Accuracy of universal formulas for percolation thresholds based on dimension and coordination number

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Recent mathematical results regarding percolation thresholds are relevant to efforts to find universal formulas for the percolation threshold. This Brief Report uses exact solutions and recent rigorous bounds for site and bond percolation thresholds to demonstrate that any universal formula based on only the dimension and the coordination number must provide estimates differing substantially from the true threshold value for some lattices.

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I. INTRODUCTION AND HISTORY

Since the early development of percolation theory, there have been efforts to find a universal formula, based on a small number of features of the underlying lattice, for predicting the values of the percolation threshold for all lattice graphs. For example, Vyssotsky, Gordon, Frisch, and Hammersley [1] studied bond percolation on eight regular two- and three-dimensional lattices, commented that "p_c appears to be little affected by differences of lattice type if the number of dimensions and coordination number are the same," and mentioned the approximation

$$p_c = \frac{d}{(d-1)q}, \tag{1}$$

where d is the dimension of the lattice and q is the coordination number (or vertex degree) of the lattice.

For site percolation, the formula

$$p_c = \frac{d}{(d-1)(q-1)} \tag{2}$$

was proposed by Sahimi *et al.* [2] for $d \geqslant 3$. An alternative formula for site models,

$$p_c = \frac{1}{\sqrt{q-1}}, \tag{3}$$

proposed by Galam and Mauger [3,4] obtained good results in two dimensions, but not for higher dimensions.

Galam and Mauger [5,6] provided excellent estimates for several lattices using the power law formula

$$p_c = p_0[(d-1)(q-1)]^{-a} d^b, \tag{4}$$

where the parameters p_0, a, and b were determined by a fit to known percolation threshold values. The lattices studied were classified into three universality classes. For the two classes of lattices with dimensions $d \leqslant 7$, $b=0$ for site percolation and $b=a$ for bond percolation. One of these classes includes the two-dimensional square, triangular, hexagonal, and dice lattices, for which $p_0=0.8889$ and $a=0.3601$ for site models and $p_0=0.6558$ and $a=0.6897$ for bond models. The other class includes the Kagomé lattice and other lattices with $3 \leqslant d \leqslant 7$, for which $p_0=1.2868$ and $a=0.6160$ for site percolation and $p_0=0.7541$ and $a=0.9346$ for bond percolation. For the lattices considered in [5], the maximum deviation of the formula from numerical estimates is ± 0.008. However, the universality classes are not precisely defined in terms of properties of the lattice graphs, so it may be unclear which class a new lattice belongs to.

In [6], Galam and Mauger extended their formula to nonregular lattices (i.e., those that do not have a single coordination number for all vertices), via the use of an effective parameter q_{eff} to replace the average coordination number q. They suggest that their formula has predicting ability for percolation thresholds which have not yet been computed: For example, if the site threshold of a lattice has been estimated, q_{eff} can be computed from the formula for site thresholds, and can be used to predict the bond threshold from the formula for bond thresholds.

Although the formulas of Galam and Mauger are in extremely good agreement with simulation estimates for the lattices studied, some numerical discrepancies have been noted in the past. Van der Marck [7] noted that, if there is to be a universal formula for percolation thresholds, it needs to be based on more information than d and q only. As examples, he provides two three-dimensional lattices with $d=3$ and $q=8$, the body centered cubic lattice and the stacked triangular lattice. Their site percolation threshold estimates are 0.246 and 0.2623 respectively, with bond percolation estimates of 0.1803 and 0.1859, respectively. Babalievski [8] investigated and confirmed a discrepancy of 0.020 in the estimate for the value of the bond percolation threshold of the ferrovariant of the dodecagonal lattice.

Researchers have considered other means of developing universal formulas for the percolation threshold, based on a minimal spanning tree approach [9–11], lattice Green functions [2], filling factors [12], and preferred directions for cluster formation [13].

II. DIMENSION AND COORDINATION NUMBER

Recent mathematical analysis of percolation on Archimedean lattices shows that percolation threshold approximation formulas based only on dimension and coordination number must necessarily have large errors for some graphs. 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 which maps one into the other.) There are exactly 11 Archimedean lattices [14]. 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 [11], van der Marck [15], Suding and Ziff [16], Ruskin and Cadilhe [17], and Wierman [18,19]—have considered various percolation models on Archimedean lattices.

We first discuss why there must be substantial errors when predicting bond percolation thresholds based only on dimension and coordination number. Four of the 11 Archimedean lattices are regular graphs with coordination number $q=3$. The exact bond percolation threshold for the (3^6) lattice, called ''hexagonal'' or ''honeycomb,'' is $1-2\sin(\pi/18)=0.6527\ldots$. This value was derived by Sykes and Essam [20] and proved by Wierman [21]. Wierman [19] used the substitution method to determine the following rigorous bounds for the bond percolation threshold for three Archimedean lattices:

$$0.7385<p_c[(3,12^2)\text{ bond}]<0.7449, \tag{5}$$

$$0.6430<p_c[(4,6,12)\text{bond}]<0.7376, \tag{6}$$

$$0.6281<p_c[(4,8^2)\text{ bond}]<0.7201. \tag{7}$$

Thus, among the Archimedean lattices with $d=2$ and $q=3$, the bond percolation thresholds can have a difference of at least 0.0858.

Furthermore, Wierman [22] constructed a sequence of planar periodic fully triangulated graphs with bond percolation thresholds converging to zero. Since the bond percolation thresholds of dual lattices add to 1, the sequence of dual lattices of these fully-triangulated lattices has percolation thresholds converging to 1. However, the dual of a fully triangulated lattice is a regular lattice with coordination number $q=3$. Therefore, bond percolation thresholds of lattices with $d=2$ and $q=3$ range between 0.6527 and 1, an interval of length 0.3473. Consequently, any bond percolation threshold estimate from any universal formula based on only the dimension and the coordination number must differ from the true threshold by at least half the length of this interval, 0.1736, for at least one lattice.

For site models, the discrepancy in predictions that can currently be proved mathematically is not as large as for bond models. For the four Archimedean lattices with $d=2$ and $q=3$ we have the following exact solutions and bounds [18,23]:

$$p_c[(3,12^2)\text{site}]=0.807\,900\,764\ldots, \tag{8}$$

$$0.707\,10\leqslant p_c[(4,8^2)\text{ site}]\leqslant 0.799\,97, \tag{9}$$

$$0.721\,73\leqslant p_c[(4,6,12)\text{site}]\leqslant 0.818\,98, \tag{10}$$

$$0.652\,703\,6\ldots\leqslant p_c(\text{hexagonal site})\leqslant 0.794\,72. \tag{11}$$

The range of values is at least the difference between the exact threshold of the $(3,12^2)$ lattice and the upper bound for the hexagonal lattice, which is 0.013 18, implying an error of at least 0.006 59 for one graph. Such errors are within the range of accuracy, 0.008, claimed by Galam and Mauger, for example. However, simulations provide estimates of approximately 0.697 043 for the site percolation threshold of the hexagonal lattice, which would imply a substantially larger error in such formulas.

Note that Galam and Mauger divide the low-dimensional lattices into two classes, with a different formula for each class. This approach may eliminate errors of the size mentioned above for site models. For bond models, however, an infinite collection of the examples must fall into one of the two classes, so there must still be substantial inaccuracy.

III. EFFECTIVE COORDINATION NUMBER

The success of the effective coordination number approach requires that the bond percolation thresholds of graphs be close if their site percolation thresholds are close. Unfortunately, the class of periodic fully triangulated graphs studied in [22] all have site percolation thresholds equal to one-half, but the bond percolation thresholds range from near zero to $2\sin(\pi/18)=0.3473\ldots$. Thus, the procedure of predicting bond thresholds from the site threshold will be inaccurate by at least 0.1736 for at least one of these lattices, for any such formula.

For example, the Galam and Mauger site threshold formulas, solved for q_{eff} when site $p_c=1/2$, give a value of $q_{\text{eff}}=5.942\,269$ for class 1 and $q_{\text{eff}}=5.639\,41$ for class 2, leading to bond threshold predictions of $p_c=0.351\,391$ for class 1 and $p_c=0.343\,475$ for class 2. Thus, there are discrepancies as large as 0.343 475, even though two formulas are used.

IV. LACK OF MONOTONICITY

In the formulas of [1–6], for fixed dimension the percolation threshold is a monotonically decreasing function of the average coordination number. A recent counterexample of Wierman [24] involves two two-dimensional lattices with bond percolation thresholds and average degrees in the same order, violating the monotonicity in the formulas: A modification of the $(3,12^2)$ lattice has bond percolation threshold between 0.695 23 and 0.698 25 and average degree $3\frac{3}{4}$, which may be compared to the hexagonal lattice, with exact bond threshold 0.6527 . . . and uniform coordination number 3. Since the difference in the thresholds is at least 0.042 53, any monotone formula must err by at least half this amount, or 0.021 26, for one of these lattices. The counterexample can be converted into site models, by the bond-to-site transformation and containment principle, for which monotone formulas must err by at least 0.021 26 also.

Furthermore, a different counterexample of Wierman [25] shows that two lattices may have bond percolation and site percolation thresholds in the opposite order. If universal formulas for bond percolation and site percolation thresholds

were monotone function of the average coordination number, this would not be possible.

V. BOND-TO-SITE TRANSFORMATION

The bond-to-site transformation converts any bond percolation model on a lattice to an equivalent site percolation model on the *line graph* or *covering graph* of the lattice. Note that for a regular graph with coordination number q, the covering graph has coordination number $2q-2$. Therefore, discrepancies will arise if the bond percolation threshold for coordination number q does not agree with the site percolation threshold for coordination number $2q-2$.

For example, the bond percolation threshold of the Kagomé lattice, which has coordination number 4, is equal to the site percolation threshold of its covering graph, which has coordination number 6. However, since the Kagomé lattice is in class 2, the Galam and Mauger formula estimates its bond threshold as 0.5162, while its covering graph has site threshold estimated as 0.4979 if it is in class 1 and 0.4775 if it is in class 2. Nearly exact mathematical bounds exist for the Kagomé lattice bond threshold [26], for which $0.5209 \leqslant p_c(\text{Kagomé bond}) \leqslant 0.5291$. Thus, the discrepancy is at least 0.0230 for the site percolation threshold of the covering graph of the Kagomé lattice.

VI. DUALITY

An important theoretical result in mathematical percolation theory, due to Kesten [27], is that bond percolation thresholds of a dual pair of periodic planar lattices sum to 1. The formula $p_c = d/(d-1)q$ satisfies this property, as a consequence of Euler's formula for planar graphs. However, the property is not satisfied for the other formulas mentioned above.

For example, the Kagomé lattice falls into Galam and Mauger's class 2 and its dual, the dice lattice, falls into class 1. Since both have average degree equal to 4, the formulas produce the estimates 0.5162 and 0.4958, respectively, which sum to 1.0120. Thus, at least one of the threshold estimates must be in error by at least 0.006. In fact, mathematical bounds of

$$0.5209 \leqslant p_c(\text{Kagomé bond}) \leqslant 0.5291 \tag{12}$$

and, consequently,

$$0.4709 \leqslant p_c(\text{dice bond}) \leqslant 0.4791, \tag{13}$$

have been proved [26]. Thus, the inaccuracy is at least 0.0037 for the Kagomé lattice and 0.0167 for the dice lattice.

VII. CONCLUSIONS AND DISCUSSION

This Brief Report reports on recent mathematical results which prove exact results and rigorous bounds for percolation thresholds, showing that the inaccuracy of universal formulas based only on the dimension and coordination number is much larger than indicated by previous evidence. In particular, any universal formula depending upon only dimension and average coordination number must err by at least 0.1736 for at least one planar lattice, as shown in Sec. II. Furthermore, any such universal formula that is monotone in the average coordination number must err by at least 0.021 26 for some graph, due to the lack of monotonicity of the percolation threshold as a function of the average coordination number. Similarly, lack of consistency with the bond-to-site transformation and planar graph duality also exposes inaccuracies in the predictions of such universal formulas. The sizes of the discrepancies established in Secs. II–VI are minimums, established by mathematical proof: Simulation estimates indicate discrepancies that are considerably larger in some cases.

It is important to note that the discrepancies exhibited are obtained with any universal formula depending only on dimension and coordination number. The mathematical results provide bounds on the accuracy of the predictions of the entire class of universal formulas. Galam and Mauger's formulas were not singled out for criticism, but used as examples precisely because they are the most accurate formulas to date.

The main theme of this Brief Report is that just dimension and average degree (or even a measure of effective average degree) are insufficient to explain the variation in percolation thresholds. The introduction of a third explanatory variable is a natural approach to this problem. The use of universality classes in Galam and Mauger's formula essentially introduces another explanatory variable to obtain better predictions, although the nature of the variable and its dependence on the lattice structure are not clearly defined.

Other approaches to developing universal formulas have been proposed, in addition to those involving dimension and average degree. However, these approaches must also deal with issues such as lack of monotonicity, consistency relative to the bond-to-site transformation, and consistency with duality for planar graphs. For example, Suding and Ziff [16] and others use a filling factor to obtain excellent estimates of site percolation thresholds of Archimedean lattices. However, they note that their method does not apply as well with nonregular graphs. In fact, the percolation behavior depends only on the adjacency structure of the lattice graph, while being independent of its planar representation. Thus, one cannot expect filling methods to fully capture the complexity of the dependence of the percolation threshold on the detailed structure of the underlying graph.

The comments in this paper demonstrate that developing accurate universal formulas for percolation thresholds is much more challenging that previously believed. Explaining the dependence of the percolation threshold on the detailed structure of the lattice is an important and interesting problem, worthy of further attention. It is hoped that this note will help influence and stimulate further research on this problem.

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