Improved site percolation threshold universal formula for two-dimensional matching lattices

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(Received 31 August 2005; published 14 December 2005)

A universal formula is proposed for predicting the site percolation threshold of two-dimensional matching lattices. The formula is slightly more accurate for these lattices than the formulas of Galam and Mauger, based on a comparison over a class of 38 lattices, and does not require two universality classes for two-dimensional lattices. The formula is constructed from the Galam-Mauger square root formula for site thresholds, by a modification which makes it consistent with the theoretical relationship between percolation thresholds of matching pairs of lattices. In the framework for evaluation of universal formulas introduced by Wierman and Naor, the formula is currently the best performing universal formula for site thresholds on this class of lattices.

DOI: 10.1103/PhysRevE.72.066116 PACS number(s): 02.50.Cw, 05.50.+q, 64.60.Ak

I. INTRODUCTION AND HISTORY

A challenge since the introduction of percolation theory has been to find a universal approximation formula, based on a small number of features of the underlying lattice, for accurately predicting the values of the percolation threshold for all lattice graphs. Site percolation universal formulas based on dimension and average coordination number have been proposed by Sahimi, Hughes, Scriven, and Davis [1] and Galam and Mauger [2–5]. Other researchers have developed universal formulas or prediction procedures for the percolation threshold based on a minimal spanning tree approach [6–8], lattice Green functions [1], filling factor [9], and preferred directions for cluster formation [10].

Recent studies have shown that the existing percolation threshold universal formulas must necessarily have large errors for some lattice graphs [11] and that it is not sufficient to base a universal formula only on dimension and average degree [12]. Universal formulas were only evaluated on an *ad hoc* basis until an evaluation framework was introduced by Wierman and Naor [13].

This article uses the evaluation framework from [13] as a tool for improving a site percolation threshold universal formula for two-dimensional lattices. Section II summarizes the evaluation criteria. Section III describes a method for modifying a universal formula that does not satisfy one of the criteria, "consistency with the matching property," to obtain a formula which does satisfy the property. In Sec. IV, this modification technique is applied to a universal formula introduced by Galam and Mauger to find a site percolation universal formula. This formula is shown to outperform the Galam-Mauger power law universal formula for two-dimensional lattices. Concluding remarks are provided in Sec. V.

II. EVALUATION CRITERIA

Wierman and Naor [13] introduced a framework for evaluation of universal formulas, giving several properties that should be satisfied by an ideal universal formula. The ideal site percolation threshold universal formula will (1) be well defined, (2) be easily computable, (3) provide values only between 0 and 1, (4) depend only on the adjacency structure of the lattice, (5) be accurate, (6) be consistent with the matching relationship, and (7) be consistent with the containment principle.

The first four properties are necessary for any reasonable formula. Accuracy of predictions is perhaps the single most important property. The last two properties ask that certain theoretical properties that have been proved for percolation thresholds hold for the predictive formulas. The concept of matching graphs was introduced by Sykes and Essam [14], and Kesten [15] proved (under rather general conditions) that the site percolation thresholds of a pair of matching graphs sum to one. The containment principle states that if one lattice is contained in a second lattice, then its percolation threshold is greater than or equal to that of the second lattice. See [13] for further discussion of the properties and the evaluation framework.

III. THE MODIFICATION TECHNIQUE

We now show a simple technique for modifying a universal formula, which is not consistent with the matching property to create a formula that is consistent with the matching property. In the following, we denote the matching graph of a graph G by G^*. Consider a universal formula $f(\cdot)$, which applies to any pair of matching lattices. We can then define a parametrized family of universal formulas $g_a(\cdot)$ by

$$g_a(G) = \frac{f(G)^a}{f(G)^a + f(G^*)^a}$$

for $a>0$. Since $(G^*)^*=G$, we have

$$g_a(G^*) = \frac{f(G^*)^a}{f(G^*)^a + f(G)^a},$$

so

$$g_a(G) + g_a(G^*) = 1.$$

Thus, all formulas in this parameterized family are consistent with the matching property.

When applying the modification technique, if the original formula f satisfies properties (1), (2), (3), and (4), then each

modified formula g_a will satisfy these properties as well.

Given a collection of lattices that have accurate percolation threshold estimates, one may solve for the value of the parameter a that minimizes some optimality criterion, such as the mean absolute error or the mean squared error between the g_a formula values and the percolation threshold estimates for the lattices.

IV. THE PROPOSED FORMULA

Let q denote the average degree of the lattice G, and q^* denote the average degree of its matching lattice. The improved universal formula of this article was derived from the Galam and Mauger [2,3] square root formula

$$f(G) = \frac{1}{\sqrt{q-1}},$$

which, with $a=1$, produces

$$g(G) = \frac{\sqrt{q^*-1}}{\sqrt{q^*-1}+\sqrt{q-1}}$$

after simplification.

We carried out the optimization using the collection of 38 lattices and their site threshold estimates given in Table I. Using either the mean absolute error or the mean squared error as optimality criteria, the optimizing value of the parameter a is very near, but slightly greater than one. The value of the optimality criterion for $a=1$ is only slightly higher than for the optimal value. Since additions to the collection of lattices or slight modifications of the site percolation threshold estimates would result in changes in the optimal value of a, and for simplicity, we have chosen to use $a=1$ in the modified universal formula.

Recall that properties (1)–(4) are not affected by the application of the modification technique. Since the original formula satisfies properties (1), (2), (3), and (4), the modified formula will satisfy these properties still, but also property (6), as intended.

In addition to the properties proved above, this formula has another advantage. It does not require two different universality classes to handle the two-dimensional lattices. The Galam-Mauger power law formula used two universality classes for two-dimensional lattices, with the classes determined empirically rather than defined as a function of properties of the lattice. The proposed formula apparently explains the behavior of the site percolation threshold of two-dimensional lattices as accurately without the need for universality classes.

A. Accuracy

We now evaluate the accuracy of this universal formula using the 38 lattices considered in Table I, which were also used to determine the optimal value of a. These are essentially all percolation threshold exact values, nearly-exact bounds, or estimates that have appeared explicitly or implicitly in the literature. Most of these lattice graphs are Archimedean lattices [16] or related lattices. The others are related to the bowtie lattice [17], denoted B.

Archimedean lattices are vertex-transitive graphs with a planar representation that is a tiling of the plane by regular polygons. (A vertex-transitive graph is one in which all vertices are equivalent, i.e., for any pair of vertices, there is a graph isomorphism that maps one into the other.) There are exactly 11 Archimedean lattices [16]. We denote each Archimedean lattice by a sequence of integers $(n_1, n_2, \ldots, n_k)$ for some k, where the n_i denote the number of sides of successive faces as one moves around a single vertex. (For conciseness, an exponent is used to indicate a number of successive faces of the same size.) Several authors—d'Iribarne, Rasigni, and Rasigni [8], van der Marck [18], Suding and Ziff [19], Ruskin and Cadilhe [20], and Wierman [21,22]—have considered various percolation models on Archimedean lattices. The exact site percolation thresholds are known for three of the Archimdean lattices: the triangular, Kagomé, and $(3,12^2)$. (See [15,23,24].) Suding and Ziff [19] estimated site percolation thresholds of all the Archimedean lattices.

The 38 lattices are listed in Table I. Galam and Mauger [4,5] and van der Marck [18] provided tables of values containing bond percolation thresholds of most Archimedean lattices and site and bond percolation thresholds of a few additional lattices. Exact bond percolation thresholds are known for the square, triangular, and hexagonal lattices, and for the bowtie lattice and its dual lattice [17,23,25]. The bowtie lattice is denoted by B. $D(G)$ denotes the dual graph of lattice graph G. The bond percolation thresholds of a dual pair of lattices sum to one. $L(G)$ denotes the line graph (or covering graph) of the lattice graph G. By the bond-to-site transformation, the bond percolation threshold of a lattice G is equal to the site percolation threshold of $L(G)$. $M(G)$ denotes the matching graph of the lattice graph G. The site percolation thresholds of a matching pair of lattices sum to one.

All values in Table I are rounded to four decimal places. In the column of actual values, values with no superscript are simulation estimates from Suding and Ziff [19]. Superscript e denotes an exact value, b denotes the average of nearly-exact upper and lower bounds, m is obtained by the matching property, v denotes a simulation estimate from van der Marcke [18], p denotes a simulation estimate from Parviainen ([26], part IV, p. 5), and d denotes a value obtained by duality of bond models and then the bond-to-site transformation.

The column labelled GM-pl provides values of the Galam-Mauger power law universal formula, which uses different formulas for two universality classes of two-dimensional lattices. In the GM-pl column, the superscript indicates the class formula which provides the closest estimate to the actual value.

B. Accuracy comparison with Galam and Mauger power law formula

We evaluate the accuracy of the formulas using three measures. The maximum error of our formula is 0.0495,

TABLE I. Comparison of values predicted by the proposed formula and the Galam and Mauger power law formula. See Sec. IV A, paragraphs 2 and 3, for an explanation of the notation for lattice names.

Lattice	q	q^*	Actual	New	Error	GM-pl	Error
$(3,12^2)$	3	21	0.8079^e	0.7597	0.0482	0.8396^2	0.0317
(4, 6, 12)	3	16	0.7478	0.7325	0.0153	0.6926^1	0.0552
$(4,8^2)$	3	14	0.7297	0.7183	0.0114	0.6926^1	0.0371
(6^3)	3	12	0.6970	0.7011	0.0041	0.6926^1	0.0044
$D(3^3,4^2)$	$\frac{10}{3}$	10	0.6471^v	0.6626	0.0155	0.6552^1	0.0081
$D(B)$	$\frac{10}{3}$	$\frac{32}{3}$	0.6653^v	0.6706	0.0053	0.6552^1	0.0101
$L(3,12^2)$	4	16	0.7405^b	0.6910	0.0495	0.6540^2	0.0865
$L(4,8^2)$	4	$\frac{34}{3}$	0.6768^p	0.6499	0.0269	0.6540^2	0.0228
(3,4,6,4)	4	9	0.6218	0.6202	0.0016	0.5985^1	0.0233
(3,6,3,6)	4	10	0.6527^e	0.6340	0.0187	0.6540^2	0.0013
$D(3,6,3,6)$	4	8	0.5848^v	0.6044	0.0196	0.5985^1	0.0137
(4^4)	4	8	0.5927	0.6044	0.0117	0.5985^1	0.0058
$L[D(B)]$	$\frac{24}{5}$	$\frac{42}{5}$	0.5955	0.5825	0.0130	0.5847^1	0.0108
$(3^4,6)$	5	8	0.5795	0.5695	0.0100	0.5478^2	0.0317
$(3^2,4,3,4)$	5	7	0.5508	0.5505	0.0003	0.5478^2	0.0030
$(3^3,4^2)$	5	7	0.5502	0.5505	0.0003	0.5478^2	0.0024
B	5	7	0.5475^v	0.5505	0.0030	0.5478^1	0.0003
(3^6)	6	6	0.5000^e	0.5000	0.0000	0.4979^1	0.0021
$D(4,6,12)$	6	6	0.5000^e	0.5000	0.0000	0.4979^1	0.0021
$D(4,8^2)$	6	6	0.5000^e	0.5000	0.0000	0.4979^1	0.0021
$D(3,12^2)$	6	6	0.5000^e	0.5000	0.0000	0.4979^1	0.0021
$M(B)$	7	5	0.4525^m	0.4495	0.0030	0.4663^1	0.0138
$M(3^3,4^2)$	7	5	0.4498^m	0.4495	0.0003	0.4663^1	0.0165
$M(3^2,4,3,4)$	7	5	0.4492^m	0.4495	0.0003	0.4663^1	0.0171
$M(4^4)$	8	4	0.4073^m	0.3956	0.0117	0.3881^2	0.0192
$L(B)$	$\frac{42}{5}$	$\frac{24}{5}$	0.4045	0.4175	0.0130	0.4324^1	0.0295
$M[D(B)]$	$\frac{32}{3}$	$\frac{10}{3}$	0.3347^m	0.3294	0.0053	0.3669^2	0.0322
$M[D(3,6,3,6)]$	8	4	0.4152^m	0.3956	0.0196	0.4204^1	0.0052
$M(3^4,6)$	8	5	0.4205^m	0.4305	0.0100	0.4029^1	0.0176
$M(3,6,3,6)$	10	4	0.3473^e	0.3660	0.0187	0.3324^2	0.0149
$M[D(3^3,4^2)]$	10	$\frac{10}{3}$	0.3529^m	0.3374	0.0155	0.3324^2	0.0205
$M(3,4,6,4)$	9	4	0.3782^m	0.3798	0.0016	0.3879^1	0.0097
$L[D(4,8^2)]$	$\frac{34}{3}$	4	0.3232^m	0.3501	0.0269	0.3053^2	0.0179
$M(6^3)$	12	3	0.3030^m	0.2989	0.0041	0.2938^2	0.0092
$M(4,8^2)$	14	3	0.2703^m	0.2817	0.0114	0.2650^2	0.0053
$L[D(3,12^2)]$	16	4	0.2595^d	0.3090	0.0495	0.2427^2	0.0168
$M(4,6,12)$	16	3	0.2522^m	0.2675	0.0153	0.2427^2	0.0095
$M(3,12^2)$	21	3	0.1921^m	0.2403	0.0482	0.2033^2	0.0112

which is considerably smaller than the 0.0865 maximum of the GM-pl formula. The mean error of our formula is somewhat smaller than that of the GM-pl formula: 0.0134 and 0.0164, respectively. The values for the median have a similar relationship: 0.0114 for our formula and 0.0124 for the GM-pl formula. Using the rating scale of Wierman and Naor [13], all these accuracy measures are in the Good range, except for the maximum error of the GM-pl formula which is rated Fair.

V. SUMMARY AND CONCLUSIONS

This paper provides an example of the use of evaluation criteria for percolation threshold universal formulas to develop an improved formula. The Galam-Mauger square root formula is modified to create a family of possible universal formulas that continue to satisfy the criteria it previously did, but are also consistent with the matching property. An optimization procedure can then be applied to select a formula

TABLE II. Summary of evaluations of site threshold universal formulas according to the Wierman-Naor criteria.

Property	New	GM-pl
Well-defined	Yes	No
Computable	Yes	Partly
Values in [0,1]	Yes	No
Adjacency	Yes	Partly
Accuracy (maximum)	Good	Fair
Accuracy (mean)	Good	Good
Accuracy (median)	Good	Good
Matching	Yes	Fair
Containment	No	No

from the family to achieve the best fit to percolation threshold estimates. Although this modification was not designed to improve the accuracy of the formula, in this case the accuracy became significantly better. This formula satisfies all the desirable properties in the Wierman and Naor [13] evaluation framework except consistency with containment, and arguably has slightly better accuracy than the Galam-Mauger power law universal formula, without the need for universality classes. (See Table II for a comparison of the two formulas.) A disadvantage of the formula is that it is valid only for a class of two-dimensional lattices—there is no concept of matching lattice in higher dimensions.

In future research on universal formulas, we hope to use the evaluation framework to systematically improve bond percolation threshold formulas. A similar approach to this paper can be applied to existing formulas that do not satisfy the duality property. A more difficult task is to develop an approach for developing formulas that satisfy the containment property. We also hope to incorporate information on the variability of degrees in the graph, as there is some evidence that degree variability explains some of the percolation threshold variability for lattices that have equal average degrees.

ACKNOWLEDGMENTS

The first author gratefully acknowledges sabbatical support from the American Society of Engineering Education and the U. S. Naval Surface Warfare Center. All authors gratefully acknowledge financial support from the Johns Hopkins University's Acheson J. Duncan Fund for the Advancement of Research in Statistics.

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