Bond Percolation Critical Probability Bounds for the Kagomé Lattice by a Substitution Method

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Abstract

A new substitution method improves bounds for critical probabilities of the bond percolation problem on the Kagomé lattice, $\mathcal{K}$. The method theoretically produces a sequence of upper and lower bounds, in which the second pair of bounds establish

$$.5182 \leq p_c(\mathcal{K}) \leq .5335.$$

1. Introduction

Percolation processes were introduced by Broadbent and Hammersley in 1957 as models for the flow of a fluid through a random medium. A *bond percolation model* is comprised of an infinite lattice graph G, with each bond independently designated as open with probability p, $0 < p < 1$, and closed with probability $q = 1 - p$. The *open cluster* containing a specific vertex $v \in G$, denoted C_v, is the set of all vertices that can be reached from v through a path of open bonds. Let P_p denote the probability measure corresponding to parameter value p. The *critical probability* of the graph G, denoted by $p_c(G)$, is defined by $p_c(G) = \inf\{p : P_p[|C_v| = \infty] > 0\}$, which is independent of the vertex v if G is connected.

Since the seminal papers on mathematical percolation theory (Broadbent and Hammersley 1957; Hammersley 1957), there has been considerable interest in determining exact values of the critical probability for specific lattices. Sykes and Essam (1964) gave a heuristic determination of exact critical probability values for the square, triangular, and hexagonal lattice bond percolation models, and the value $\frac{1}{2}$ for the triangular lattice site

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percolation model. Verifying these values was a focus of research for nearly two decades. Even now, their method has not been completely justified.

The first rigorous determination of the critical probability of a periodic graph was due to Kesten (1980), who proved that the critical probability of the square lattice bond model is $\frac{1}{2}$. Wierman (1981) verified the values conjectured by Sykes and Essam for the triangular and hexagonal lattice bond model critical probabilities. The critical probabilities of two lattices for which no values were previously conjectured were found by Wierman (1984). The key aspects of these proofs were the use of planar graph duality, and (for graphs that are not self-dual) use of the star-triangle transformation. However, only these few cases currently have rigorous solutions, and there is no general method for rigorously determining critical probability values. There are only a few techniques for generating bounds on the critical probability of other graphs, and these provide unsatisfying results. In no case do they provide bounds that completely determine the leading digit of the critical probability value. For example, prior to this work, the Kagomé lattice bond model was known to satisfy $.4045 \leq p_c(\mathcal{K}) \leq .6180$. (See Wierman 1988.) The purpose of this paper is to introduce a rigorous method for determining much more accurate bounds for two-dimensional bond percolation models.

A key aspect of the proofs of Wierman (1981, 1984) is use of the star-triangle transformation, which was a crucial tool in Sykes and Essam's derivation for the triangular and hexagonal lattice bond models. Ottavi (1979) also used the star-triangle transformation to compute upper and lower bounds for the Kagomé lattice, by a non-rigorous argument. In each case, two lattices are related by a substitution of portions of one lattice into the other, while applying an appropriate transformation to the parameters in the percolation model. In the cases considered by Wierman (1981, 1984), transformations provide the equivalence of two models, while in Ottavi's case an exact transformation does not exist. Motivated by this previous work, we propose a modified 'substitution method' which can be rigorously verified. The method has the advantage of providing both upper and lower bounds. In fact, by considering larger portions of the lattices as the basic units of substitution, sequences of upper and lower bounds are obtained. While the computations become increasingly unwieldy, the first two bounds have been computed for the Kagomé lattice, and suggest that the bounds converge rapidly to the true critical probability value, although there is no proof of convergence.

To illustrate the method, and familiarize the reader with the basic ideas, we begin §2 by calculating the first of the sequence of upper and lower bounds for the Kagomé lattice: $.5182 \leq p_c(\mathcal{K}) \leq .5413$. The best previous upper bound, derived by the contraction principle of Wierman (1988), was $p_c(\mathcal{K}) \leq .6180$, while the best lower bound was by containment

FIG. 1. The Kagomé lattice.

in the bowtie lattice, giving $p_c(\mathcal{K}) \geq .4045$. Later in §2, the upper bound is improved further, to $p_c(\mathcal{K}) \leq .5335$, by computing the second bound in the sequence.

The bounds obtained contradict an early Monte Carlo estimate of $.449 \pm .032$ by Dean (1963), and a renormalization group method estimate of .4697 by Murase and Yuge (1979). A Monte Carlo estimate of .526 by Neal (1972) is consistent with these bounds. It is rare to have sufficiently accurate rigorous bounds to rule out such estimates.

The substitution method introduced and applied to the Kagomé lattice in §2 may also be applied to other lattices. Preliminary work on the pentagon lattice bond percolation model indicates substantial improvement over the best previous bounds, obtained by Wierman (1988) by the contraction principle. Research in progress is investigating the possibility of extending the method to site percolation models, and suggests that the best current bounds for the square lattice site model may be improved.

Some necessary definitions and background material are included in the description of the substitution method presented in §2. The proof itself is given in §3. It shows the equivalence of two partial orders on the set of probability measures on a partially ordered set.

2. Kagomé Lattice Computations

We begin by illustrating the computation of bounds for the Kagomé lattice bond percolation critical probability, deferring the justification for the computations until §3. The Kagomé lattice is shown in Figure 1. It arises as the dual graph of the dice lattice, and also as the covering graph or line graph of the hexagonal lattice.

FIG. 2. Superposition of a triangle and a three-star.

Comparison with the Hexagonal Lattice

Note that the Kagomé lattice may be partitioned into disjoint triangles. By substituting a three-star for each triangle in $\mathcal{K}$, we obtain the graph $\mathcal{H}^\star$, which may be recognized as a subdivision of the hexagonal lattice $\mathcal{H}$ with one vertex subdividing each edge of $\mathcal{H}$. Since the critical probability of bond percolation on $\mathcal{H}$ is exactly $1-\sin\frac{\pi}{18}$ (see Wierman 1981), the bond percolation critical probability of $\mathcal{H}^\star$ is $q_0 = \{1 - 2\sin\frac{\pi}{18}\}^{1/2} \approx .807901$. In the remainder of this section, we first construct two probability measures on partitions of the vertices on the boundary of the triangle and the three-star, derived from the bond percolation models on the Kagomé and subdivided hexagonal lattices. We introduce a concept of stochastic ordering which allows us to compare these probability measures, and determine a parameter value p_L so that the probability measure corresponding to percolation on $\mathcal{K}$ is stochastically smaller than that associated with $\mathcal{H}^\star$ with parameter .807901, and a parameter value p_U such that the reverse holds. In §3, we show that p_L and p_U are in fact lower and upper bounds for $p_c(\mathcal{K})$.

Boundary Partitions

Consider a three-star and a triangle superimposed as in Figure 2, denoting the vertices on the boundary by A, B, and C. Any configuration (a designation of bonds as open and closed) on the triangle partitions the boundary vertices $\{A, B, C\}$ into clusters of vertices which are connected by open bonds, and similarly for configurations on the three-star. Each such *boundary partition* may be denoted by a sequence of vertices and vertical bars, where vertices are in distinct open clusters if and only if they are separated by a vertical bar.

The percolation model on the Kagomé lattice with parameter p induces a probability measure on the set of boundary partitions, in which the probability of a particular boundary partition is the sum of the probabilities of all configurations on the triangle which produce that boundary partition. Simple calculations show that this probability measure, which we denote by P_p^K, is given by

$$P_p^K[ABC] = 3p^2(1-p) + p^3,$$
$$P_p^K[AB \mid C] = P_p^K[AC \mid B] = P_p^K[A \mid BC] = p(1-p)^2,$$
$$P_p^K[A \mid B \mid C] = (1-p)^3.$$

Similarly, a different probability measure on the boundary partitions is determined by the percolation model on the subdivision of the hexagonal lattice with parameter q. We denote this probability measure by P_q^H, and compute that

$$P_q^H[ABC] = q^3,$$
$$P_q^H[AB \mid C] = P_q^H[AC \mid B] = P_q^H[A \mid BC] = q^2(1-q),$$
$$P_q^H[A \mid B \mid C] = 3q(1-q)^2 + (1-q)^3.$$

We will compare these two probability measures to derive the critical probability bounds for the Kagomé lattice.

The Partition Lattice

For two boundary partitions π and σ, we say that σ *dominates* π, denoted $\pi \leq \sigma$, if any two elements u and v that are in a cluster in π are also in a cluster in σ. Equivalently, $\pi \leq \sigma$ if and only if every cluster of π is wholly contained in a cluster of σ, or, conversely, every cluster of σ fully decomposes into clusters of π. If this is the case, π is called a *refinement* of σ. The set of boundary partitions on a given graph, when ordered by refinement, is a partially ordered set which is in fact a lattice, called the *partition lattice*.

In our example above, we see that ABC dominates each of $AB \mid C$, $AC \mid B$, and $A \mid BC$ in the refinement ordering, which in turn each dominate $A \mid B \mid C$.

Stochastic Ordering of Probability Measures on Partially Ordered Sets

Let $(S, \leq)$ be a finite partially ordered set (also called a *poset*). A function $P : S \to [0,1]$ is a *probability measure on S* if $P(s) \geq 0$ for all $s \in S$ and $\sum_{s \in S} P(s) = 1$. P may be defined on subsets of S by $P[A] = \sum_{s \in A} P(s)$. (Note that we use the same notation for the probability measure and its frequency function.)

A *filter* in a partially ordered set S is a subset $F \subset S$ such that if $g \geq f$ and $f \in F$, then $g \in F$. For $A \subset S$, the set $\{x \in S : x \geq a$ for some $a \in A\}$ is a filter, denoted $F(A)$, called the *filter generated by A*.

For two probability measures P and Q defined on a partially ordered set S, we say that P is *stochastically smaller* than Q, denoted $P \leq_S Q$, if for each filter F, $P[F] \leq Q[F]$. If the partially ordered set is a subset of the real line with the usual ordering, this definition agrees with the usual concept of stochastic ordering. Note that two probability measures may be incomparable with respect to the stochastic partial ordering $\leq_S$. Any filter is generated by its minimal elements. Thus, it is not necessary to check the inequality for filters generated by all subsets, but only for the filters generated by sets called anti-chains (in which all elements are incomparable).

Computation of Bounds

In §3, it is shown that if $P_p^K \leq_S P_{q_0}^H$, then p is a lower bound for the critical probability of the bond percolation model on the Kagomé lattice, and that if $P_{q_0}^H \leq_S P_p^K$, then p is an upper bound for the critical probability of the bond percolation model on the Kagomé lattice. Therefore, to compute a lower bound for $p_c(\mathcal{K})$, we solve for the largest p satisfying the following four inequalities: from the filter consisting of only ABC,

$$3p^2(1-p) + p^3 \leq q_0^3;$$

from the filters generated by one, two, or all three of $AB \mid C$ and $AC \mid B$ and $A \mid BC$,

$$\begin{aligned} p(1-p)^2 + 3p^2(1-p) + p^3 &\leq q_0^2(1-q_0) + q_0^3 \\ 2p(1-p)^2 + 3p^2(1-p) + p^3 &\leq 2q_0^2(1-q_0) + q_0^3 \\ 3p(1-p)^3 + 3p^2(1-p) + p^3 &\leq 3q_0^2(1-q_0) + q_0^3. \end{aligned}$$

(The filter generated by $A \mid B \mid C$ consists of the entire partially ordered set, which has probability one in both measures.) Numerical solution of the inequalities produces the upper bound

$$p_c(\mathcal{K}) \leq .5413.$$

Reversing all four inequalities and solving, we obtain the lower bound

$$p_c(\mathcal{K}) \geq .5182.$$

Sequences of Bounds

By partitioning the Kagomé lattice into larger regions, and carrying out the same process of substitution of corresponding regions of the $\mathcal{H}^*$ lattice, a sequence of bounds may be obtained.

To illustrate, a second pair of bounds for $p_c(\mathcal{K})$ may be obtained by considering a region consisting of two adjacent triangles, shown in Figure 3.

FIG. 3. Superposition of a pair of triangles and a pair of three-stars, used in determining the second set of critical probability bounds.

For the percolation model on $\mathcal{K}$ with parameter p, the probability measure P_p^K is given by:

$$P_p^K[ABCD] = [3p^2(1-p)+p^3]^2,$$

$$\begin{aligned} P_p^K[ABC \mid D] = P_p^K[ABD \mid C] = P_p^K[ACD \mid B] = \\ = P_p^K[BCD \mid A] = [3p^2(1-p)+p^3]p(1-p)^2, \end{aligned}$$

$$P_p^K[AB \mid CD] = 2[3p^2(1-p)+p^3]p(1-p)^2 + p^2(1-p)^4,$$

$$\begin{aligned} P_p^K[AC \mid B \mid D] = P_p^K[AD \mid B \mid C] = P_p^K[BD \mid A \mid C] = \\ = P_p^K[BC \mid A \mid D] = p^2(1-p)^4, \end{aligned}$$

$$\begin{aligned} P_p^K[AB \mid C \mid D] = P_p^K[CD \mid A \mid B] = \\ = p(1-p)[4p(1-p)^3 + (1-p)^4 + p^2(1-p)^2] + (1-p)^4p^2. \end{aligned}$$

For the percolation model on $\mathcal{H}^*$ with parameter q_0, we determine $P_{q_0}^H$ to be:

$$P_{q_0}^H[ABCD] = q_0^6,$$

$$\begin{aligned} P_{q_0}^H[ABC \mid D] = P_{q_0}^H[ABD \mid C] = P_{q_0}^H[ACD \mid B] = \\ = P_{q_0}^H[BCD \mid A] = q_0^5(1-q_0), \end{aligned}$$

$$P^H_{q_0}[AB \mid CD] = q_0^4(1-q_0^2),$$

$$P^H_{q_0}[AC \mid B \mid D] = P^H_{q_0}[AD \mid B \mid C] = P^H_{q_0}[BD \mid A \mid C] =$$
$$= P^H_{q_0}[BC \mid A \mid D] = q_0^4(1-q_0)^2,$$

$$P^H_{q_0}[AB \mid C \mid D] = P^H_{q_0}[CD \mid A \mid B] =$$
$$= q_0^2[(1-q_0)^2 + 2q_0(1-q_0)(1-q_0^2)].$$

Numerical solution of the inequalities generated by all filters provide the bounds

$$.5182 \leq p_c(\mathcal{K}) \leq .5335.$$

The upper bound is an improvement over the first calculation, but the lower bound is identical, since the inequality generated by the filter consisting of $ABCD$ is equivalent to that in the first step, and is the active constraint. The smallest region that will produce an improvement in the lower bound is a ring of six triangles in $\mathcal{K}$, for which the computations have not been completed.

If one considers a sequence of larger regions, each a union of copies of its predecessor, one will obtain monotone sequences of upper and lower bounds. It is not known if these sequences converge to the true critical probability value, although the computational results suggest rapid convergence.

3. Justification

The Flow Ordering

Let Q be a probability measure on a partially ordered set $(S, \leq)$. If $s \in S$ with $Q[s] > 0$, and $t \in S$ with $t < s$, we may construct a new probability measure P by moving probability mass x, $0 < x < Q[s]$, from s to t. Formally, define P by letting $P[s] = Q[s] - x$, $P[t] = Q[t] + x$, and $P[u] = Q[u]$ for $u \neq s, t$. Since the construction moves probability downward in the poset (from one element to another that it dominates), we say that P is constructed from Q by a *downward flow.*

The concept of downward flow leads to a partial ordering on the set of probability measures on the poset $(S, \leq)$. We call a finite sequence of downward flows a *flow sequence.* A flow sequence on a subset F of S moves probability only between elements of F, leaving the probability measure unchanged elsewhere. Define the *flow ordering*, $\leq_F$, by letting $P \leq_F Q$ if and only if P may be constructed from Q using a flow sequence.

The downward flow operation may be interpreted in terms of random variables. The probability measure Q is the distribution of an S-valued random variable X. A downward flow moving probability mass x in Q from s to t, where $s > t$, produces a probability measure which is the distribution of the S-valued random variable which takes the value X if $X \neq s$ or if $B_{x,s,t} = 0$, and the value t if $X = s$ and $B_{x,s,t} = 1$, where $B_{x,s,t}$ is a Bernoulli random variable, independent of X, with $P[B_{x,s,t} = 1] = x/Q(s)$. We will denote this random variable by $X * B_{x,s,t}$. Thus, if $P \leq_F Q$ and X has distribution Q, there exist Bernoulli random variables B_{x_i,s_i,t_i}, $i = 1, 2, \dots, n$, (corresponding to a flow sequence) such that $X * B_{x_1,s_1,t_1} * \cdots * B_{x_n,s_n,t_n}$ has distribution P.

Inequalities Between Percolation Probabilities

Consider probability measures P_p^K and P_q^H on a partition lattice derived from percolation models on the Kagomé and $\mathcal{H}^*$ lattices. Fix the parameter values p and q so that $P_p^K \leq_F P_q^H$. We will construct related bond percolation models on $\mathcal{K}$ and $\mathcal{H}^\star$ by the following procedure.

Superimpose $\mathcal{K}$ on $\mathcal{H}^*$ so that each triangle in $\mathcal{K}$ exactly contains one three-star of $\mathcal{H}^*$. Construct the percolation model on $\mathcal{H}^\star$ as usual, by declaring each edge to be open with probability q, independently of all other edges. This creates a random boundary partition X_σ with probability distribution P_q^H on the set of boundary vertices of each star-triangle pair σ in $\mathcal{H}^*$.

Since $P_p^K \leq_F P_q^H$, there is a flow sequence which produces P_p^K from P_q^H. Thus, for each star-triangle pair σ there exist independent Bernoulli random variables (independent of those for other star-triangle pairs) B_{σ,x_i,s_i,t_i} such that $Y_\sigma = X_\sigma * B_{\sigma,x_1,s_1,t_1} * \cdots * B_{\sigma,x_n,s_n,t_n}$ has distribution P_p^K exactly.

Define vertices u and w of $\mathcal{K}$ to be in the same open cluster if and only if there exists a sequence of vertices $u = v_0, v_1, v_2, \dots, v_{k-1}, v_k = w$ for some k, such that for each $i = 1, 2, \dots, k$, v_{i-1} and v_i are on a common star-triangle pair σ and are in the same boundary partition set in Y_σ. With this definition, for each connected subgraph C in $\mathcal{K}$, the probability that C is an open cluster is identical in the model just described and in the bond percolation model on the Kagomé lattice with parameter p.

Let $C(\mathcal{H}^*)$ denote the open cluster in $\mathcal{H}^*$ containing a fixed vertex $v \in \mathcal{K}$, and let $C(\mathcal{K})$ denote the open cluster in $\mathcal{K}$ containing v. By construction, the boundary partition of each triangle in $\mathcal{K}$ is a refinement of the boundary partition of the corresponding three-star in $\mathcal{H}^*$. Therefore, $u \in C(\mathcal{K})$ implies $u \in C(\mathcal{H}^*)$, so $C(\mathcal{K}) \subset C(\mathcal{H}^*)$. If $q < p_c(\mathcal{H}^*)$, then $P_q^H[|C(\mathcal{H}^*)| = \infty] = 0$, so $P_p^K[|C(\mathcal{K})| = \infty] = 0$ also. Thus, $q < p_c(\mathcal{H}^*)$ implies $p < p_c(\mathcal{K})$.

It follows that to compute a lower bound for $p_c(\mathcal{K})$ it is sufficient to find the largest value of p such that P_p^K is smaller than $P_{q_0}^H$ in the flow ordering. Similar reasoning applies to the determination of upper bounds. In order to conveniently compute such values of p, in the following we show that the flow ordering is equivalent to the stochastic ordering.

Combinations of Flow Sequences

Let f and g be flow sequences on a poset $(S, \leq)$. For $\lambda \in [0, 1]$, define λf to be the sequence of flows which moves probability mass λa from s to t whenever f moves a from s to t. Define $f + g$ to be the downward flow sequence which moves $a + b$ from s to t whenever f moves a and g moves b from s to t.

Suppose Q_f and Q_g are the probability measures obtained from Q by applying the downward flow sequences f and g respectively. Then the measure Q_λ, corresponding to $f_\lambda = \lambda f + (1-\lambda)g$, satisfies $Q_\lambda[s] = \lambda Q_f[s] + (1 - \lambda)Q_g[s]$ for all $s \in S$, so is a linear function of λ at each element of S.

Equivalence of Stochastic Ordering and Flow Ordering

It is easy to see that if P is obtained from Q by a flow sequence, then P is stochastically smaller than Q. (It suffices to check this for a single downward flow.) We next show that the converse is true, so, in fact, the partial orders $\leq_S$ and $\leq_F$ on the set of probability measures are equivalent.

Let P and Q be probability measures on a partition lattice S, satisfying $P \leq_S Q$. The *excess* of Q relative to P at a set V of elements of S is defined by $e_{Q/P}(V) = \max \{Q[V] - P[V], 0\}$. Similarly, the deficit of Q relative to P on V is defined by $d_{Q/P}(V) = \max \{P[V] - Q[V], 0\}$.

Suppose that there does not exist a flow sequence which produces P from Q. Consider the set $\mathcal{F}$ of filters F for which no flow sequence on F can produce a probability Q' from Q which satisfies $Q'[s] \geq P[s]$ for all $s \in F$. $\mathcal{F}$ is non-empty, since the entire poset S is in $\mathcal{F}$ by hypothesis.

Let A be a minimal filter in $\mathcal{F}$ (when $\mathcal{F}$ is ordered by set inclusion). Consider the probability measure Q' obtained from Q by a flow sequence on A which minimizes the sum of deficits (of Q' relative to P) of elements in A. If there exist elements of A which are not minimal and have positive excesses, allow the excess to flow downward so that only minimal elements of A have positive excesses. This cannot increase the deficit sum, since it removes probability only from elements with positive excesses. It also cannot decrease the deficit sum, since the original flow sequence minimizes the deficit sum. Denote the resulting flow sequence by f_0 and the corresponding probability measure by Q_0.

If Q_0 has no positive excess relative to P at any element of A, then since by hypothesis there is an element with a positive deficit, the filter A satisfies $P[A] > Q_0[A]$. However, the flow sequence f_0 kept all Q-probability in A while constructing Q_0, so $Q_0[A] = Q[A]$, which implies that $P[A] > Q[A]$. This exhibits a filter for which the stochastic ordering condition fails, so $P \leq_S Q$ does not hold.

If Q_0 has a positive excess relative to P at an element of A, let E denote the set of elements with positive excesses and D denote the set of elements with positive deficits.

Note that the set $A \setminus E$ is a filter, since all elements of E are minimal in A. By the minimality of A, there exists a flow sequence f_1 on $A \setminus E$ which produces a probability measure Q_1 satisfying $Q_1[s] \geq P[s]$ for all $s \in A \setminus E$.

Consider the flow sequences $f_\lambda = \lambda f_0 + (1-\lambda) f_1$, where $0 < \lambda < 1$, denoting the resulting probability measures by Q_λ.

If $s \in A \setminus (E \cup D)$, we have $P[s] = Q_0[s] \leq Q_1[s]$ and thus by linearity $Q_\lambda[s] \geq P[s] = Q_0[s]$ for all λ.

If $s \in E$, then by definition $Q_0[s] > P[s]$. Although $Q_1[s]$ may be less than $P[s]$, by linearity there exists $\epsilon_s > 0$ such that $Q_\lambda[s] \geq P[s]$ for all $\lambda < \epsilon_s$. Since E is a finite set, there exists ϵ_E such that for all $s \in E$ and for all $\lambda \leq \epsilon_E$ we have $Q_\lambda[s] \geq P[s]$.

If $s \in D$, then $Q_0[s] < P[s]$ and $Q_1[s] \geq P[s]$, so $Q_\lambda[s]$ is a strictly increasing function of λ, and thus the deficit of Q_λ relative to P at s is strictly decreasing as a function of λ.

Thus, for $\lambda \leq \epsilon_E$, Q_λ has no positive deficits relative to P except at elements of D, at which the deficits are strictly decreasing functions of λ. Hence, each f_λ, $0 < \lambda < \epsilon_E$, is a flow sequence on A which produces a smaller sum of deficits at elements of A than f_0. Since this is a contradiction, there actually is no element s with $e_{Q_0/P}(s) > 0$.

Therefore, if there is no flow sequence that can obtain P from Q, there exists a filter A such that $P[A] > Q[A]$, so $P \leq_S Q$ does not hold. Hence, the partial orderings $\leq_F$ and $\leq_S$ on the set of probability measures on a poset S are equivalent.

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