An Improved Upper Bound for the Site Percolation Threshold of the $(4, 8^2)$ Archimedean Lattice

John C. Wierman
Department of Applied Mathematics & Statistics
Johns Hopkins University

Abstract

Percolation models are infinite random graph models which have applications to phase transitions and critical phenomena. In the site percolation model, each vertex in an infinite graph G is retained independently with probability p and deleted otherwise. The percolation threshold is the critical probability $p_c(G)$ such that if $p > p_c(G)$ there is positive probability that the random subgraph induced by the retained vertices has an infinite connected component, while the probability that all of its components are finite is one if $p < p_c(G)$. There are few lattice graphs for which the site percolation threshold is exactly known, and rigorous bounds for unsolved lattices are very imprecise. The substitution method for computing bounds for the more common class of bond percolation models must be modified to apply to site models. Some modifications will be illustrated with an application to the $(4, 8^2)$ Archimedean lattice, which is a vertex-transitive tiling of the plane by squares and regular octagons. An improved upper bound, $p_c^{site}(4, 8^2) < 0.785661$, is obtained.

1 Introduction

Percolation models were introduced in the 1950s to explain aspects of fluid flow in a random medium. By associating the randomness with the medium, they provide an alternate perspective to diffusion models, which associate the randomness with the fluid. The physical and biological sciences have found percolation models particularly valuable in studying phemomena in which a threshold value of a parameter separates regimes with substantially different qualitative behavior, such as solid versus liquid phases, conduction or insulation of heat or electricity, or epidemic or quarantine of a disease. Consequently, many variations of the model have been created for a variety of applications. The mathematical theory of percolation models mainly employs concepts from probability, graph theory, and combinatorics. For comprehensive references on aspects of mathematical

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percolation theory, see the monographs by Grimmett [4], Bollobás and Riordan [3], and Hughes [6].

1.1 Site and Bond Percolation Models

The two classical types of percolation models are site models and bond models. Given an infinite graph G, the *site percolation model* on G retains each vertex in G stochastically independently with probability p. Traditionally, retained vertices are called "open." The object of study is the random subgraph G_p of G induced by the set of open vertices. In the *bond percolation model* on an infinite graph G, each edge is open with probability p, and the random subgraph G_p consisting of the set of open edges and their endpoints is studied.

For both site percolation models and bond percolation models, the focus is on connectivity properties of the random subgraph G_p. Of particular interest is the set of retention probability parameter values p for which an infinite component exists. As a consequence of the stochastic independence in the model, Kolmogorov's zero-one law implies that there exists a *percolation threshold* $p_c(G)$ such that all components of G_p are finite with probability one if $p < p_c(G)$, while there exists an infinite component of G_p with probability one if $p > p_c(G)$. The interpretation of the percolation threshold as a phase transition point, corresponding to a melting or freezing temperature, for example, is a reason for the intense interest in percolation models in science and engineering research and applications.

The value of the percolation threshold is highly dependent on the infinite graph, and, unfortunately, is exactly known for a very small set of common graphs. The bond percolation thresholds of the square, triangular, and hexagonal lattices [7, 16] are $1/2$, $2\sin(\pi/18)$, and $1 - 2\sin(\pi/18)$, respectively, and the site percolation threshold of the triangular lattice [8] is $1/2$. Although a few other common lattices are exactly solved, most knowledge of percolation threshold values is in the form of estimates derived in extensive simulation studies in the physics literature. This article is focused on issues relating to the derivation of mathematically rigorous bounds for site percolation thresholds, about which even less is known than for bond percolation thresholds.

Motivated by applications to atomic lattice structures, typical infinite graphs that are considered have substantial symmetries in structure. A well-studied class is the set of eleven Archimedean lattices, which are vertex-transitive tilings of the plane by regular polygons. A naming system for these lattices lists the number of edges in the sequence of polygons around a vertex in the lattice, with exponents indicating successive repetitions. As examples, the square lattice is the (4^4) lattice, and the lattice considered in this article is the $(4, 8^2)$ lattice. (For a discussion of the eleven Archimedean lattices, see the beautiful monograph by Grünbaum and Shephard [5].) The most familiar Archimedean lattices are the square, triangular, and hexagonal lattices mentioned above. Bounds for unsolved bond percolation thresholds of Archimedean lattices typically provide intervals of length less than 0.07, and in two cases determine the leading 2 and 3 digits. In comparison, all bounds for unsolved Archimedean lattice site percolation thresholds provide intervals longer than 0.09. We will discuss some issues related to this disparity, illustrate them with the $(4, 8^2)$ Archimedean lattice, and derive a

slightly improved upper bound for its site percolation threshold.

1.2 Substitution Method

Nearly all of the most accurate percolation threshold bounds have been derived by the substitution method. The method has been quite successfully applied to bond percolation models [17, 18, 21, 22, 24, 27, 28, 30, 31, 32], but less progress has been made for site percolation models [19, 22]. Section 2 will discuss reasons why bounding site percolation thresholds is more difficult in principle, and discuss difficulties applying the substitution method to site percolation models.

The substitution method derives upper and lower bounds for the percolation threshold of an unsolved lattice by comparing probabilities of connections in finite subgraphs with those of a percolation model on another lattice for which the percolation threshold is exactly known or precisely bounded. The two percolation models are compared using stochastic ordering. In the remainder of this section, we give a description of the basic ideas of the method needed later in this article, and a brief summary of computational reductions that make the computations more efficient. For more extensive summaries of the substitution method, see [26, 32]

For bond percolation models, the two lattices that are to be compared must be decomposed into isomorphic edge-disjoint subgraphs, called *substitution regions*, to provide independence of their connection probabilities. For site percolation models, the substitution regions must be vertex-disjoint. For both types of models, all substitution regions must have the same number of boundary vertices, i.e., vertices which are adjacent to at least one vertex outside the substitution region. Figure 1 illustrates two substitution regions to be considered for a comparison later in this article.

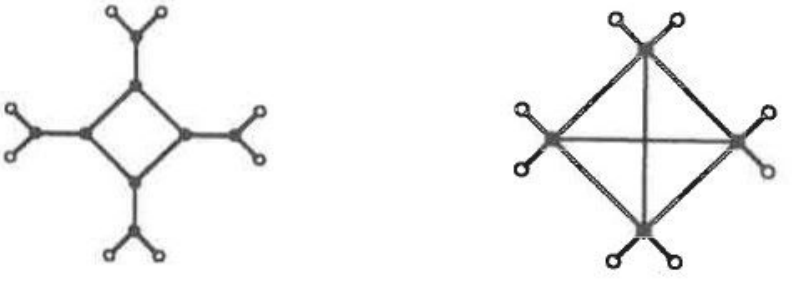

Figure 1: Substitution regions with eight boundary vertices for a comparison considered later in this article. The boundary vertices are indicated by open circles.

A configuration of a bond percolation model is a designation of every edge as open or closed. Each configuration on a substitution region partitions the set of boundary vertices into blocks which are connected by open paths within the substitution region. By summing the probabilities of configurations that produce a partition, a probability is obtained, in the form a polynomial function of the retention probability parameter, for each partition in each of the two percolation models. Thus, the connection probabilities in each substitution region form a probability measure on the set of partitions of boundary vertices.

A partition is a *refinement* of another if all its blocks are contained in blocks of the other. The set of partitions can be partially ordered by refinement, forming the *partition lattice*.

The probability measures are compared by stochastic ordering, i.e., inequalities between probabilities of upsets in the partition lattices. Since the upset probabilities of the unsolved model are increasing functions, while the upset probabilities for the comparison model are constant (evaluated at its percolation threshold or the value of a bound), the problem can be reduced to solving upset probability equations. The upper and lower bounds for the percolation threshold are the largest and smallest solutions, respectively, of the set of upset probability equations.

Carrying out the neceassary calculations to derive rigorous bounds would at first glance appear to be impossible, since the number of upset probability equations to solve grows super-exponentially. For example, for eight boundary vertices, there are at least $2^{1701} \approx 1.127 \times 10^{512}$ equations to solve. To modify a colloquial expression, the problem might be called "finding two needles in a haystack." The haystack is the set of equations, while the needles are the two that produce the extremal solutions. The solution method is to "throw away large parts of the haystack," i.e., prove that the solutions cannot come from large sets of upset probability equations.

Several computational reductions have been developed to allow the calculations to be completed. An efficient "graph-welding" technique allows the probabilities for the equations to be calculated recursively [10]. If the lattice graphs are planar, consideration can be restricted to non-crossing partitions [12]. Symmetry considerations allow partitions to be grouped together into classes, and it is proved that the desired solutions must be determined by upsets that consist only of entire classes [11]. Determining stochastic ordering can be converted into a network flow problem, which can be solved symbolically in MATLAB [10]. With these reductions, bounds can be computed for planar bond percolation threshold bounds for substitution regions with eight boundary vertices.

2 Diferences Between Site and Bond Models

There has been considerably more success at finding exact solutions and accurate rigorous bounds for bond percolation models than for site percolation models. In this section, we provide numerical results to show this, and discuss theoretical reasons as possible explanations for the difference in results.

Bond percolation threshold values are generally more accurately known than site percolation threshold values. For example, while the square lattice is perhaps the lattice most well-studied in percolation theory, its bond percolation threshold is exactly known to be $1/2$, while the best bounds for its site percolation threshold are

$$0.556 < p_c^{site}(square) < 0.679492.$$

Similarly, the bond percolation threshold of the hexagonal lattice is known to be $1 - 2\sin(\pi/18) = 0.652703...$, but the best bounds for the site percolation

threshold are

$$0.652703 \leq p_c^{site}(hexagonal) < 0.743359,$$

which are the most accurate bounds for any unsolved Archimedean lattice site model. In contrast, much more accurate bond model threshold bounds have been obtained for two Archimedean lattices:

$$0.522551 < p_c^{bond}(3,6,3,6) < 0.526490$$

and

$$0.740084 < p_c^{bond}(3,12^2) < 0.740761.$$

These bounds disprove two conjectures of Tsallis [15] and determine the leading two and three digits, respectively, of the bond percolation thresholds.

There are theoretical reasons why site models are more difficult to deal with than bond models. By a bond-to-site transformation, the bond percolation model on a graph G is equivalent to a site percolation model on the line graph of G. Since there exist graphs that are not line graphs, by Beinecke's theorem [1], not every site model is equivalent to a bond model. Thus, site models are more general than bond models. Consequently, bond models have some additional structure to exploit than site models. While the nature of this additional structure is unclear, most exact percolation threshold solutions have been obtained for planar bond percolation models using properties involving graph duality.

More specifically, to apply the substitution method to site percolation models, there are several difficulties:

[1] There are fewer "useful" exactly-solved site models to use as comparisons. Although every solved bond model is equivalent to a site model, which therefore is also solved, the line graphs of the bond models are typically nonplanar. Inability to apply the reduction to non-crossing partitions may increase the computational effort tremendously.

[2] Vertex-disjoint substitution regions are needed to apply the substitution method. In practice, it is often difficult to decompose an unsolved lattice into isomorphic vertex-disjoint substitution regions that are appropriate for a comparison with an exactly-solved lattice.

[3] To achieve vertex-disjoint substitution regions, edges between the regions must be subdivided by inserting "ghost vertices" which are considered to be always open. The ghost vertices serve as the boundary vertices. Typically, the number of boundary vertices for a substitution region for a site model is larger than that for the same region in a bond model on the same lattice, which could greatly increase the computational burden to complete the substitution method calculations.

[4] Since there are fewer vertices than edges in a typical subgraph, there are fewer random elements in the corresponding site model than in the corresponding bond model. For this reason, larger substitution regions are needed for site models than for bond models to have comparable randomness to obtain comparably accurate bounds. However, use of larger substitution regions further increases the number of boundary vertices.

While substitution method calculations for site percolation models have not become efficient, some adaptations have been found to help circumvent some of the difficulties mentioned above. These will be applied to the Archimedean $(4, 8^2)$ lattice in Section 3.

[1] Multiple-stage substitutions may be used. This approach helps deal with non-planarity, by removing different diagonal edges from faces in stages to produce a planar comparison lattice or to produce the line graph of a solved bond percolation model. However, it is difficult to discover multi-stage comparisons that will be likely to provide accurate bounds.

[2] The set of ghost boundary vertices that are adjacent to a specific vertex in the substitution region are either all connected to each other (if the vertex is open) or completely disconnected (if the vertex is closed). This allows us to consider only partitions of the vertices in the "internal boundary" of the substitution region, except that for blocks of size one we must distinguish between open and closed vertices. The structure of this augmented partition lattice currently needs to be analyzed on a case-by-case basis. However, it does have the advantage that, by considering partitions of fewer vertices, it has a smaller number of upsets, making substitution method calculations less extensive.

3 The $(4, 8^2)$ Lattice

3.1 Previous Results

The $(4, 8^2)$ lattice, which is often called the "bathroom tile" lattice, is one of the eleven Archimedean tilings. The notation $(4, 8^2)$ refers to the fact that a square and two octagons meet at each vertex. The $(4, 8^2)$ lattice is illustrated in Figure 2. Note that the lattice is not a line graph, since it contains the three-star as an induced subgraph, which is forbidden by Beinecke's theorem.

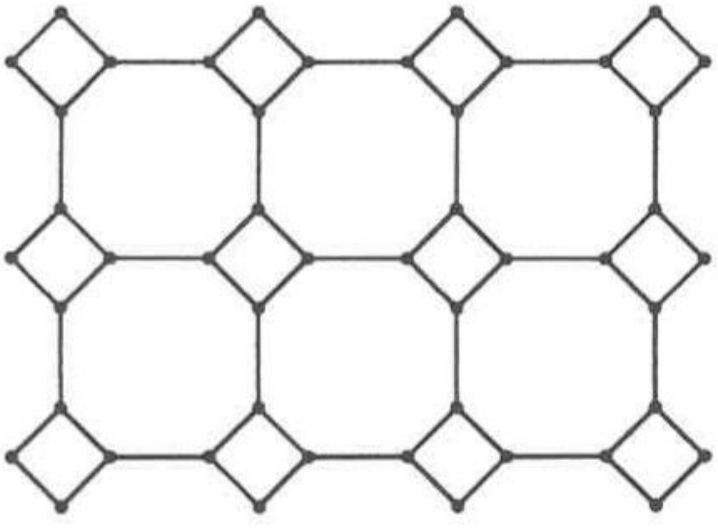

Figure 2: An induced subgraph of the $(4, 8^2)$ lattice.

Two methods for deriving bounds have been applied previously to the site

percolation threshold of the $(4, 8^2)$ lattice.

The grouping method [9] provided an upper bound: The endpoints of each edge between squares in the $(4, 8^2)$ lattice can be viewed as a single vertex in a new graph, and is considered to be open if and only if both original vertices are open, producing a square lattice. If there is an infinite open component in this square lattice site percolation model, then there is an infinite open component in the $(4, 8^2)$ lattice site model. Therefore,

$$p_c^{site}(4, 8^2) \leq \sqrt{p_c^{site}(square)}.$$

The smallest upper bound for the square lattice site percolation threshold [19] is 0.679492, so

$$p_c^{site}(4, 8^2) \leq 0.824313.$$

Note that Suding and Ziff [14] estimated $p_c^{site}(square)$ to be 0.5927460 by Monte Carlo simulation, so if the exact value were determined to be near this value, the bound for the $(4, 8^2)$ lattice by this method could not be lowered to less than 0.7698. Since their simulation estimate for $p_c^{site}(4, 8^2)$ is 0.729724, this method is unlikely to produce a very sharp upper bound.

The line graph of a square lattice with each edge subdivided has a bond percolation threshold equal to $1/\sqrt{2}$. The resulting graph is a $(4, 8^2)$ lattice with diagonals inserted in every square. By comparing this graph with the $(4, 8^2)$ lattice using the substitution method, [20] obtained the best numerical bounds:

$$0.707106 < \frac{1}{\sqrt{2}} \leq p_c^{site}(4, 8^2) < 0.79997.$$

However, an improved upper bound for the square lattice site percolation threshold could provide a smaller upper bound than 0.79997 for $p_c^{site}(4, 8^2)$.

3.2 An Improved Upper Bound

In this subsection, we illustrate the issues mentioned above by applying the substitution method to derive bounds for the site percolation threshold of the $(4, 8^2)$ lattice. The first issue is to find a useful comparison lattice, i.e., a lattice with somewhat similar structure for which the site percolation threshold is exactly known or accurately bounded. Since the $(4, 8^2)$ lattice has four-fold rotational symmetry, a natural choice is the line graph of the square lattice, which consists of a square lattice with diagonal edges inserted in half of the squares in a checkerboard pattern. By the bond-to-site transformation, its site percolation threshold is exactly $1/2$.

We use a two-stage substitution process to obtain the $(4, 8^2)$ lattice from the line graph of the square lattice. The first stage removes diagonal edges from half of the squares containing diagonals in the line graph, while the second stage replaces the diagonal edges from the other half of such squares with a subgraph that converts the graph into the $(4, 8^2)$ lattice.

3.2.1 The First-Stage

Each of the two lattice graphs must be decomposed into isomorphic vertex-disjoint substitution regions, with all substitution regions having the same number of boundary vertices. Figure 3 shows a decomposition of the line graph of the square lattice, denoted L, which may be visualized as a square lattice with both diagonal edges inserted in alternating squares in a checkerboard pattern. By the bond-to-site transformation, the site percolation threshold of L is equal to the bond percolation threshold of the square lattice, which is exactly $1/2$. L is to be compared to an intermediate graph, denoted H. Figure 3 also shows H, in which some of the diagonal edges have been deleted from L, decomposed into substitution regions.

In order to decompose L and H into vertex-disjoint substitution regions, a ghost vertex is inserted to subdivide each edge that crosses the boundary of a substitution region. The two substitution regions, with their boundary vertices, are shown in Figure 4.

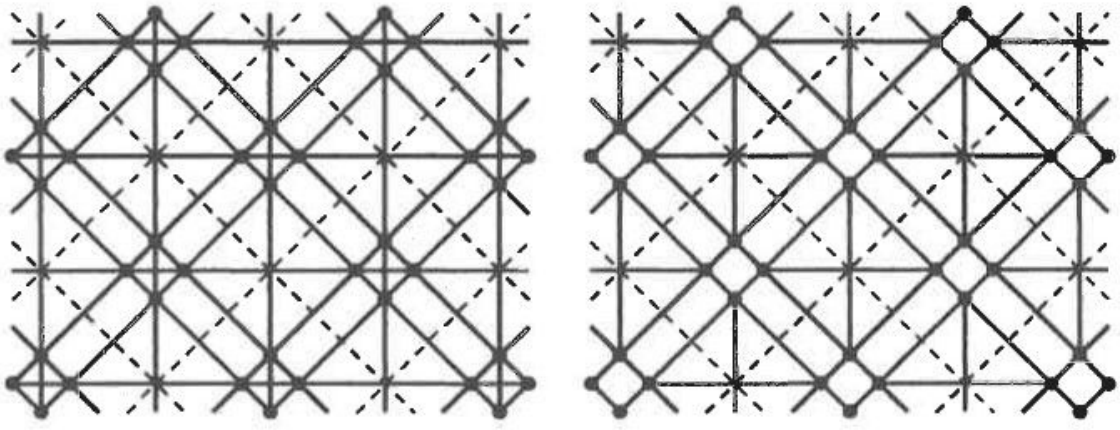

Figure 3: An illustration of the first stage of the substitution. Dashed lines indicate the decomposition of the lattices into vertex disjoint substitution regions. Left: The line graph of the square lattice, drawn with squares of different edge-lengths so vertex locations correspond to those in the $(4, 8^2)$ lattice. Right: Diagonal edges have been removed from the small squares in the line graph of the square lattice.

Notice that each of the substitution regions has 12 boundary vertices, so the partition lattice of boundary vertices is extremely large. However, we may consider a much smaller *augmented partition lattice* based on partitions of the four vertices in the *internal boundary*, i.e., the non-boundary vertices which are adjacent to boundary vertices. The reduction to the internal boundary is possible because the boundary vertices are grouped in triples, with each triple adjacent to only one internal boundary vertex. Consequently, the boundary vertices in a triple are either all connected to each other or completely disconnected.

To describe the augmented partition lattice, we introduce the following notation. Suppose that the internal boundary vertices are labeled A, B, C, and D, in cyclic order. In our notation for a partition, let the upper case letter for a vertex indicate that the vertex is open, and the lower case letter indicate that it is

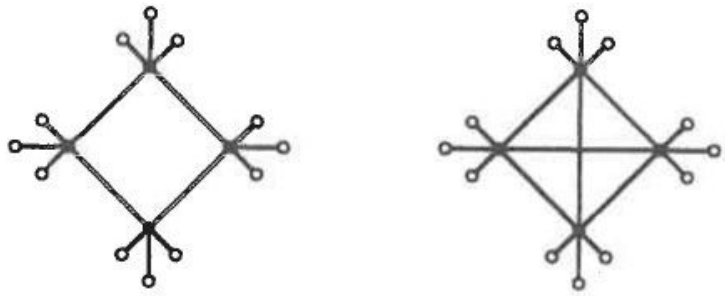

Figure 4: Substitution regions for the first-stage of the calculation of the bounds. Left: A subgraph of the intermediate graph. Right: A subgraph of the matching graph of the square lattice.

closed. A partition is denoted by a sequence of letters and vertical bars, where the bars separate sets of vertices (called *blocks*) which are connected by open paths in the substitution region. If two or more vertices are connected, they must be open. However, if a vertex is not connected to any other, it may be either open or closed, which is indicated by an upper or lower case letter, respectively. Thus, in general, the elements of the augmented partition lattice are all set partitions of $\{A, B, C, D\}$ augmented by partitions in which any block of size one may indicate that the vertex is closed. For example, for a general substitution region with four internal boundary vertices, in addition to $AB|C|D$, the augmented partition lattice could also contain $AB|C|d$, $AB|c|D$, and $AB|c|d$.

We now apply the substitution method to derive an upper bound for $p_c^{site}(H)$. The substitution regions are illustrated in Figure 4. Each includes a square with three ghost vertices added as boundary vertices at each corner of the square. The substitution region for L also includes both diagonals of the square.

Since there are four vertices in the regions, there are only $2^4 = 16$ configurations. A further simplification is that there are only six symmetry classes which have positive probability. Instead of considering partitions of the 12 boundary vertices, we consider the augmented partitions of four vertices. The augmented partitions are grouped into symmetry classes by rotation. The probability measure on the augmented partitions for L is given by:

$$P[ABCD] = p^4.$$
$$P[ABC|d] = P[ABD|C] = P[ACD|B] = P[A|BCD] = p^3(1-p).$$
$$P[AC|b|d] = P[a|BD|c] = p^2(1-p)^2.$$
$$P[A|b|C|d] = P[a|B|c|D] = 0.$$
$$P[AB|c|d] = P[a|BC|d] = P[a|b|CD] = P[AD|b|c] = p^2(1-p)^2.$$
$$P[A|b|c|d] = P[a|B|c|d] = P[a|b|C|d] = P[a|b|c|D] = p(1-p)^3.$$
$$P[a|b|c|d] = (1-p)^4.$$

The probability measure on the augmented partitions for H is given by:

$$P[ABCD] = p^4.$$

$$P[ABC|d] = P[ABD|c] = P[ACD|b] = P[a|BCD] = p^3(1-p).$$
$$P[AC|b|d] = P[a|BD|c] = 0.$$
$$P[A|b|C|d] = P[a|B|c|D] = p^2(1-p)^2.$$
$$P[AB|c|d] = P[a|BC|d] = P[a|b|CD] = P[AD|b|c] = p^2(1-p)^2.$$
$$P[A|b|c|d] = P[a|B|c|d] = P[a|b|C|d] = P[a|b|c|D] = p(1-p)^3.$$
$$P[a|b|c|d] = (1-p)^4.$$

Define the *class lattice* to be the set of symmetry classes, partially ordered by refinement, in which one class is a refinement of a second class if any partition in the first class is a refinement of any class in the second. By the symmetry reduction in [11], the upsets which provide the largest and smallest solutions are upsets in the class lattice. Figure 7 (on the left) provides the Hasse diagram of the class lattice of the augmented partitions on four vertices which have a positive probability in one or both of the probability measures.

We are now prepared to determine an upper bound for $p_c^{site}(H)$. Notice that the only difference between the two probability measures is for the two classes represented by $AC|b|d$ and $A|b|C|d$. From this fact, we see that the two probability measures give equal probabilities for the four upsets generated by class $ABCD$, by class $ABC|d$, by class $AB|c|d$, and by class $A|b|c|d$. Since we fix the parameter of the site percolation model on L at its percolation threshold, $1/2$, and the upset probabilities for H are increasing functions, $1/2$ is the solution to the upset probability equations for all four of these upsets.

There are only four other upsets in the class lattice, generated by class $AC|b|d$, by class $A|b|C|d$, by classes $AC|b|d$ and $AB|c|d$, and by classes $A|b|C|d$ and $AB|c|d$. The upset probability functions for the upsets generated by the second and fourth of these are equal, so again have the solution $1/2$. The upset probability equations for the first and third upsets, respectively, are

$$p^4 + 4p^3(1-p) = 7/16$$

and

$$p^4 + 4p^3(1-p) + 4p^2(1-p)^2 = 11/16.$$

Their solutions (rounded up) are 0.577962 and 0.586668, respectively. Therefore, the smallest and largest solutions produce the bounds

$$0.500000 \leq p_c^{site}(H) < 0.586668.$$

3.2.2 The Second Stage

In the second stage of the upper bound derivation, we compare the $(4, 8^2)$ lattice to the intermediate lattice H, setting the vertex-retention parameter of H at the upper bound value that was calculated during the first stage.

The intermediate lattice H may be decomposed into vertex-disjoint substitution regions in a different way, with each substitution region replaced by a different substitution region that produced the $(4, 8^2)$ lattice. Figure 5 shows the decompositions of the two lattices, with the generic substitution regions shown

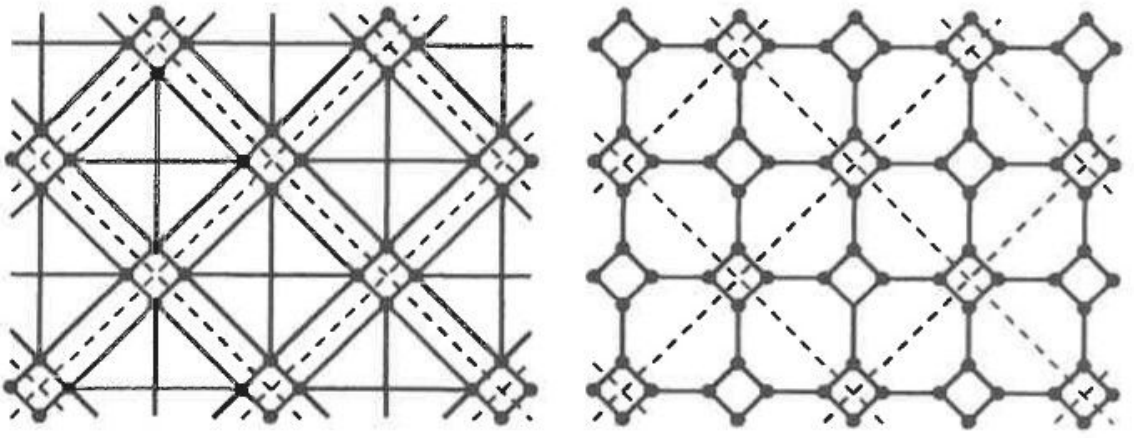

Figure 5: A different decomposition of the lattice graphs. Dashed lines partition the lattices into vertex disjoint regions. Left: The intermediate lattice H. Right: The $(4, 8^2)$ lattice.

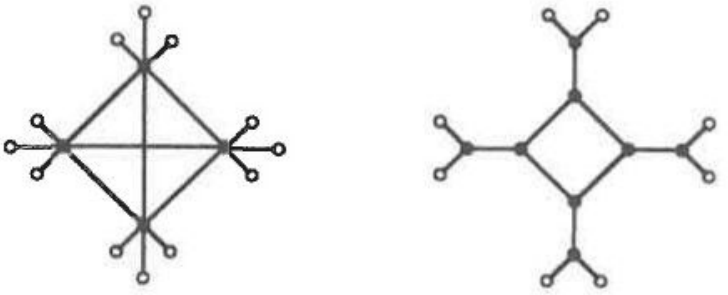

Figure 6: Substitution regions for the second stage of the calculation of the bounds. Left: A subgraph of the intermediate graph H. Right: A subgraph of the $(4, 8^2)$ lattice.

in Figure 6. The probability measure for the substitution region in H was calculated in the first stage. The probability measure for the substitution region in the $(4, 8^2)$ lattice is somewhat more complicated, but can be calculated relatively easily from the 2^8 configurations on its eight internal vertices.

The probability distribution for the substitution region of the $(4, 8^2)$ lattice is:

$$P[]ABCD] = p^8.$$

$$P[ABC|D] = P[BCD|A] = P[CDA|B] = P[DAB|C] = p^7(1-p).$$

$$P[ABC|d] = P[BCD|a] = P[CDA|b] = P[DAB|c] = p^6(1-p).$$

$$\begin{aligned} P[AB|c|D] = P[BC|d|A] = P[CD|a|B] = P[DA|b|C] \\ = P[AB|C|d] = P[BC|D|a] = P[CD|A|b] = P[DA|B|c]. \\ = p^5(1-p)^2. \end{aligned}$$

$$P[AB|c|d] = P[a|BC|d] = P[a|b|CD] = P[DA|b|c] = p^4(1-p)^2.$$

$$P[AB|C|D] = P[A|BC|d] = P[A|B|CD] = P[DA|B|c] = p^6(1-p)^2.$$

$$P[AC|B|d] = P[a|BD|C] = P[D|AC|b] = P[A|BD|c] = p^6(1-p)^2.$$

$$P[AC|b|d] = P[a|BD|c] = p^6(1-p)^2 + 2p^5(1-p)^3.$$

$$P[A|B|C|D] = p^4[(1-p)^4 + 4p(1-p)^3 + 2p^2(1-p)^2].$$

$$P[A|B|C|d] = P[a|B|C|D] = P[A|b|C|D] = P[A|B|c|D]$$
$$= p^3(1-p)[(1-p)^4 + 4p(1-p)^3 + 4p^2(1-p)^2].$$

$$P[A|B|c|d] = P[a|B|C|d] = P[a|b|C|D] = P[A|b|c|D]$$
$$= p^2(1-p)^2[(1-p)^4 + 4p(1-p)^3 + 5p^2(1-p)^2 + 2p^3(1-p)].$$

$$P[A|b|C|d] = P[a|B|c|D]$$
$$= p^2(1-p)^2[(1-p)^4 + 4p(1-p)^3 + 6p^2(1-p)^2 + 2p^3(1-p)].$$

$$P[A|b|c|d] = P[a|B|c|d] = P[a|b|C|d] = P[a|b|c|D] = p(1-p)^3.$$

$$P[a|b|c|d] = (1-p)^4.$$

The class lattice for the augmented partitions that have positive probability in either the model for H or the model for the $(4, 8^2)$ lattice is shown in Figure 7.

Since we do not know the exact site percolation threshold of H, we must evaluate the probability measure for site percolation on H at its lower bound of $1/2$ to derive a lower bound for the $(4, 8^2)$ lattice and at its upper bound of 0.586668 to derive an upper bound for the $(4, 8^2)$ lattice. While there are considerably more upsets in this class lattice than for the first stage, we can reduce consideration to a small number of upsets for each bound.

It is sufficient to consider only one upset to determine that this comparison does not improve the best previous lower bound for the $(4, 8^2)$ lattice. The class represented by $A|b|c|d$ is simply the event that at least one of the vertices A, B, C, or D is open. In both models, this probability is $1 - (1-p)^4$. Thus, when substituting $1/2$ in the probability measure corresponding to H, the corresponding upset equation is $1 - (1-p)^4 = 1 - (1/2)^4$. The solution $1/2$ is smaller that the previous lower bound of 0.707106, so the smallest solution is also.

We now show that we may reduce consideration to only six upsets to derive an upper bound for the $(4, 8^2)$ lattice. From the first stage, recall that only six classes have positive probability in the probability measure corresponding to H. An upset U that has a minimal class other than one of these six classes will have the same probability in the model for H as some upset V generated by a subset of these classes. However, in the probability measure for the $(4, 8^2)$

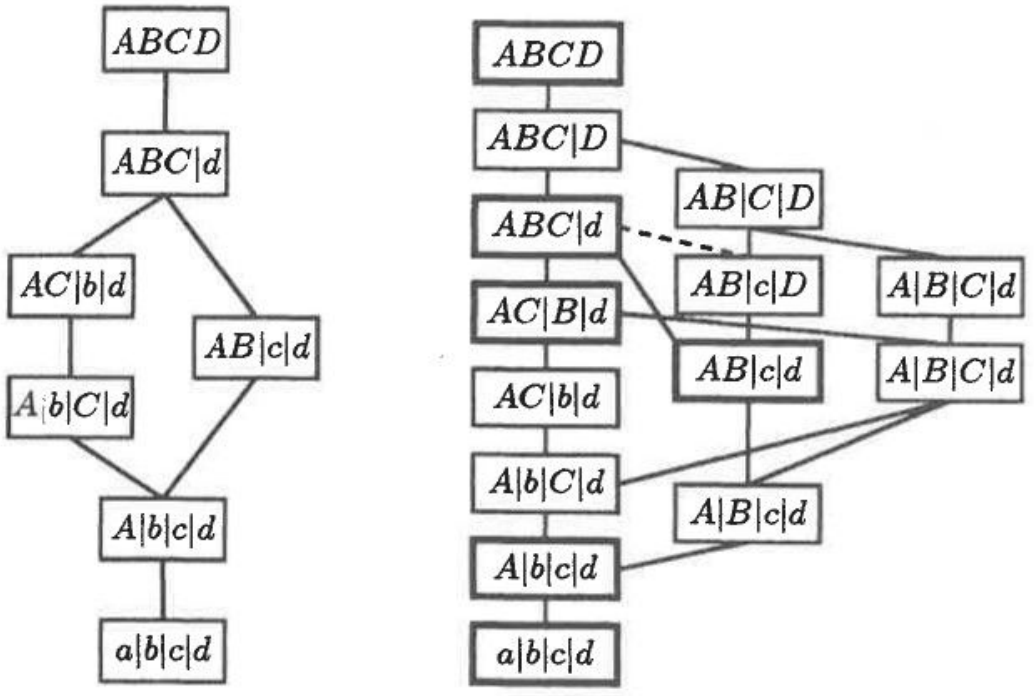

Figure 7: Hasse diagrams for the class lattices for the two stages of substitutions, in which one representative partition is shown, while the others in the class are obtained by rotations. Left: The Hasse diagram for the partitions in the first stage substitution. Right: The Hasse diagram for the partitions in the second stage. Bold rectangles indicate partitions with positive probability in both models.

lattice, the probability of U will be larger than that of V. Hence, upset U will have a smaller solution than upset V. Since we seek the largest upset probability equation solution, consideration can be reduced to upsets generated by the six classes.

The six classes generate only six non-trivial upsets. We list the representatives of the classes which generate these upsets, along with the solutions to their upset probability equations. Since we are deriving an upper bound, the solutions are rounded up.

$ABCD$	0.765943
$ABC\|d$	0.765943
$AC\|b\|d$	0.780963
$AB\|c\|d$	0.765943
$AC\|b\|d$ and $AB\|c\|d$	0.785661
$A\|b\|c\|d$.	0.586668

Selecting the largest solution, we have established that $p_c^{site}(4, 8^2) < 0.785661$, which is slightly smaller than the previous upper bound .79997 of [20]. Together with the previous lower bound of [20], we have

$$0.707106 \leq p_c^{site}(4, 8^2) < 0.785661.$$

The length of the interval between the bounds was reduced by 15%. Furthermore, the interval is shorter than that for the hexagonal lattice, so provides the most

accurate bounds for any unsolved Archimedean lattice site percolation threshold.

4 Summary and Further Research Directions

The substitution method has mainly been developed with bond percolation models in mind. In particular, it may have been tailored to be more applicable to bond models in the attempt to disprove the conjectured exact values by Tsallis.

In order to adapt the method to derive improved percolation threshold bounds for site percolation models, there are several issues to consider. There is a need to determine the useful structure of the augmented partition lattice. Developing approaches for discovering two-stage comparisons that will be computationally feasible and produce more accurate bounds would be useful. It would be helpful to determine reductions that produce a small class of equations that are sufficient to determine the percolation threshold bounds. Finally, one would like to understand when bounds will and will not improve for larger substitution regions. Knowledge regarding these issues could be exploited to improve site percolation threshold bounds first for other Archimedean lattices and then for broader classes of lattices.

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References

[1] Beineke, L. W. (1968) Derived graphs and digraphs. *Beiträge zur Graphentheorie*, (H. Sachs, H.-J. Voss, and H.-J. Walter, eds.), Teubner, Leipzig, 17–33.

[2] van den Berg, J. and Ermakov, A. (1996) A new lower bound for the critical probability of site percolation on the square lattice. *Random Structures & Algoritms* 8, 199–212.

[3] Bollobás, B. and Riordan, O. (2006) *Percolation*, Cambridge University Press.

[4] Grimmett, G. (1999) *Percolation*, Springer.

[5] Grünbaum, B. and Shephard, G. C. (1987) *Patterns and Tilings*, W. H. Freeman.

[6] Hughes, B. (1996) *Random Walks and Random Environments, Volume 2: Random Environments*, Oxford University Press.

[7] Kesten, H. (1980) The critical probability of bond percolation on the square lattice equals 1/2. *Communications in Mathematical Physics* 74, 41–59.

[8] Kesten, H. (1982) *Percolation Theory for Mathematicians*, Birkhäuser.

[9] Łuczak, T. and Wierman, J. C. (1988) Critical probability bounds for two-dimensional site percolation models, *Journal of Physics A: Mathematical and General* 21, 3131–3138.

[10] May, W. D. and Wierman, J. C. (2003) Recent improvements to the substitution method for bounding percolation thresholds. *Congressus Numerantium* 162, 5–25.

[11] May, W. D. and Wierman, J. C. (2005) Using symmetry to improve percolation threshold bounds. *Combinatorics, Probability and Computing* 14, 549–566.

[12] May, W. D. and Wierman, J. C. (2007) The application of non-crossing partitions to improving percolation threshold bounds. *Combinatorics, Probability and Computing* 17, 285–307.

[13] Riordan, O. and Walters, M. (2007) Rigorous confidence intervals for critical probabilities. *Phys. Rev. E* 76, 011110.

[14] Suding, P. N. and Ziff, R. M. (1999) Site percolation thresholds for Archimedean lattices. *Physical Review E* 60, 275–283.

[15] Tsallis, C. (1982) Phase diagram of anisotropic planar Potts ferromagnets: A new conjecture. *Journal of Physics C* 15, L757–L764.

[16] Wierman, J. C. (1981) Bond percolation on honeycomb and triangular lattices, *Advances in Applied Probability* 13, 293–313.

[17] Wierman, J. C. (1990) Bond percolation critical probability bounds for the kagomé lattice by a substitution method. *Disorder in Physical Systems* (G Grimmett and D J A Welsh, eds.), Oxford University Press, 349–360.

[18] Wierman, J. C. (1992) Equality of the bond percolation critical exponents for two pairs of dual lattices, *Combinatorics, Probability & Computing* 1, 95–105.

[19] Wierman, J. C. (1995) Substitution method critical probability bounds for the square lattice site percolation model. *Combinatorics, Probability and Computing* 4, 181–188.

[20] Wierman, J. C. (2001) Site percolation critical probability bounds for the $(4, 8^2)$ and $(4, 6, 12)$ lattices. *Congressus Numerantium* 150, 117–128.

[21] Wierman, J. C. (2002) Bond percolation critical probability bounds for three Archimedean lattices, *Random Structures and Algorithms* 20, 507–518.

[22] Wierman, J. C. (2002) An improved upper bound for the hexagonal lattice site percolation critical probability. *Combinatorics, Probability and Computing* 11, 629–643.

[23] Wierman, J. C. (2003) Upper and lower bounds for the kagome lattice bond percolation critical probability, *Combinatorics, Probability and Computing* 12, 95–111.

[24] Wierman, J. C. (2015) An improved upper bound for the bond percolation threshold of the cubic lattice. *Proceedings of the 2015 Joint Statistics Meetings*, American Statistical Association, 3610–3620.

[25] Wierman, J. C. and Yu, G. (2016) Rigorous bounds relating bond percolation thresholds of two three-dimensional lattices, *Congressus Numerantium* 227, 157–176.

[26] Wierman, J. C. (2016) Tight bounds for the bond percolation threshold of the $(3, 12^2)$ lattice, *Journal of Physics A: Mathematical and Theoretical* 49, 475002.

[27] Wierman, J. C. (2017) Bounds for bond percolation thresholds of Archimedean lattices with degree three, *Journal of Physics A: Mathematical and Theoretical* 50, 295001.

[28] Wierman, J. C. (2017) Strict inequalities between bond percolation thresholds of Archimedean lattices. *Congressus Numerantium* 229, 231–244.

[29] Wierman, J. C. (2017) On bond percolation threshold bounds for Archimedean lattices with degree three, *Journal of Physics A: Mathematical and Theoretical* 50, 295001.

[30] Wierman, J. C.; Nathan, A.; and Lim, E. (2012) Bond percolation threshold bounds for planar lattices with generators with four boundary vertices. *Congressus Numerantium* 213, 169–183.

[31] Wierman, J. C. and McCarthy, S. (2015) An upper bound for the bond percolation threshold of the cubic lattice. *Congressus Numerantium* 224, 135–146.

[32] Wierman, J. C.; Yu, G.; and Huang, T. (2015) A disproof of Tsallis' bond percolation threshold conjecture for the kagome lattice. *Electronic Journal of Combinatorics* 22, P2.52.