2Z}[(x+1)^{L-2} + (x-1)^{L-2}]x^{-\frac{L}{2}} \qquad (7)$$

In the thermodynamic limit $L \gg 1$, the second term in brackets is negligible and Eq.(7) simplifies to $R = \frac{2}{x+1}$. Using the Eq.(5) we obtain $\varepsilon = -\frac{x-1}{x+1}$, where $\varepsilon = E/JL$

Expected value of the acceptance ratio of metropolis update:

$$R = \varepsilon + 1$$

Expected value of the acceptance ratio of the heat bath update:

$$R_{HB} = \frac{1}{2}\frac{1-\varepsilon^2}{1+\varepsilon^2}$$

ISING MODEL

One-dimensional Ising model defined by the Hamiltonian function

$$H = -J\sum_{i=1}^{L} S_i S_{i+1}, \quad (1)$$

Where the coupling constant $J > 0$ and $S_i = \pm 1$ are Ising spins, located at the sites of a one-dimensional chain lattice of L sites with periodic boundary conditions.
We convert model (1) to bond variables. To this end, we define for a bond connecting sites i and $i+1$ the 'charge',

$$Q_i = \frac{1}{2}(S_i S_{i+1} + 1), \quad (2)$$

Which takes values of 0 (for $S_i \neq S_{i+1}$) and 1 (for $S_i = S_{i+1}$). In this notation, Eq.(1) takes the form

$$H = -2J\sum_{i=1}^{L} Q_i + JL, \qquad (3)$$

Where the sum is taken over the bonds of the lattice.

XY MODEL

One-dimensional XY model defined by the Hamiltonian function

$$H_{XY} = -J\sum_{i=1}^{L}\cos(S_i - S_{i+1})$$

Where the coupling constant $J > 0$ and $S_i \in [0, 2\pi)$.

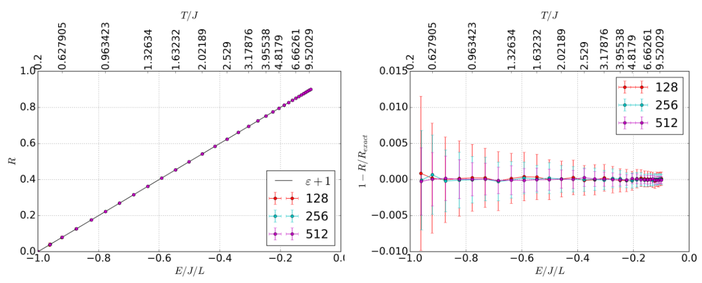
METROPOLIS ALGORITHM

A Monte Carlo simulation constructs an ergodic random walk in the configuration space of a model, $\cdots \to \mu \to \nu \to \cdots$, with the transition probabilities satisfying the detailed balance condition [3]. The stationary distribution of the random process reproduces the equilibrium Gibbs distribution of the model (1) at a fixed value of temperature T.

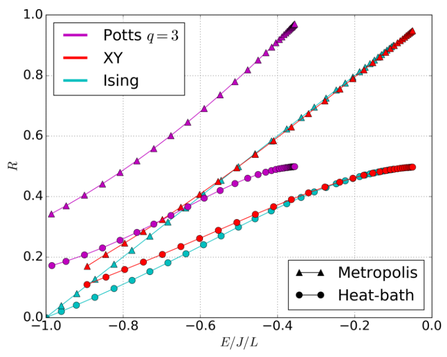
Metropolis algorithm. An elementary update of the local Metropolis algorithm [1] proceeds in two steps: (i) select a random site $j \in [1, L]$,and (ii) flip its spin, $S_j \to -S_j$, with the probability $p(\mu \to \nu) = \min\left(1, e^{-\beta\Delta E}\right), where\ \Delta E = E_\nu - E_\mu$ is the energy difference between the original and updated states. [4]

Heat bath algorithm. The heat bath algorithm differs from the Metropolis algorithm only in that a spin-flip update is accepted with the probability [4]:

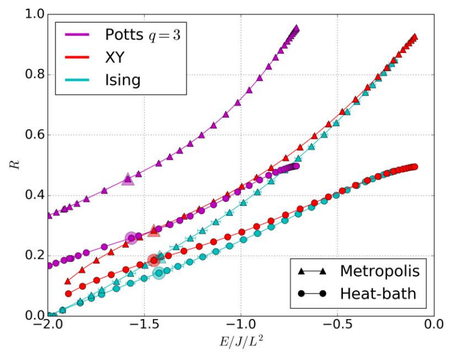
$$p(\mu \to \nu) = \frac{e^{-\beta E_\nu}}{e^{-\beta E_\nu} + e^{-\beta E_\mu}}$$



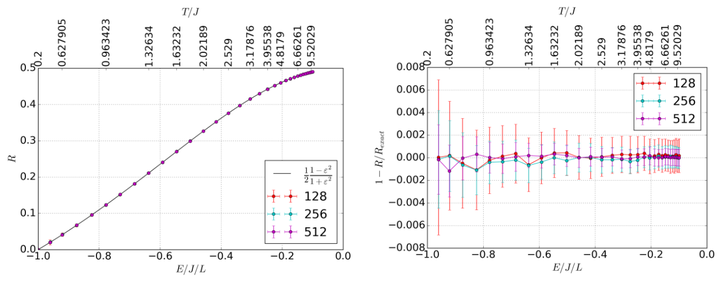
ONE-DIMENSIONAL ISING MODEL, METROPOLIS ALGORITHM



ACCEPTANCE RATIO FOR ALL ONE-DIMENSIONAL MODELS



ACCEPTANCE RATIO FOR ALL TWO-DIMENSIONAL MODELS



ONE-DIMENSIONAL ISING MODEL, HEAT-BATH ALGORITHM

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[1] N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller, and E. Teller, *Equations of State Calculations by Fast Computing Machines*, J. Chem. Phys. **21**(6), 1087 (1953).
[2] see, *e.g.,* R.J. Baxter, *Exactly Solved Models in Statistical Mechanics*, Academic Press, 1982, and references therein
[3] see, *e.g.*, K. Binder and D.P. Landau, *A Guide to Monte Carlo Simulations in Statistical Physics*, Cambridge University Press, 2009, and references therein.
[4] see, *e.g.*, W. Janke, *Monte Carlo Methods in Classical Statistical Physics*, Lect. Notes Phys. **739**, 79–140 (2008) // *Computational Many Particle Physics*, eds. H. Fehske, R. Schneider, A. Weiße, Springer, 2008.