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Note on the Metropolis Monte Carlo Method on Random Lattices

N.Tsuda [†]

Department of Physics, Tokyo Institute of Technology
Oh-okayama, Meguro, Tokyo 152, Japan

and

A.Fujitsu, [‡] T.Yukawa [§]

National Laboratory for High Energy Physics (KEK)
Tsukuba, Ibaraki 305, Japan

848442

Abstract

Efficiency of algorithms in the Metropolis Monte Carlo method is examined for the problem of random walks on random lattices. Three types of algorithms, which satisfy the detailed balance, are considered. The efficiency mainly depends on the relative easiness in obtaining geometrical factors and Boltzmann factors. The most efficient algorithm for the dynamical triangulation of random surfaces is suggested.

[†]E-mail address: ntsuda@phys.titech.ac.jp

[‡]Permanent address: Information Systems and Technology Center The University of Aizu
Tsuruga, Ikki-machi, Aizu-Wakamatsu City Fukushima, 965-80 Japan
E-mail address: a-fujitu@u-aizu.ac.jp

[§]E-mail address: yukawa@theory.kek.jp

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Simulations of random walks by the Monte Carlo method are considered in most of the case on regular lattices [1]. If one wishes to study the problem on random lattices, the detailed balance equation should be modified so that the inhomogeneity in the coordination number of each lattice site is taken into account. The detailed balance equation between state A and B, in general cases, is given by

$$\frac{W_A}{t_A} P_{A \rightarrow B} = \frac{W_B}{t_B} P_{B \rightarrow A}, \quad (1)$$

where $P_{A \rightarrow B}$ is the transition probability from states A to B which is chosen to bring the system towards the equilibrium distribution $\{W_A\}$. Inhomogeneity of the lattice space is accounted by the geometrical factors t_A and t_B . For each state A there exist a set of nearest neighbor states $\mathbf{B} = \{B_i\} (i = 1, 2, \dots, t_A)$ which are connected to the state A by one step move, *i.e.* t_A is the number of states of A. In the random walk problem states A and B are specified by a pair of nearest neighbor sites x_i and $x_{i+\hat{\mu}_i}$ between which the random walker moves. Here $\hat{\mu}_i$ represents one of the t_A directions of the nearest-neighbour sites of x_i . Thus the factor t_A is the same for any state in the regular lattice, while for the random lattice it varies by states.

There are many solutions for eq.(1), which give the same value for the ratio of two transition probabilities

$$\frac{P_{A \rightarrow B}}{P_{B \rightarrow A}} = \frac{t_A}{t_B} \frac{W_B}{W_A}. \quad (2)$$

Among those we shall compare three types of algorithms, which are selected as typical cases. They are classified according to the relative easiness of obtaining geometrical factors and Boltzmann factors.

Case I

This is the simplest case occurring when geometrical factors and Boltzmann factors are readily obtained. Standard choice of the Metropolis algorithm will work well in this case; the transition probability $P_{A \rightarrow B}$ is chosen to be

$$\min \left\{ 1, \frac{t_A}{t_B} \cdot \frac{W_B}{W_A} \right\}. \quad (3)$$

Case II

When it takes much longer time to obtain Boltzmann factors than geometrical factors or *vice versa*, the Metropolis Monte Carlo procedure could be split into two parts in order to reduce the time consuming calculations; namely, first perform the Metropolis Monte Carlo with the probability

$$\min \left\{ 1, \frac{t_A}{t_B} \right\}. \quad (4)$$

Only when it is accepted, repeat the Monte Carlo procedure with the probability

$$\min \left\{ 1, \frac{W_B}{W_A} \right\}. \quad (5)$$

Figure 1: Example of a random graph. Proper states are represented by white circles, while improper states are black circles. Transition takes place only between proper states.

In this way we can avoid the calculation of $\frac{W_B}{W_A}$ for a rejected move. When the calculation of geometrical factors are more time consuming, the order of two Monte Carlo procedures should be interchanged.

Case III

There exist certain problems which require a great deal of computing time to obtain the geometrical factor t_A . In such cases calculations of t_B for the transition between states A and B are waste of time since the move is not always accepted by the Monte Carlo procedure. Simulation of quantum gravity by the dynamical triangulation method [2] is one of such problems. In the dynamical triangulation a state A corresponds to a specific graph of d -dimensional hyper-surface triangulated by equilateral d -simplices. The transition between state A and B are performed by one of so-called *moves*. Although each move is known to conserve the topology, the resulting state B does not necessarily fulfill conditions of the proper PL-manifold. The check of proper manifold condition is the most time consuming step in this method. To know the geometrical factor t_A all the graphs B must be checked. The third algorithm is made in the following way so that the calculation of geometrical factors is unnecessary. For each graph A choose a set of graphs $C = \{C_i\}$ ($i = 1, 2, \dots, n_A$), which may be obtained by one step move from the graph A , but not necessary the proper graphs. As far as the set of graphs C contains the set of proper graphs B as a subset, the choice is free. This situation is illustrated in Figure 1. Now, perform the Metropolis Monte Carlo with the probability

$$\min \left\{ 1, \frac{n_A}{n_B} \cdot \frac{W_B}{W_A} \right\}. \quad (6)$$

Only when this move is accepted make the manifold check of resulting graph B . The probability of passing this check is t_A/n_A . The ratio of transition probability,

$$\min \left\{ 1, \frac{n_A}{n_B} \cdot \frac{W_B}{W_A} \right\} \times \frac{t_A}{n_A} : \min \left\{ 1, \frac{n_B}{n_A} \cdot \frac{W_A}{W_B} \right\} \times \frac{t_B}{n_B} = t_A W_B : t_B W_A, \quad (7)$$

then satisfies eq.(2). In the above procedure it is important for the efficiency to choose an appropriate set C so that t_A/n_A is reasonably closer to 1.

In this note we have considered three types of algorithms of the Metropolis Monte Carlo simulation on random lattices. Selection of the most efficient algorithm depend strongly on the relative easiness of obtaining geometrical factors and Boltzmann factors. We propose an algorithm which does not require geometrical factors, and thus suites for the dynamical triangulation of quantum gravity.

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