Incorporating variability into an approximation formula for bond percolation thresholds of planar periodic lattices

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(Received 28 July 2006; published 17 January 2007)

Approximation formulas to predict values for bond percolation thresholds of periodic graphs make use of certain features of lattice graphs such as dimension and average degree. We show that a relationship exists between the average and second-moment of the degree of a graph and the average degree of its line graph. Using this relationship together with the well-known bond-to-site transformation between the bond percolation model on a graph and the site percolation model on its line graph, we create a new approximation formula that improves the accuracy of bond percolation threshold predictions.

DOI: 10.1103/PhysRevE.75.011114 PACS number(s): 02.50.Cw, 05.50.+q, 64.60.Ak

I. INTRODUCTION

Bond percolation thresholds are exactly known for only a few lattice graphs [1–4], while much of our knowledge of numerical threshold values has been derived by simulations, e.g., Ref. [5]. To explain the simulation results, considerable research has been devoted to the derivation of approximation formulas which provide predicted percolation threshold values that are close to the true percolation threshold. See, e.g., Ref. [6–18]. These universal formulas, as they have been called, are based on a small number of features of the lattice graph, typically the dimension d and average vertex degree q.

One universal formula worth noting for bond percolation models was suggested by Vyssotsky, Gordon, Frish, and Hammersley (VGFH) [19], who studied bond percolation on eight regular two- and three-dimensional lattice graphs. Their universal formula

$$\tilde{p}_c = \frac{d}{(d-1)q}$$

is based on dimension and average vertex degree, so the predicted percolation threshold $\tilde{p}_c$ is the same for different lattice graphs if d and q are the same.

Galam and Mauger [8,9] provided the power law formula

$$\tilde{p}_c = p_0[(d-1)(q-1)]^{-a}d^b, \tag{1}$$

which we denote by GM-pl. With different values of the parameters p_0, a, and b, it approximates both bond and site percolation thresholds. The parameter values were determined by a fit to exactly known or precisely estimated percolation threshold values for several lattices, which were classified into three "universality classes." One of these classes included the two-dimensional square, triangular, hexagonal, and dice lattices, for which $p_0=0.6558$ and $a=b=0.6897$ for bond models. For the kagomé lattice and the other regular lattices with $3\leq d\leq 7$ they considered, $p_0=0.7541$ and $a=b=0.9346$ for bond percolation. (A third class, which we will not consider here, consisted of lattices in eight or more dimensions.)

One motivation for our investigation is the fact that several lattice graphs with the same dimension and average degree nevertheless have a relatively wide range of bond percolation threshold values. This suggests that there may be another feature of the lattice graph, in addition to dimension and average degree, that affects the value of the percolation threshold. Some previous research suggests that variability of the vertex degree may play a role [20,21], although the appropriate measure of variability is not obvious.

The remainder of this paper is organized as follows. Section II provides several items of background information about percolation thresholds and universal formulas. In Sec. III, we derive a formula for the average degree of a line graph in terms of the average degree and second moment of the degree of the underlying graph. In Sec. IV, we introduce an approximation formula which incorporates variability into a bond percolation threshold universal formula. Our formula uses the second moment of the vertex degree, which essentially uses the variance as the measure of variability. The use of the second moment is justified by the bond-to-site transformation, by showing that if site threshold formulas are a function of the average degree, then bond threshold formulas should be a function of the second moment of the degree. We also compare the accuracy of our formula to that of the VGFH and GM-pl formulas, and evaluate it on the basis of criteria developed by Wierman and Naor [22]. Concluding remarks and directions for further research are discussed in Sec. V.

II. BACKGROUND

A. Periodic planar lattice graphs

We will consider only percolation models defined on infinite planar two-dimensional graphs that are periodic according to the definition of Kesten [2]. To summarize briefly, a periodic graph has finitely many edges incident to each vertex, is connected, contains no loops, and may be imbedded in R^2 in such a way that each coordinate vector is a period for the image and every compact set of R^2 intersects only finitely many edges. A planar graph may be imbedded in the plane with no intersections of edges except at their endpoints. We restrict to two-dimensions, since all exact bond threshold solutions and the majority of simulation estimates for bond models are for two-dimenional lattices.

B. Evaluation criteria

Wierman and Naor [22] proposed that universal formulas should satisfy certain "desirable" properties so that the for-

mulas are consistent with properties that are proved to be true for percolation models. Briefly stated, bond percolation universal formulas should be unambiguously defined, be a function of graph parameters that are easily computed, take only values between zero and one, be as accurate as possible, and be consistent with the duality relationship, containment principle, contraction principle, and subdivision of edges. Wierman and Naor [22] illustrate the use of the criteria in the evaluation of two bond threshold formulas and two site threshold formulas. No existing formula satisfies or performs well on all of the criteria.

C. Incorporating duality

Wierman, Naor, and Cheng [23] introduced a technique for incorporating the matching property into a universal formula for site percolation thresholds. The technique can be adapted to incorporate duality into a bond percolation threshold approximation formula. Consider a planar graph G, and denote its dual graph by $D(G)$. From any bond threshold approximation formula for planar graphs $f(\cdot)$, we can define a parametrized family of universal formulas $g_a(\cdot)$ by

$$g_a(G) = \frac{f(G)^a}{f(G)^a + f[D(G)]^a}.$$

The modified formulas $g_a(\cdot)$, will each satisfy the duality property

$$g_a(G) + g_a[D(G)] = 1,$$

while other desirable properties of the original formula $f(\cdot)$ are preserved. We can optimize over the parameter a by choosing the value a^* which minimizes the average error for a set of lattices for which there are percolation threshold exact values or reliable estimates. In the application to site models, the modified formula was considerably more accurate than the original formula. We will apply this modification technique in the development of our bond threshold formula.

D. Bond-to-site transformation

From any lattice graph G, we may construct a new graph $L(G)$, called the "line graph" or "covering graph," by placing a vertex of $L(G)$ on each edge of G, and placing an edge between two vertices of $L(G)$ if the corresponding edges the corresponding vertices represent are adjacent in G.

By the well-known bond-to-site transformation [24], a bond percolation model on a graph G is equivalent to the site percolation model on its line graph $L(G)$. Thus, the bond percolation threshold of G is equal to the site percolation threshold of $L(G)$, i.e.,

$$p_c(G_{\text{bond}}) = p_c[L(G)_{\text{site}}].$$

Ideally, bond and site threshold universal formulas should be consistent with this relationship. Since most site percolation universal formulas are functions of the average vertex degree of the graph, to obtain consistency, a bond percolation universal formula for a lattice graph should depend on the average degree of its line graph. For this reason, in the next section we derive an expression for the average degree of the line graph in terms of characteristics of the original graph. For consistency with the bond-to-site transformation, a bond percolation formula should depend on these characteristics.

III. THE AVERAGE DEGREE OF A LINE GRAPH

We now derive a formula for the average degree of a line graph $L(G)$ in terms of the degrees of vertices in the underlying graph G. Note that in the remainder of this paper we use d to denote degree rather than dimension. Note also that the following derivation applies to a finite graph, but can be extended to an infinite periodic graph by considering the limit as a rectangular region is expanded.

Note that every vertex z in $L(G)$ corresponds to an edge in G with two end vertices, say u_z and v_z. Since z is connected to the vertices of $L(G)$ corresponding to all the other edges incident to u_z and v_z, the vertex degree $d(z)$ of every $z \in L$ is

$$d(z) = [d(u_z) - 1] + [d(v_z) - 1] = d(u_z) + d(v_z) - 2.$$

Thus, $q(L)$, the average degree of the line graph $L(G)$, is

$$q(L) = \frac{\sum_{z \in L(G)} d(z)}{|\mathcal{V}[L(G)]|} = \frac{\sum_{z \in L(G)} [d(u_z) + d(v_z) - 2]}{|\mathcal{V}[L(G)]|},$$

where $|\mathcal{V}[L(G)]|$ denotes the number of vertices in $L(G)$.

We wish to express this summation in terms of the degrees of vertices in G. First, by construction of the line graph, the number of vertices in $L(G)$ is equal to the number of edges in G, denoted by $|\mathcal{E}(G)|$. Secondly, since there are $d(v)$ edges incident to each vertex $v \in G$, then the term $d(v)$ appears in the sum above $d(v)$ times. Therefore,

$$q(L) = \frac{\sum_{v \in G} d(v)^2 - 2|\mathcal{E}(G)|}{|\mathcal{E}(G)|} = \frac{2\sum_{v \in G} d(v)^2/|\mathcal{V}(G)|}{2|\mathcal{E}(G)|/|\mathcal{V}(G)|} - 2.$$

Since each edge has two endpoints, we recognize the denominator in this expression as the average degree of G, $E[d]$. The numerator is the average squared degree, or second moment of the degree, $E[d^2]$. Thus, we obtain the formula

$$q(L) = 2\left(\frac{E[d^2]}{E[d]} - 1\right).$$

We have shown that the average degree of a line graph $L(G)$ is a function of the first and second moments of the vertex degree of G. By the standard identity $\text{Var}(d) = E[d^2] - E[d]^2$, it is a function of the mean and variance of the degree of G.

IV. A BOND MODEL APPROXIMATION FORMULA INCORPORATING VARIABILITY

A. The formula

To interpret the result of the previous section in terms of universal formulas, we may state that if site model formulas

use average vertex degree, then second moment or variance of degree must be a factor in bond model formulas. However, the authors are not aware of any bond model universal formula that incorporates the vertex degree variance or second moment.

Note that the expression derived for $q(L)$ includes the ratio $E[d^2]/E[d]$. For a regular lattice, i.e., a lattice with uniform degree, this ratio is equal to the average degree. If the lattice has variability in the degree of its vertices, then this ratio is greater than the average degree. From this observation, a simple way to incorporate variability into a bond percolation universal formula is to start with an existing formula based on average degree and substitute the ratio for the average degree. If this approach is used to modify the VGFH formula, we obtain

$$\frac{2}{\left(\frac{E[d^2]}{E[d]}\right)}.$$

However, this formula does not satisfy the duality property for planar lattices. (Consider the kagomé and dice lattices, for example.) The formula may be modified as described in Sec. II C to incorporate duality, then simplified algebraically. The optimum value of the exponent was numerically determined to be 0.9145. (Note that a minimum average error rounding to 0.0040 was obtained for the interval of values $0.9097 \leq a \leq 0.9160$.) As a result, we propose a new bond percolation approximation formula, denoted WNS, given by

$$\tilde{p}_c(G) = \frac{\left(\frac{E[d^2_{D(G)}]}{E[d_{D(G)}]}\right)^{0.9145}}{\left(\frac{E[d^2_G]}{E[d_G]}\right)^{0.9145} + \left(\frac{E[d^2_{D(G)}]}{E[d_{D(G)}]}\right)^{0.9145}},$$

where the subscript on d indicates the lattice graph considered.

B. Evaluation and comparison with the VGFH and GM-pl formulas

Table I shows evaluations of the WNS, VGFH, and GM-pl formulas on planar periodic graphs using the Wierman-Naor criteria. Note that, for this class of graphs, the WNS formula satisfies exactly the same theoretical criteria as the VGFH formula. It is important to point out, however, that because of the planarity restriction, the WNS formula is undefined for any graph of dimension greater than 2. On the other hand, the VGFH and GM-pl formulas do not require planarity, so they apply to a much wider class of lattice graphs than the WNS formula.

However, the WNS formula has a considerable advantage in accuracy for the class of planar periodic graphs, where it performs substantially better than either the VGFH or the GM-pl formula. The accuracy evaluation in Table I is based on data from Table II, which shows values for percolation threshold estimates using WNS, VGFH, and GM-pl, and compares them with exact and simulated values for the threshold for 21 lattices.

TABLE I. A comparison of the WNS, VGFH, and GM-pl bond threshold approximation formulas according to the Wierman-Naor criteria.

Property	WNS	VGFH	GM-pl
Well-defined	Yes	Yes	No
Computable	Yes	Yes	Partly
Values in $[0,1]$	Yes	Yes	No
Adjacency	Yes	Yes	Partly
Accuracy (maximum)	0.0109	0.0737	0.0607
	Excellent	Fair	Fair
Accuracy (mean)	0.0040	0.0235	0.0147
	Excellent	Good	Good
Accuracy (median)	0.0019	0.0196	0.0093
	Excellent	Good	Excellent
Duality	Yes	Yes	Fair
Containment	No	No	No
Contraction	No	No	No
Subdivision	No	No	No

Note that the WNS formula has smaller or equal errors than the VGFH formula for all 21 lattice graphs, and smaller errors than the GM-pl formula for all but one of the 21 lattices. The WNS formula significantly reduces the maximum error to 0.0109, from 0.0737 for the VGFH formula and 0.0607 for the GM-pl formula. The mean error is reduced by 83% from 0.0235 for VGFH and 73% from 0.0147 for GM-pl. Median error is reduced comparably by the WNS formula, to 0.0019 from 0.0196 with VGFH and 0.0093 with GM-pl.

The WNS formula improves accuracy by distinguishing between lattices that have the same average degree. For example, the $(3,12^2)$, $(4,6,12)$, $(4,8^2)$, and hexagonal lattices all have average degree 3—in fact, all vertices of these lattices have degree three. Thus, the VGFH formula gives the same estimate 0.6666… for the bond percolation threshold of all four lattices. Even though the second moment of the degree of all these lattices are identical, equal to 9, the fact that their dual lattices have second moments ranging from 36 to 54 causes their WNS bond percolation threshold estimates to range from 0.6527 to 0.7320. Similar distinguishing between lattices occurs for the lattices of average degree $\frac{10}{3}$, 4, 5, and 6.

V. CONCLUDING REMARKS

We have proposed a bond percolation threshold approximation formula for planar lattices, derived using mathematical principles. We derived a formula for the average degree of a line graph in terms of the average degree and second moment of the degree of its underlying graph. To be consistent with the bond-to-site transformation, this implies that if average degree is a factor in predicting site percolation thresholds, then the second moment of the degree or, equivalently, the variance of the degree, is a factor in predicting bond percolation thresholds. To be consistent with the duality

TABLE II. Estimates of bond model threshold values for 21 lattices using the WNS and VGFH universal formulas. The percolation threshold values given are exact values proved for the square lattice by Kesten [1], the triangular and hexagonal lattices by Wierman [3], the bowtie lattice and its dual lattice by Wierman [4], rounded to four decimal places. The values for the kagomé and dice lattices are from simulations by Ziff and Suding [25]. The values for all other lattices are from simulations by Parviainen [5]. Parviainen's values for the Kagomé and $(3,12^2)$ lattices agree with the predictions of Scullard and Ziff [26].

Lattice	$E[d]$	$E[d^2]$	Value	WNS	WNS error	VGFH	VGFH error	GM-pl	GM-pl error
$(3,12^2)$	3	9	0.7404	0.7320	0.0084	0.6667	0.0737	0.7541^2	0.0137
$(4,6,12)$	3	9	0.6937	0.6937	0.0000	0.6667	0.0270	0.6558^1	0.0379
$(4,8^2)$	3	9	0.6768	0.6749	0.0019	0.6667	0.0101	0.6558^1	0.0210
Hexagonal	3	9	0.6527	0.6534	0.0007	0.6667	0.0140	0.6558^1	0.0031
D(Bowtie)	3.3333	11.3333	0.5955	0.5959	0.0004	0.6000	0.0045	0.5897^1	0.0058
$D(3^2,4,3,4)$	3.3333	11.3333	0.5859	0.5873	0.0014	0.6000	0.0141	0.5897^1	0.0038
$D(3^3,4^2)$	3.3333	11.3333	0.5804	0.5873	0.0069	0.6000	0.0196	0.5897^1	0.0093
$D(3^4,6)$	3.3333	12	0.5657	0.5745	0.0088	0.6000	0.0343	0.5897^1	0.0240
Kagomé	4	16	0.5244	0.5269	0.0025	0.5000	0.0250	0.5162^2	0.0082
$(3,4,6,4)$	4	16	0.5248	0.5139	0.0109	0.5000	0.0248	0.5162^2	0.0086
Square	4	16	0.5000	0.5000	0.0000	0.5000	0.0000	0.4958^1	0.0042
$D(3,4,6,4)$	4	17	0.4752	0.4861	0.0109	0.5000	0.0248	0.4958^1	0.0206
Dice	4	18	0.4756	0.4731	0.0025	0.5000	0.0250	0.4958^1	0.0202
$(3^4,6)$	5	25	0.4343	0.4255	0.0088	0.4000	0.0343	0.4066^1	0.0277
$(3^3,4^2)$	5	25	0.4196	0.4127	0.0069	0.4000	0.0196	0.4066^1	0.0310
$(3^2,4,3,4)$	5	25	0.4141	0.4127	0.0014	0.4000	0.0141	0.4066^1	0.0075
Bowtie	5	26	0.4045	0.4041	0.0004	0.4000	0.0045	0.4066^1	0.0021
Triangular	6	36	0.3473	0.3466	0.0007	0.3333	0.0140	0.3486^1	0.0013
$D(4,8^2)$	6	40	0.3232	0.3251	0.0019	0.3333	0.0101	0.3203^2	0.0029
$D(4,6,12)$	6	44	0.3063	0.3063	0.0000	0.3333	0.0270	0.3203^2	0.0140
$D(3,12^2)$	6	54	0.2596	0.2680	0.0084	0.3333	0.0737	0.3203^2	0.0607

property for bond percolation thresholds of planar graphs, we use a technique to produce an estimator consistent with duality from one that is not. The resulting comparison of values estimated by our formula with exact or accurate simulated values shows that the combination of duality and second moment of vertex degree is valuable in improving the accuracy of bond percolation approximation formulas for planar lattices.

Further research, in progress, is applying similar techniques to predict site percolation model thresholds. Current site model universal formulas are typically based on average degree, and thus do not distinguish between lattices with the same average degree. Preliminary results indicate that incorporating variance into site model universal formulas will lead to improved performance. Another direction of research in progress is incorporating variability into universal formulas for percolation thresholds in higher dimensions, where the duality and matching techniques cannot be used.

ACKNOWLEDGMENT

This research was supported by the Acheson J. Duncan Fund for the Advancement of Research in Statistics.

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