A proposal for the estimation of percolation thresholds in two-dimensional lattices

LETTER TO THE EDITOR

A proposal for the estimation of percolation thresholds in two-dimensional lattices

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Abstract. We propose a method to calculate percolation thresholds p_c and their error bars Δp_c of two-dimensional (2D) lattices. The characteristic feature of our method is an efficient extraction of information from the results of Monte Carlo (MC) simulations. We apply this method to some 2D systems such as a square, Kagomé and dice lattice, Penrose tiling and a Penrose dual lattice. Our method enables us to estimate thresholds very accurately even when we use the MC data obtained from fairly small sizes. For instance, we achieve three significant figures for p_c from the MC data obtained from lattices with sizes less than 300×300 and the increment 0.002 of p.

One of the central themes in the investigation of percolation problems is the evaluation of percolation thresholds p_c (Shante and Kirkpatrick 1971, Stauffer 1985). Exact derivation of p_c is possible only when the lattice under consideration has some topological advantage (Sykes and Essam 1963, 1964). Examples of lucky cases in this sense include bond percolation in a square, triangular and honeycomb lattice and site percolation in a Kagomé lattice. Except for these lucky cases, the determination of percolation thresholds p_c depends on the Monte Carlo (MC) simulations and some other methods such as the transfer matrix method (Derrida and De Seze 1982, Saleur and Derrida 1985). In any method for estimating p_c numerically, the most important factor is the efficiency of extracting significant information from the data obtained for systems of finite sizes. On noting this point, it is a purpose of this letter to propose a technique to derive an extremely accurate value of p_c and its error bar for a given two-dimensional (2D) lattice.

The outline of this letter is as follows. We first give a definition of several kinds of percolating clusters and study probabilities $R_N(p)$ that we find these percolating clusters. On the basis of the assertion that $R_N(p)$ is approximated by an error function, we introduce the concept of effective thresholds $p_c(N)$ for a system of size N, and we give relations which $p_c(N)$ should satisfy. Then we show the way in which $p_c(N = \infty)$ and its error bar Δp_c are estimated by adapting finite-size scaling for the extrapolation from the results of finite systems. We apply our method to bond and site percolation in some 2D lattices such as a square, Kagomé and dice lattice, Penrose tiling and a Penrose dual lattice.

Here it is worth mentioning the following point. As for Penrose tiling and its dual lattice, we pick up a portion of a given N such that the frequency of each

vertex is almost equal to the corresponding infinite system. When this consideration is made, the dependence of the results on a choice of origin becomes practically insignificant.

Suppose we have a system composed of N elements, being either bonds or sites depending on whether we are interested in bond or site percolation. We choose M elements at random out of the N elements and regard them as intact while the other $N - M$ elements are assumed to be broken. Then, the problem of percolation is to ask if we find a percolating cluster of intact elements at a given concentration $p \equiv M/(N + M)$.

A cluster could percolate rightward from left to right, or downward from top to bottom. We define the following probabilities:

$R_N^R(p)$: the probability that we find a rightward percolating cluster;

$R_N^D(p)$: the probability that we find a downward percolating cluster;

$R_N^I(p)$: the probability that we find a cluster percolating both rightward and downward;

$R_N^U(p)$: the probability that we find either a rightward percolating cluster or a downward percolating cluster, and

$$R_N^A(p) \equiv \tfrac{1}{2}[R_N^R(p) + R_N^D(p)].\tag{1}$$

The notation R, D, I, U and A respectively denotes rightward, downward, intersection $(I = R \cap D)$, union $(U = R \cup D)$ and average.

From the definitions, we have the following relations:

$$R_N^R(p) + R_N^D(p) = R_N^I(p) + R_N^U(p)\tag{2}$$

$$R_N^I(p) \leqslant R_N^A(p) \leqslant R_N^U(p)\tag{3}$$

where the equal signs hold when $N \to \infty$ in (3).

For each definition of $R_N^X(p)$, X being either A, I or U, we have $R_N^X(0) = 0$ and $R_N^X = 1$, and $R_N^X(p)$ changes from zero to unity as p increases from zero to unity. In an infinite system, this change takes place only at the percolation threshold $p_c = p_c(N = \infty)$ so that $R_\infty^X(p) = 0$ for $p < p_c$ and $R_\infty^X(p) = 1$ for $p > p_c$. In other words, $dR_\infty^X(p)/dp = \delta(p - p_c)$. When the size N is finite, the change is continuous. There are some arguments (Stauffer 1985; Efros 1986) that, for p not very far from p_c, $dR_N^X(p)/dp$ is well approximated by a Gaussian function

$$\frac{dR_N^X(p)}{dp} = \frac{1}{\sqrt{2\pi}\,\Delta_N^X}\exp\left[-\frac{1}{2}\left(\frac{p - p_c^X(N)}{\Delta_N^X}\right)^2\right]\tag{4}$$

where $p_c^X(N)$ is the value of p at which $R_N^X(p)$ becomes $\tfrac{1}{2}$; Δ_N^X is the standard deviation which is expected to decrease when N increases. The character X may denote either I, U or A. From (4), we have

$$p_c^I(N) \geqslant p_c^A(N) \geqslant p_c^U(N).\tag{5}$$

Let us denote by L^d a dual lattice of an initial lattice L. Then, we superpose both lattices on the same plane and assume that, at each concentration, a bond of L^d is intact or broken if the corresponding bond of L is broken or intact, respectively. Under this condition, the concentration q of intact bonds in L^d is given by $q = 1 - p$ where p is the concentration of intact bonds in L. Then, we can prove the following relation for bond percolation:

$$R_N^A(p; \text{bond}; L) + R_N^A(q; \text{bond}; L^d) = 1.\tag{6}$$

Remembering that $R_N^A(p)$ is $\frac{1}{2}$ at the effective threshold $p_c^A(N)$, we can derive from (6) that

$$p_c^A(N; \text{bond}; L) + p_c^A(N; \text{bond}; L^d) = 1 \tag{7}$$

which is the finite-size version of the well known relation

$$p_c(\infty; \text{bond}; L) + p_c(\infty; \text{bond}; L^d) = 1. \tag{8}$$

Similar relations naturally hold for site percolation between an initial lattice and its matching lattice.

An important outcome of relation (7) is that, for some special kinds of lattices of finite sizes, the effective thresholds $p_c^A(N)$ are determined exactly if appropriate care is taken of the boundaries. For instance, since a square lattice is self-dual, it follows immediately from (7) that, for all values of N,

$$p_c^A(N; \text{bond}; \text{square}) = \frac{1}{2}. \tag{9}$$

It is also possible to show, by making use of (8) and the star-triangle transformation (Skyes and Essam 1963), that

$$R_N^A(p_c(T); \text{bond}; \text{triangular}) = R_N^A(p_c(H); \text{bond}; \text{honeycomb}) = \frac{1}{2} \tag{10}$$

where $p_c(T)$ and $p_c(H)$ are respectively the percolation thresholds of an infinite triangular and honeycomb lattice. Equation (10) then proves that, for all values of N,

$$p_c^A(N; \text{bond}; \text{triangular}) = p_c^A(\infty; \text{bond}; \text{triangular}) \tag{11a}$$

$$p_c^A(N; \text{bond}; \text{honeycomb}) = p_c^A(\infty; \text{bond}; \text{honeycomb}). \tag{11b}$$

Since a Kagomé lattice is a covering lattice of a honeycomb lattice, we have, for all values of N,

$$p_c^A(N; \text{site}; \text{Kagomé}) = p_c^A(\infty; \text{bond}; \text{honeycomb}). \tag{12}$$

Equations (9), (11) and (12) assert that $p_c^A(N)$ is independent of N for the above-mentioned lattices. As we shall see in what follows, our numerical analyses of other lattices imply that this seems to be the case in all the examples we study.

We now apply the method thus described to five different 2D lattices; a square and Kagomé lattice, periodic with single-valued coordination, the coordination number being $z = 4$; a dice lattice, periodic with mixed-valued coordination, $z = 3$ and 6, the average $\bar{z}$ being 4; Penrose tiling, non-periodic with mixed-valued coordination, $z = 3$, 4, 5, 6, and 7, the average $\bar{z}$ being 4; and a Penrose dual lattice, non-periodic with single-valued coordination, $z = 4$.

In order to determine $R_N(p)$ of a given problem, we carry out n runs of MC simulations for a given concentration p. If we find a percolating cluster in each of m out of n runs, we equate $R_N(p)$ to m/n. We repeat this process for different values of p with each increment of 0.002. Then $R_N(p)$ is given as a function of p at discrete p values as expressed by filled and open circles and open squares in figure 1 for 'average', 'union' and 'intersection', respectively, for a Penrose lattice of size approximately 300×300. The curves fitted to (4) are illustrated by full curves. The fittings are remarkable, thus suggesting that the assumption of the Gaussian function is validated.

The effective thresholds $p_c^A(N)$ determined from this curve fitting are listed in table 1 both for bond and site percolation of the five 2D lattices (Yonezawa *et al* 1989). It is readily seen from the table that the effective threshold $p_c^A(N)$ is almost independent of N for all ten cases, thus indicating that $p_c^A(N)$ as defined in the above for a finite
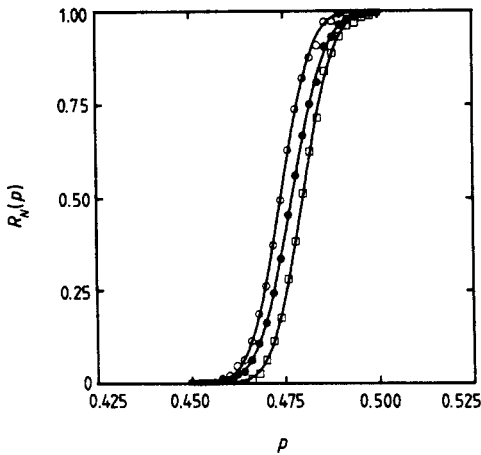
Figure 1. Probabilities $R_N^A(p)$ (●), $R_N^I(p)$ (□) and $R_N^U(p)$ (○) for the bond problem in Penrose tiling with $N \simeq 100\,000 \simeq 310 \times 310$. The corresponding curves are obtained by the least-mean-square fitting on assuming the error function. Note that the scale on the p axis is very minute.
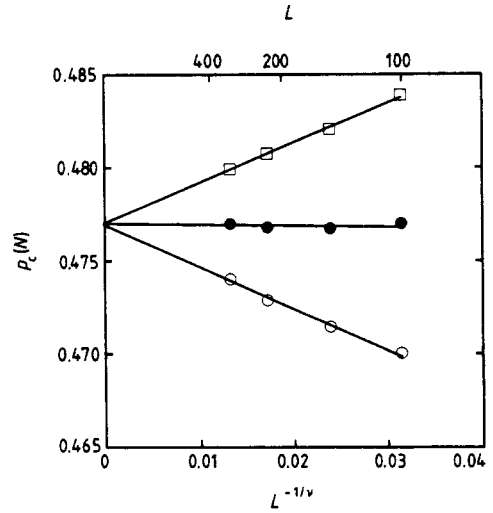
Figure 2. Three thresholds $p_c^A(N)$ (●), $p_c^I(N)$ (□) and $p_c^U(N)$ (○). $L^{-1/\nu}$ ($=N^{-1/2\nu}$) for the bond problem in Penrose tiling.

Table 1. Threshold $p_c^A(N)$ of the bond and site problems for five different lattices of different sizes.

	$N \simeq$	Square	Kagomé	Dice	Penrose	Penrose dual
Bond	10 000	0.5000	0.5244	0.4757	0.4770	0.5234
	20 000	0.4999	0.5244	0.4759	0.4768	0.5234
	50 000	0.5001	0.5246	0.4759	0.4768	0.5235
	100 000	0.5000	0.5243	0.4759	0.4770	0.5233
Site	5 000	0.5929	0.6529	0.5857	0.5845	0.6376
	10 000	0.5928	0.6524	0.5853	0.5841	0.6377
	20 000	0.5928	0.6526	0.5852	0.5842	0.6379
	50 000	0.5930	0.6527	0.5854	0.5840	0.6379

system gives a very reliable estimate of the percolation threshold in an infinite system. This is examined for bond percolation in a square lattice and for site percolation in a Kagomé lattice since the exact thresholds are known for these cases. From the table, we can observe that, even when the size is as small as 20×20 or 30×30, the effective threshold in either case gives three significant figures.

When compared with the previous MC simulations for the estimation of p_c, our method is advantageous in the following three points.

(i) Each MC run requires a relatively short CPU time. For instance, one MC run of size $N \simeq 100\,000$ bonds takes 0.5 s even for disordered systems by HITAC M682H (a *scalar* processor).

(ii) The CPU time is nearly proportional to size N, which is remarkable in these kinds of simulations.

(iii) It is possible to obtain a considerably accurate value of p_c even from the simulations of a fairly small size. If we take 100 MC runs of size $N \simeq 5000$ sites as an example, they need only three seconds and give three significant figures for p_c.

To the best of the authors' knowledge, the above three aspects guarantee that the efficiency of our method proposed in this letter is higher than that of any other existing method due to computer simulations.

In order to estimate the percolation thresholds of an infinite system, we extrapolate $p_c^X(N)$ to $N \to \infty$ by making use of a relation due to the scaling hypothesis (Stanley 1971):

$$p_c^X(N) = p_c + A^X L^{-1/\nu} \tag{13}$$

where $X = A$, U or I; $\nu = \frac{4}{3}$, and A^X is a constant, A^I being positive and A^U being negative, while A^A is expected to be zero.

In figure 2, $p_c^X(N)$ for $X = A$, U and I are plotted against $L^{-1/\nu}$, where the diameters of circles or the edges of squares give a measure for the magnitude of error bars, the errors originating from the curve fitting. We choose the extrapolated value $p_c^A(\infty)$ of $p_c^A(N)$ into $N \to \infty$ as an estimated percolation threshold of an infinite system. The differences $|p_c^I(\infty) - p_c^A(N)|$ and $|p_c^A(\infty) - p_c^U(N)|$ provide a measure for the magnitude of the error bar to the estimated value $p_c^A(\infty)$. The error bar thus determined is less than 0.0003 and accordingly the estimated value of $p_c^A(\infty)$ has three significant figures.

The thresholds determined from our simulations are compared with some previous results in table 2. When previously proposed values for thresholds exist (Sykes and Essam 1963, Reynolds *et al* 1980, Saleur and Derrida 1985, Lu and Birman 1987, Hori 1989), the agreement between these values and our results is remarkable, which shows

Table 2. Thresholds p_c derived from our simulations compared with previous results. As explained in the text, our results for the threshold are derived from 500 MC runs for each p of each size, the largest being 100 000 bonds and 50 000 sites.

	Bond		Site	
	Our result	Previous results	Our result	Previous results
Square	0.5001 ± 0.003	0.5†	0.5930 ± 0.0001	$0.5928 \pm 0.0006\|$
Kagomé	0.5244 ± 0.0002	0.524430‡	0.6527 ± 0.0002	0.652704†
Dice	0.4760 ± 0.003	0.475570‡	0.5851 ± 0.0004	—
Penrose	0.4770 ± 0.0002	0.483 ± 0.005§	0.5837 ± 0.0003	—
Penrose dual	0.5233 ± 0.0002	—	0.6381 ± 0.0003	—

† Exact value.
‡ Exact value of Hori (1989). The value of the percolation threshold for the bond problem p_c in a Kagomé lattice is derived as follows. By a generalised star-triangle transformation, the bond problem in a Kagomé lattice is transformed to the mixed bond-site problem in a honeycomb lattice. Then we can get the equation

$$a^2(3 - 2a)p_c^3 - 3a^2(1 - a)p_c^2 - 3a^2 p_c + 1 = 0$$

where a^2 is the exact percolation threshold for the bond problem in a honeycomb lattice, i.e. $a = (1 - \sin \pi/18)^{1/2} = 0.807\,900\,76\ldots$. The solution of the above equation gives the exact p_c for the bond problem in a Kagomé lattice, $p_c = 0.524\,408\,76\ldots$.
§ 20 MC runs for 90 000 bonds (Lu and Birman 1987).
‖ The transfer matrix method (Derrida and De Seze 1982).

the usefulness of our method. The thresholds for bond percolation in a Kagomé lattice and in a dice lattice satisfy the required relation (7), and so do the thresholds for bond percolation in a Penrose lattice and in a Penrose dual lattice. This also lends support to the validity of our method. A comprehensive description of our method will be published elsewhere (Yonezawa *et al* 1989).

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