Site percolation thresholds on triangular lattice with complex neighborhoods

Krzysztof Malarz*

AGH University of Science and Technology, Faculty of Physics and Applied Computer Science, al. Mickiewicza 30, 30-059 Kraków, Poland (Dated: July 3, 2020)

We determine thresholds $p_c$ for random site percolation on triangular lattice for neighborhoods containing nearest (NN), next-nearest (2NN), next-next-nearest (3NN), next-next-next-nearest (4NN) and next-next-next-next-nearest (5NN) neighbors, and their combinations forming regular hexagons (3NN+2NN+NN, 5NN+4NN+NN, 5NN+4NN+3NN+2NN, 5NN+4NN+3NN+2NN+NN). We use a fast Monte Carlo algorithm, by Newman and Ziff, for obtaining the dependence of the largest cluster size on occupation probability. The method is combined with a method, by Bastas et al, of estimating thresholds from low statistics data. The estimated values of percolation thresholds are $\hat{p_c}(4NN) = 0.192450(36)$, $\hat{p_c}(3NN+2NN) = 0.232020(36)$, $\hat{p_c}(5NN+4NN) = 0.140250(36)$, $\hat{p_c}(3NN+2NN+NN) = 0.215459(36)$, $\hat{p_c}(5NN+4NN+NN) = 0.131660(36)$, $\hat{p_c}(5NN+4NN+3NN+2NN) = 0.117460(36)$, $\hat{p_c}(5NN+4NN+3NN+2NN+NN) = 0.115740(36)$. The method is tested on the standard case of site percolation on triangular lattice, where $p_c(3NN) = p_c(2NN) = p_c(3NN) = p_c(5NN) = \frac{1}{2}$ is recovered with five digits accuracy $\hat{p_c}(3NN) = 0.4999971(36)$ by averaging over thousand lattice realizations only.

Keywords: sites percolation; triangular lattice; complex neighborhoods; Newman–Ziff algorithm; Bastas et al method; finite size scaling hypothesis

I. INTRODUCTION

The percolation theory [1, 2]—introduced in the middle ‘50 of twentieth century [3, 4]—was recently applied in various fields of science ranging from agriculture [5] via studies of polymer composites [6], materials science [7], oil and gas exploration [8], quantifying urban areas [9] to transportation networks [10] (see Ref. 11 for review).

Usually, one assumes that the system percolates, when a cluster of occupied neighboring sites spans between borders of the system. This happens when the occupation probability $p$ is greater than or equal to the percolation threshold $p_c$. The value $p_c$ is uniquely defined in the limit of infinite system size. The value of $p_c$ depends on network topology as well as on sites’ neighborhood. By a site neighbourhood we mean a geometrical zone consisting of $z$ sites near the considered site. The sites may lie in the first, second, etc., coordinations zones. Percolation thresholds are known for many regular lattices $d$-dimensional spaces (with $d$ up to 13) and for complex networks. One can find a list of known percolation thresholds in Ref. 12 and references therein.

In most cases only sites in the first coordination zone are included to site’s neighborhood. There are some exceptions, however, where people consider neighborhoods consisting of several coordination zones, i.e. next-nearest neighbors, next-next-nearest neighbors, etc on hypercubic [13, 14], cubic [15, 16] or square [17–19] lattices. Much less is know on percolation threshold values for complex neighborhoods on other low-dimensional lattices.

In this paper we try to fill this gap by estimating values of the percolation thresholds for several complex neighborhoods on triangular lattice. To that end we use a fast algorithm for percolation by Newman and Ziff [20] and a low sampling technique by Bastas et al. [21]. We determine percolation thresholds for random site percolation with several neighborhoods containing the nearest neighbors (NN), the next-nearest neighbors (2NN), the next-next-nearest neighbors (3NN), the next-next-next-nearest neighbors (4NN) and the next-next-next-next-nearest neighbors (5NN). All considered cases are schematically sketched in Fig. 1.

II. METHODS

A. Newman–Ziff method

The idea behind the algorithm by Newman and Ziff [20] is based on the observation that some quantities can be calculated in the $(n, N)$ ensemble easier than in the $(p, N)$ ensemble. $N$ stands for the size of the system, $n$ for the number of occupied sites (or bonds) and $p$ for site (or bond) occupation probability. The relation between the two ensembles is similar to the relation between $G(n, N)$ [22, 23] and $G(p, N)$ [24] ensembles known from the construction of classical random graphs. In thermodynamic limit ($N \to \infty$) these two approaches give the same results for $p = n/N$. The Authors [20] give several examples of quantities $\overline{A}(n, N)$ which can be quickly computed in the $(n, N)$ ensemble by a recursive method. The algorithm by Newman and Ziff [20] is based on a recursive construction of states with $(n+1)$ occupied sites (or bonds) from states with $n$ occupied sites (or bonds). In a single step one adds a single site (or bond) and one applies union/find algorithm. The algorithm is very efficient.

Once the quantity $\overline{A}(n, N)$ is determined for $n =...
1, 2, · · · , N, one can also reconstruct its counterpart in
the (p, N) ensemble by the following equation:

\[ A(p; N) = \sum_{n=1}^{N} \overline{A}(n; N)B(n; N, p), \]  

where

\[ B(n; N, p) = \binom{N}{n} p^n (1 - p)^{N-n}. \]

For large N and for n ∼ O(N) one can approximate the
Bernoulli distribution function by the Gauss curve:

\[ G(n; \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma^2} \exp \left( -\frac{(n-\mu)^2}{2\sigma^2} \right), \]

with the expected value \( \mu = pN \) and variance \( \sigma^2 = p(1-p)N \).

**B. Bastas et al method**

The algorithm by Bastas et al. [21] relies on the scaling
hypothesis [25, 26] which states that in the vicinity of a
phase transition, many observables obey the following
scaling law

\[ A(p; L) = L^{-x} \cdot F\left( (p - p_c)L^{1/\nu} \right), \]

where \( x \) and \( \nu \) are some characteristic exponents, \( L \) is
the linear dimension of the system (\( L \sim N^{1/d} \)) and \( F \) is a
universal scaling function [1, p. 71]. The product \( A(p; L) \cdot L^x \)
is equal to \( F(0) \) for \( p = p_c \) and thus it does not depend
on the linear system size \( L \). Therefore the curves \( L^x \cdot A(p; L) \)
plotted for various values of \( L \) should intercept
in one point exactly at \( p = p_c \). Instead of searching
this crossing point the idea is to minimize the pairwise
difference

\[ \Lambda(p, x) = \sum_{i \neq j} [H(p; L_i) - H(p; L_j)]^2, \]

where \( H(p; L) \) is either \( L^x \cdot A(p; L) \) [27] or \( H(p; L) =
L^x \cdot A(p; L) + 1/(L^x \cdot A(p; L)) \) [21] and \( i, j \) enumerate
available system sizes \( L \).

The minimization of \( \Lambda(x, p) \) may be reduced to a
single-value function \( \lambda(p) \) minimization for any observ-
able \( A \) which does not require scaling along \( A \) axis by a
factor \( L^x \) in order to achieve statistical invariance of the
shape \( A(p; L) \) for various values of \( L \). Such a situation
occurs for instance when one chooses the (top-bottom)
wrapping probability function as \( A \) [15]. A similar re-
duction may be achieved also for any observable \( A \) for
which the value of the exponent \( x \) is known (note, that
for wrapping probability function the scaling exponent is
just \( x = 0 \)). An example of such an observable \( A \) is the
probability that a randomly selected site belongs to the
largest cluster

\[ P_{max} = S_{max}/N, \]

where \( S_{max} \) is the size of the largest cluster (i.e. the
number of sites which belong to it) and \( N = L^2 \). For
\( P_{max} \) the scaling exponent \( x = \beta/\nu \)

\[ P_{max}(p; L) = L^{-\beta/\nu} \cdot F\left( (p - p_c)L^{1/\nu} \right) \]

with exponents \( \beta = \frac{5}{36} \) and \( \nu = \frac{4}{7} \) [1, p. 54].

Here, to estimate the percolation thresholds \( \tilde{p}_c \) we min-
imize function

\[ \lambda(p) = \sum_{i \neq j} [H(p; L_i) - H(p; L_j)]^2 \]
TABLE I: Random site triangular lattice percolation thresholds estimations $\hat{p}_c$ for various complex neighborhoods. The middle column indicates the total number $z$ of sites forming the neighborhood.

| neighborhood | $z$ | $\hat{p}_c$ |
|--------------|-----|-----------|
| NN           | 6   | 0.499971(36) |
| 2NN          | 6   | $p_c$(NN) |
| 3NN          | 6   | $p_c$(NN) |
| 4NN          | 12  | 0.192450(36) |
| 5NN          | 6   | $p_c$(NN) |
| 3NN+2NN      | 12  | 0.232020(36) |
| 5NN+4NN      | 18  | 0.140250(36) |
| 3NN+2NN+NN   | 18  | 0.215459(36) |
| 5NN+4NN+NN   | 24  | 0.131660(36) |
| 5NN+4NN+3NN+2NN | 30 | 0.117460(36) |
| 5NN+4NN+3NN+2NN+NN | 36 | 0.115740(36) |

with $H(p;L) = L^{\beta/\nu} \cdot P_{\text{max}}(p;L) + 1/[L^{\beta/\nu} \cdot P_{\text{max}}(p;L)]$.

III. RESULTS

In Fig. 2 we show the charts representing the dependence of $(P_{\text{max}}(p;L)) \cdot L^{\beta/\nu}$ on the sites occupation probabilities $p$ for various neighborhoods and various linear system sizes $L$. The brackets denote averaging over $R = 10^5$ independent simulations. The abscissas of the points where curves intercept estimate the percolation thresholds $\hat{p}_c$. Abscissas of the subsequent points are separated by $\Delta p = 10^{-5}$. Unfortunately, each pair of curves intercept in different points. In contrast, the curves representing the dependence $\lambda(p)$ have clearly visible minima (see Fig. 3). The abscissa of this minimum estimates the percolation threshold $\hat{p}_c$. Due to discretization of available values of $p$ with a step $\Delta p$, we can only estimate position of the true minimum, and thus also the true percolation threshold $p_c$, up to the step size $|\hat{p}_c - \Delta p \cdot \hat{p}_c + \Delta p| \geq p_c$. The assumption that the true percolation threshold $p_c$ is uniformly distributed in these intervals increases uncertainty of its estimation as $U(p_c) = 2k\Delta p/\sqrt{3}$. We assume the coverage factor $k = 3$ [28]. The obtained percolation thresholds $\hat{p}_c$ together with their uncertainties are gathered in Table I.

IV. CONCLUSIONS

In this paper we estimated percolation thresholds $\hat{p}_c$ for random site triangular lattice percolation and for neighborhoods containing NN, 2NN, 3NN, 4NN and 5NN. The estimated values of percolation thresholds are collected in Table I. As a triangular lattice with 2NN (3NN, 5NN) neighbors may be mapped onto independent interpenetrated triangular lattices but with $\sqrt{3}$ (2, 3) times larger lattice constant the percolation thresholds $p_c(2NN) = p_c(3NN) = p_c(5NN)$ are exactly equal to $p_c(3NN)$.

We adopted the algorithm by Newman and Ziff [20] and the technique by Bastas et al. [21] to estimate these values.

In the algorithm by Newman and Ziff [20] we replaced the Bernoulli probability distribution function with a Gaussian $\mathcal{B}(n; N, p) \approx \mathcal{G}(n; \mu, \sigma)$ with $\mu = pN$ and $\sigma = \sqrt{p(1-p)N}$. Based on hypothesis of critical exponents universality we simplified the Bastas et al. [21] algorithm by reducing the problem of minimization of a multidimensional function $\Lambda(p, x)$ to a problem of minimization of a single-valued function $\lambda(p)$ by using the fact that one knows the exact value of the critical exponent $x = \beta/\nu = 45/28$ for $P_{\text{max}}$ in two dimensions.

Percolation thresholds for lattices with complex neighborhoods have been very recently successfully applied for many problems on square [5, 29, 30] and cubic [31–36] lattices. We believe that the results presented in this paper can also be applied to practical problems. For instance, the site-bond percolation in square, triangular, and honeycomb lattices [5] may be used to predict the minimal pathogen susceptibility to prevent the propagation of Phytophthora zoospores on Mexican chili plantations. The site percolation threshold for square lattices with complex neighbourhoods [17, 18] is known to give quite good prediction. The $p_c$ values obtained in this work may also be helpful in searching for universal formulas for percolation thresholds in the spirit of recent attempts by Xun and Ziff [13].

[1] D. Stauffer and A. Aharony, *Introduction to Percolation Theory*, 2nd ed. (Taylor and Francis, London, 1994).
[2] J. Wierman, Percolation theory, in *Wiley StatsRef: Statistics Reference Online* (American Cancer Society, 2014) pp. 1–9.
[3] S. R. Broadbent and J. M. Hammersley, *Percolation processes: I. Crystals and mazes*, Mathematical Proceedings of the Cambridge Philosophical Society 53, 629–641 (1957).
[4] J. M. Hammersley, *Percolation processes: II. The connective constant*, Mathematical Proceedings of the Cambridge Philosophical Society 53, 642–645 (1957).
[5] J. E. Ramirez, C. Pajares, M. Martinez, I. R. Rodriguez Fernandez, E. Molina-Gayosso, J. Lozada-Lechuga, and A. Fernandez Tellez, Site-bond percolation solution to preventing the propagation of Phytophthora zoospores on plantations, Physical Review E 101, 032301 (2020).
[6] Q. Zhang, B.-Y. Zhang, B.-H. Guo, Z.-X. Guo, and J. Yu, High-temperature polymer conductors with self-assembled
FIG. 2: Dependencies of $\langle P_{\text{max}}(p; L) \rangle \cdot L^{3/\nu}$ on occupation probability $p$.
FIG. 3: Dependencies of $\langle \lambda (p) \rangle$ on occupation probability $p$. The minima give estimates of the percolation thresholds $\hat{p}_c$. 

[20] M. E. J. Newman and R. M. Ziff, Fast Monte Carlo algorithm for site or bond percolation, Physical Review E 64, 016706 (2001).

[21] N. Bastas, K. Kosmidis, P. Giazitzidis, and M. Maragakis, Method for estimating critical exponents in percolation processes with low sampling, Physical Review E 90, 062101 (2014).

[22] P. Erdős and A. Rényi, On random graphs. I, Publications Mathematicae 6, 290–297 (1959).

[23] P. Erdős and A. Rényi, On the evolution of random graphs, Publications of the Mathematical Institute of the Hungarian Academy of Sciences 5, 17–61 (1960).

[24] E. N. Gilbert, Random graphs, The Annals of Mathematical Statistics 30, 1141–1144 (1959).

[25] V. Privman, Finite-size scaling and numerical simulation of statistical systems, edited by V. Privman (World Scientific, Singapore, 1990) pp. 1–98.

[26] D. P. Landau and K. Binder, A Guide to Monte Carlo Simulations in Statistical Physics, 2nd ed. (Cambridge UP, Cambridge, 2005).

[27] N. Bastas, K. Kosmidis, and P. Argyrakis, Explosive site percolation and finite-size hysteresis, Physical Review E 84, 066112 (2011).

[28] B. N. Taylor and C. E. Kuyatt, Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results, Tech. Rep. (NIST, 1994).

[29] V. Negi and R. C. Picu, Elastic-plastic transition in stochastic heterogeneous materials: Size effect and triaxiality, Mechanics of Materials 120, 26–33 (2018).

[30] L. Keeney, C. Downing, M. Schmidt, M. E. Pemble, V. Nicolosi, and R. W. Whatmore, Direct atomic scale determination of magnetic ion partition in a room temperature multiferroic material, Scientific Reports 7, 1737 (2017).

[31] D. Soto-Gomeze, L. Vazquez Juiz, P. Perez-Rodriguez, J. Eugenio Lopez-Periago, M. Paradela, and J. Koestel,
Percolation theory applied to soil tomography, Geoderma 357, 113959 (2020).

[32] A. Avella, A. M. Oles, and P. Horsch, Defect-induced orbital polarization and collapse of orbital order in doped vanadium perovskites, Physical Review Letters 122, 127206 (2019).

[33] W. W. Erikson, Thermal decomposition of ammonium perchlorate using Monte Carlo methods, Journal of Energetic Materials 37, 222–239 (2019).

[34] B. G. Ueland, N. H. Jo, A. Sapkota, W. Tian, M. Masters, H. Hodovanets, S. S. Downing, C. Schmidt, R. J. McQueeney, S. L. Bud’ko, A. Kreyssig, P. C. Canfield, and A. I. Goldman, Reduction of the ordered magnetic moment and its relationship to Kondo coherence in Ce$_{1-x}$La$_x$Cu$_2$Ge$_2$, Physical Review B 97, 165121 (2018).

[35] J. Jeong, K. J. Park, E.-J. Cho, H.-J. Noh, S. B. Kim, and H.-D. Kim, Electronic structure change of NiS$_{2-x}$Se$_x$ in the metal-insulator transition probed by X-ray absorption spectroscopy, Journal of the Korean Physical Society 72, 111–115 (2018).

[36] T. Moench, P. Friederich, F. Holzmueller, B. Rutkowski, J. Benduhn, T. Strunk, C. Koerner, K. Vandewal, A. Czyrska-Filemonowicz, W. Wenzel, and K. Leo, Influence of meso and nanoscale structure on the properties of highly efficient small molecule solar cells, Advanced Energy Materials 6, 1501280 (2016).