

# Research on Percolation of 2D-Lattice Models based on Monte Carlo Method

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## Abstract

In the passage, we describe in detail two efficient algorithms for studying site percolation on any lattice. The algorithm can measure an observable quantity in a percolation system for all values of the site occupation probability from zero to one in an amount of time that scales linearly with the size of the system. This passage investigates a number of issues in percolation theory, including the position of the percolation transition for site percolation on the square lattice, the size of the giant component for site percolation on random graphs as well as the exponential behavior near critical point. Lastly, we use an example to demonstrate the value of percolation in varying fields.

## 1 Introduction

Percolation Theory<sup>[1]</sup> was first proposed by Broadbent and Hammersley during their research on the flow of fluids through porous media. Noticeably, there are numerous natural phenomena concerning percolation process, e.g. the flow of oil through porous rock, spread of forest fire, propagation of epidemic diseases, etc. Common features of these phenomena reside in the fact that there are two distinctive macro-states in the system: impermeable vs. permeable or nonconductive vs. conductive. Moreover, the transition between varying macro-states depends on either occupation probability or particle concentration.

In the view of mathematics and physics, percolation generally refers to simplified lattice models of random systems shown in Fig.1, along with the nature of connectivity in them. There are three kinds of percolation models: site percolation, bond percolation as well as site-bond

percolation. In the paper, we only talk about the site percolation.

In site percolation, every site on a specified lattice is independently either “occupied,” with probability  $p$ , or not with probability  $1-p$ . The occupied sites form contiguous clusters that have some interesting properties. In particular, system shows a continuous phase transition at a finite value of  $p$  which, on a regular lattice, is characterized by the formation of a cluster large enough to span the entire system from one side to the other in the limit of infinite system size.

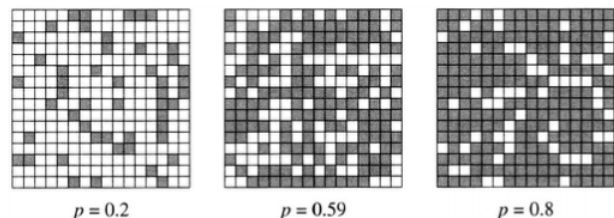


Fig.1: 2D site percolation model with occupation probability  $p=0.2, 0.59, 0.8$  respectively

Percolation threshold is a critical value of the occupation probability  $p_c$ . Regard the cluster large enough to span the entire system from one side to the other as an open cluster. Below the threshold, open cluster would not exist; while above it, there might exist. The existence of open cluster will change the properties of the system, as mentioned before: impermeable vs. permeable or nonconductive vs. conductive etc.

Despite decades of effort, no exact solution of the site percolation problem yet exists in the simplest two-dimensional square lattice, so numerical simulations have found wide use in this field.

In the paper, we investigate a number of issues in percolation theory based on Monte Carlo method, including the position of the percolation transition for site percolation on the square lattice, and the size of the giant component for site percolation on random graphs and we also mention the exponential behavior near critical point.

## 2 Model

According to Kolmogorov's zero-one law<sup>[2]</sup>, we know that for an infinite system, given site occupied probability  $p$ , the probability of a open cluster  $q$  is either 1 or 0.

$$\begin{cases} p > p_c & q = 1 \\ p < p_c & q = 0 \end{cases} \quad (1)$$

However, noticing that it is impossible to simulate an infinite system, so we would focus on discussing finite-size systems. In this case, the relation between  $p$  and  $q$  can still be approximately satisfied. Besides,  $q$  is a non-decreasing function of  $p$ , so there must be a threshold value  $p_c$ .

Firstly, consider a two-dimension  $N \times N$  lattice, each element of the lattice stands for a site. We assume the bond between each element is connected. Fig2. shows that the sites colored

black are blocked. While the others colored white or blue are open and they can connect with their neighboring sites and thus form a cluster. When the cluster reaches both ends of the lattice, we say the lattice percolates.

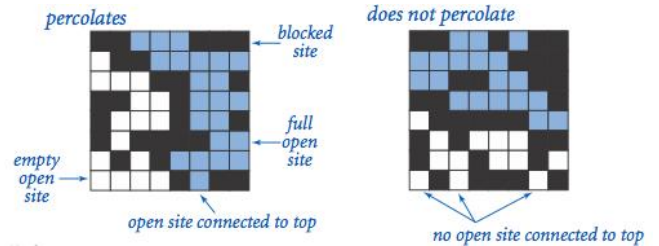


Figure 2: Left: 2D percolation model which percolates; Right: 2D percolation model which not percolates

## 3 Algorithm

For finite-size  $N \times N$  lattice, define  $p$  as the site-open probability (occupation probability) of each site and  $q$  as the percolation probability of lattice. We applied random experiments to varying size of  $N \times N$  lattice. And for each scale, we use a set of occupation probabilities to test percolation probability.

We have to go through the following procedures in single experiment:

- a. Use a  $N \times N$  structure array to represent  $N \times N$  lattice. Then Initialize the array, "1" stands for a open site, while "0" stand for a blocked site.
- b. Search for a sequence of "1" which connects an open passage in the array. This open passage stands for the open cluster in lattice.

### 3.1 Initialization

Set a site-open probability  $p$ .

Each element of the array is initialized with a random real number ranging from 0 through 1. If the random real number is greater than  $p$ , then this element stand for a open site and would be given the value "1", otherwise the element is blocked with the value "0". In Fig3. , you can

see an initialized 10×10 lattice.

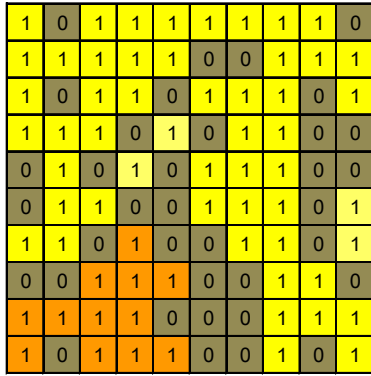


Figure 3: Initialization with site-open probability  $p=0.6$ , yellow site: open passage, grey site: blocked area

### 3.2 Search for Percolation

There are two algorithms involved in this part: wave detection algorithm and Hoshen-Kopelman Algorithm<sup>[3]</sup>. Each algorithm has its merits and drawbacks, so here we use the two algorithms for different intention.

#### a. Wave Detection Algorithm

In this method, we use the idea of wave-front expansion. As shown in Fig4. , the number of each site stands for the order of wave.

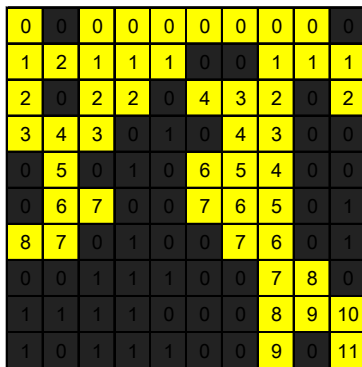


Figure 4: Wave Detection Algorithm

To begin with, we detect all the open sites in the first row and regard them as the first wave with the value “0”. Then the second wave starts. It contains all the other open sites and they can be reached within a step from the first wave. The second wave is

valued “1” . We should notice that the  $k^{\text{th}}$  wave is also derived from  $(k-1)^{\text{th}}$  wave. The  $k^{\text{th}}$  wave will be valued “k”. Not only does the value stand for the order of the wave, but also it shows the length of an open passage starting from the first row.

The advantage of this method is that it can find the shortest passage leading to percolation. While the disadvantage resides in complexity of wave detection, each time we have to go through all the sites in the structure array to find the next wave front.

#### b. Hoshen-Kopelman Algorithm

This algorithm labels every open site in the structure array in the first palce with the value “1”.

Then we start searching for cluster. When going through a brand-new open site, we check if there exist a neighboring open cluster. If there do exist, then the site would be labeled just as the open cluster. So all in all, in Fig5., every cluster shares the same label.

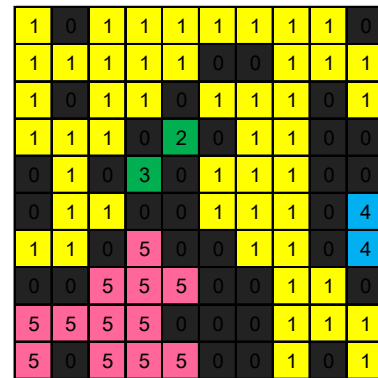


Figure 5: Hoshen-Kopelman Algorithm

The strength of Hoshen – Kopelman Algorithm attributes to its success in calculating the site number of the biggest open cluster. We will use it to investigate the size of the giant component for site percolation on random graphs.

## 4 Results and Analysis

Our simulation involves site percolation on two dimension  $N \times N$  square lattice with varying sizes ranging from  $N=4, 10, 20, 30, 50$  and  $75$ . In **Sec.4.1**, we look into the relation between site-open probability and percolation probability. While in **Sec.4.2**, the size of the giant component for site percolation has been taken into consideration. In order to fit into practical application, the exponential behavior near critical point will be discussed in **Sec.4.3**.

## 4.1 Percolation probability

Fig.6 shows the relation between independently site-occupied probability and percolation probability for systems of a variety of sizes.

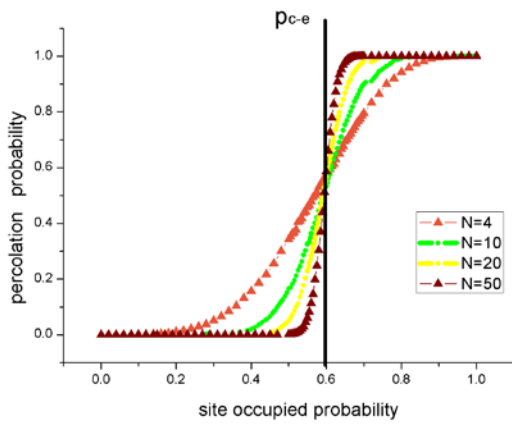


Figure 6: the relation between site occupied probability and percolation probability when the scale of lattice is  $N=4, 10, 20, 50$ , respectively.

From Fig.6, we can see the curves cross remarkably at the same point, in agreement with empirical value of percolation threshold  $p_{c-e}=0.5927$  (the subscript e stands for empirical value). By means of the software Origin, we can obtain percolation threshold in our simulation  $p_{c-s}=0.59303$  (the subscript s stands for simulation result). The error is pretty small, for the expected behavior is already well represented by the mean value, which is derived from the considerable amount of statistics we could reach in this simple case.

Different from site percolation, the exact

solution to the threshold of bond percolation is  $p_{c-t}=0.5$  (the subscript t stands for theoretical value), smaller than that of site percolation. It is easy to illustrate this phenomenon by noting the different availability of neighboring element in each case. As for bond percolation, there are six element available for connecting, while in site percolation, there are only four. So it is nature that bond percolation is easier to happen, compared to site percolation.

Also, In Fig.6, we can see each curve has different rising tendency. In specific, the bigger the lattice size, the quicker the curves increase around critical point. In order to observe the tendency precisely, we applied the following formula to lattice of different sizes.

$$\frac{\Delta q}{\Delta p} = \frac{1}{p|_{q=1^-} - p|_{q=0^+}} \quad (2)$$

The result demonstrating the relation between system size and rate of the slope is shown in Fig7. It is a straight line with positive slope. In other word, the bigger size of lattice, the bigger rate of the slope. With this tendency, the rate of slope will be  $\infty$  when  $N = \infty$ , which represent discontinuity in derivative equation of  $q$  (i.e.  $q$  will be a segmented function). So we can easily draw the Kolmogorov's zero-one law in Eq.(1).

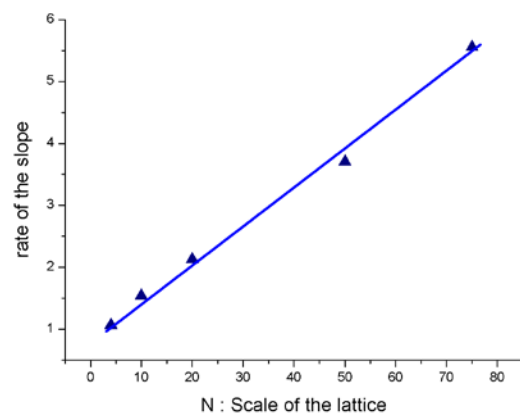


Figure 7: rate of the slope during the increasing section in Fig6. The slope have been taken from lattice scales ranges from  $N=4, 10, 20, 50, 75$

## 4.2 size of cluster

Through percolation theory, we define the average cluster size  $S$  and the size  $S_M$  of the largest cluster of each configuration. In this section, we put emphasis on  $S_M$  and the average cluster size  $S$  will be discussed later.

Fig.8. and Fig.9 show the relation between site-occupied probability and the size of the largest cluster.  $L$  is the total number of sites in the lattice.

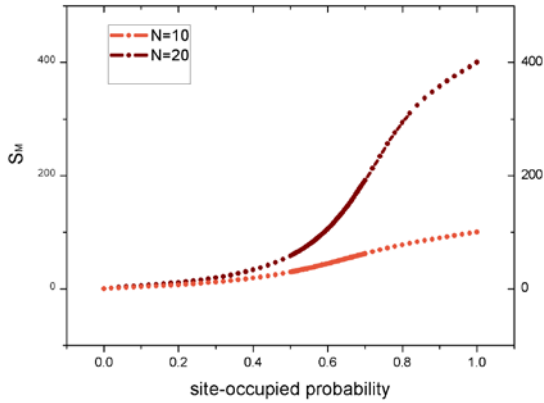


Figure8: the relation between site-occupied probability and  $S_M$  in lattice  $N=10$  and  $N=20$

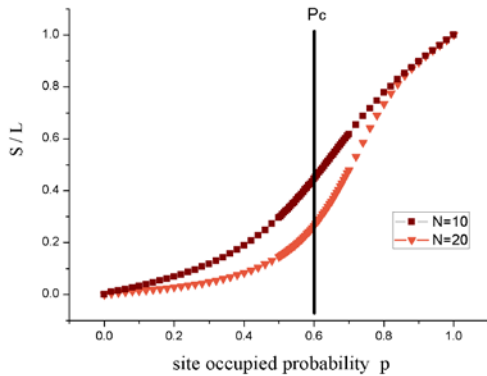


Figure 9: the relation between site-occupied probability and  $S_M/L$  in lattice  $N=10$  and  $N=20$

From Fig.8 and Fig.9, it is easy to find out that  $S_M$  is comparable to the size of the system. In Fig.9, we can see turning points in both curves near percolation threshold.

## 4.3 critical exponents

Lastly, we focus on discussing the critical

exponent around threshold. Before showing the results, some important concepts must be introduced at first.

- 1)  $S$ : the average cluster size
- 2)  $P_\infty$  (percolation probability): with certain site-occupied probability  $p$ , the probability of occupying the cluster with the size of  $\infty$  is called percolation probability  $P_\infty$ .
- 3)  $\xi$  (the average spanning length): for each configuration,  $\xi$  stands for the longest distance between two independent clusters on average.

According to percolation theory, when  $|p-p_c| \ll 1$  (i.e. near critical point) in the infinite system,  $S$ ,  $\xi$ , and  $P_\infty$  satisfy the following relations.

$$S(p) \sim (p-p_c)^{-\gamma} \quad (3)$$

$$P_\infty(p) \sim (p-p_c)^\beta \quad (4)$$

$$\xi(p) \sim (p-p_c)^{-\nu} \quad (5)$$

And  $\gamma$ ,  $\beta$ ,  $\nu$  are positive exponents. While in finite-sized systems where  $\xi$  is comparable to the scale of the system  $N$ , we now have:

$$\xi(p) \sim N \sim (p-p_c)^{-\nu} \quad (6)$$

$$P_\infty(p=p_c) \sim N^{-\beta/\nu} \quad (7)$$

$$S(p) \sim N^{-\gamma/\nu} \quad (8)$$

With these behaviors, we can put percolation theory into practical use since they relate the macroscopic properties of the compound system with their microscopic state (i.e. percolation threshold).

### 4.3.1 Application

One attractive feature of percolation theory is that many difficult and interesting phase transition problems are simplified by it. Taken the charge-injection in insulating polymer<sup>[5]</sup> as an example.

By injecting certain amount of conductive particles into a insulating polymer, the polymer could become conductive due to percolation.  $\sigma$

is defined as the conductivity of the polymeric matrix, while  $\epsilon$  represents dielectric constant. When the volume of injected particles  $v$  exceeds the critical volume  $v_c$ , conductivity  $\sigma$  increases greatly as shown in Fig.10.

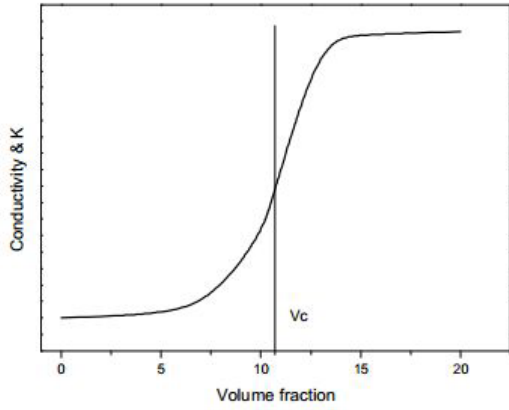


Figure 10: Percolation phenomenon of conductive particles filled polymer composites

So despite the low concentration of conductive particles, polymer composites can be a good conductor once the volume of conductive particles exceeds critical volume. In contrast with Eq(3)(4)(5), the function for  $\sigma$  and  $\epsilon$  are given below:

$$\sigma = \sigma_m (v_c - v)^{-\alpha} \quad (9)$$

$$\epsilon = \epsilon_m (v_c - v)^{-\beta} \quad (10)$$

So Through percolation theory, we can work out the critical volume of a compound system and other exponential properties around it.

## 5 Conclusion

We have described in detail two algorithms for studying site percolation on square lattice that can calculate the value of an observable quantity for all values of the site occupation probability ranging from zero to one. The percolation threshold given by our simulation is  $p_{c-s}=0.5933$ , which is close to the empirical value. We also find turning point of  $S_M$  in site percolation.

Moreover, the exponential behavior near critical point is discussed in the passage to illustrate wide use of percolation theory. In that part, percolation theory is verified to be effective in addressing practical problems, e.g. charge-injection into insulating polymer. The conductivity of polymer composites changes vastly around critical point. The results can also be applied in many other fields including granular materials, composite materials, polymers, concrete, aerogel and other porous media etc.

## References

- [1] D. Stauffer and A. Aharony, Introduction to Percolation Theory(1992)
- [2] A Doll. Kolmogorov's Zero-One Law, 《Formalized Mathematics》 (2009)
- [3] J Hoshen. The Enhanced Hoshen-Kopelman Algorithm for Cluster Analysis(1976)
- [4] F Lux. Models proposed to explain the electrical conductivity of mixtures made of conductive and insulating materials. 《 Journal of Materials Science》 (1993)