Estimating Critical Probabilities Using Bond Percolation Simulations

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1 Introduction

Many areas of graph theory have interesting and practical applications, such as in modeling information networks, social interactions, and physical materials. One such area is percolation theory, which is a sub-area of graph theory and probability theory that studies the properties of random subgraphs that emerge when edges in specific lattices or graphs are independently retained with some probability p [Gri99].

Specifically, under the bond percolation model, given a lattice graph G and a probability p, each edge in G is retained with probability p (and said to be open). The subgraph produced by this process is particularly interesting, as for certain values of p, large connected components can become spontaneously more-likely to appear. Moreover, for infinite lattices in particular it is interesting to study the critical probability p_c, which is the probability p at which an infinitely large open cluster has a nonzero chance of appearing.

While the critical probabilities for some infinite lattices such as the 2-dimensional square and triangle lattices have been directly proven [Kes80, Gri99], finding these values for higher-dimensional lattices remains an open problem. Instead, many have turned to upper and lower bounds, and random simulations to estimate these critical probabilities.

In this paper, we consider estimations for the critical probability, denoted p_c, of the 2-dimensional infinite square lattice by directly proving that $0 < p_c(2) < 1$, and give a brief overview of how its exact value was found. Additionally, we simulate bond percolation on the 2-dimensional square and triangle lattices, 3-dimensional cube lattice, and some complete graphs to provide estimations of their critical probabilities and compare these values to directly proven or accepted estimated results.

2 Background

It should be noted that there are two main models for percolation: bond percolation and site percolation. While bond percolation focuses on retaining opened edges in a lattice with probability p, site percolation models study the behavior of lattices when vertices are considered opened or closed. In this paper, we will only consider bond percolation, which is considered to have more accessible results. However it is interesting to briefly note that p_c of a lattice in the bond percolation model is less than or equal to p_c of the same lattice in the equivalent site percolation model [Gri99, Thm. 1.33].

2.1 Lattices

When discussing bond percolation, we are most often interested in studying the behavior of open components on infinite lattices, however, we do consider finite simulations to describe

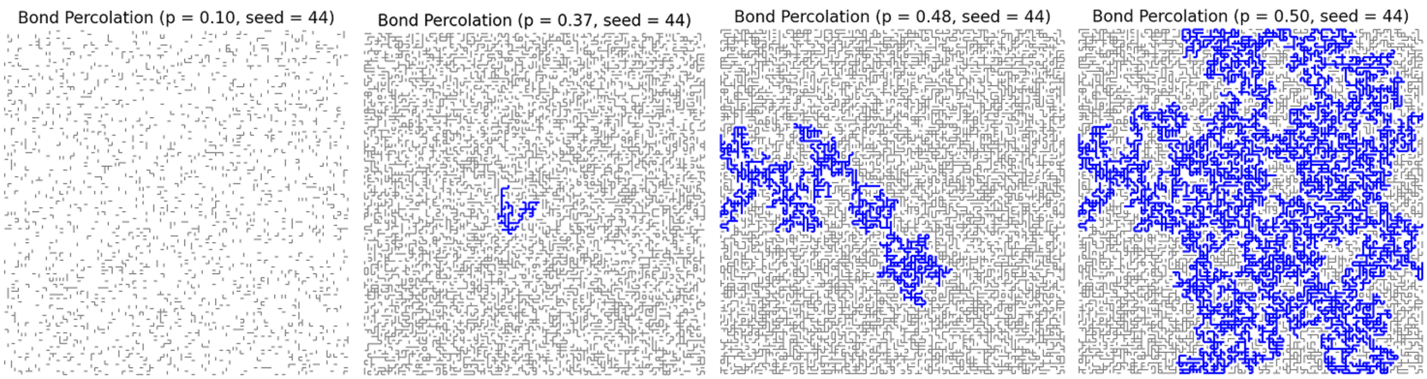

Figure 1: Simulation of bond percolation with different percolation probabilities in a 100x100 square lattice. Gray edges signify open edges, and blue edges are part of the connected open component containing the origin.

approximate values in infinite graphs in Section 4. First, a graph is called planar if it can be drawn on a plane without any of its edges crossing [W$^+$01, pg. 235]. Let the graph $\mathbb{L}^d$ represent the d-dimensional cubic lattice, which is a plane graph where $\mathbb{Z}^d$ is its set of vertices and its edge set consists of all pairs of vertices with a Euclidean distance of one.

The dual of a planar graph G is the plane graph G' that is constructed by placing vertices on the faces of G, and adding edges between two vertices in G' only if their corresponding faces in G are adjacent [W$^+$01, pg. 236]. Note that $\mathbb{L}^2$ is a special planar graph that is self-dual, which means that it is isomorphic to its planar dual. This can be seen as every vertex in $\mathbb{L}^2$'s dual is positioned in the center of a unit face, which corresponds to the set $\{x + (\frac{1}{2}, \frac{1}{2}) | x \in \mathbb{Z}\}$ [Gri99, pg. 17]. Additionally, every pair of vertices with a Euclidean distance of one will also be connected. Therefore, we can define an obvious isomorphism to shift the vertices (and corresponding edges) in this dual by $\frac{1}{2}$ units in both dimensions to recover $\mathbb{L}^2$.

2.2 Probability

While this paper takes a mostly graph theory centric approach to percolation, we must also introduce some concepts from probability theory to properly analyze the behavior of random configurations of open edges in a lattice.

Let $\Omega = \Pi_{e \in E(\mathcal{L})}\{0, 1\}$ denote the configuration space, which is the set of all possible assignments ω that denote what state the edges in our lattice $\mathcal{L}$ can take on. For any edge $e \in E(\mathcal{L})$, e is open in our lattice if $\omega(e) = 1$ and closed otherwise. Therefore, each ω fully realizes a bond percolation process across all edges in our lattice. Next, let $K(\omega)$ denote the set of open edges under the configuration ω. To simulate bond percolation independently across all edges, we can generate an independent and uniformly distributed random variable $X(e) \in [0, 1]$ for each edge. Then, for any fixed $p \in [0, 1]$ we can define $\eta_p \in \Omega$

$$\eta_p = \begin{cases} 1 & \text{if X(e) < p,} \\ 0 & \text{if X(e) } \geq \text{ p. [Gri99, } Eq.\ q.4] \end{cases} \tag{1}$$

Therefore, as p increases, the set of open edges in the first process must be a subset of the set of open edges in the newest process. This acts like a fixed seed that will continue to percolate all bonds in progressive configurations of the lattice until all edges are open.

3 Critical Probability

The most important question of percolation theory on infinite lattices is finding the critical probability p_c, at which there is a nonzero probability that an infinite open cluster appears when open edges are kept with this probability. This value serves as a threshold between a sub-critical phase where a lattice contains small sparely distributed open components, and a super-critical phase where a single infinite connected component is likely to exist. The probability that a vertex belongs to such an infinite open cluster C is called the percolation probability, and is denoted as

$$\theta(p) = P_p(|C| = \infty) \text{ [Gri99}, Eq.\ 1.6]. \tag{2}$$

Without loss of generality, it has been shown that we can assume C refers to the open cluster containing the origin of a lattice [Gri99]. Using this definition, we can explicitly define the critical probability of the d-dimensional cubic lattice as

$$p_c(d) = \sup\{p \mid \theta(p) = 0\} \text{ [Gri99}, Eq.\ 1.8]. \tag{3}$$

It will be important to show that $\theta(p)$ is non-decreasing. Consider that for each $p \in [0, 1]$ we have defined $\eta_p(e)$. It is clear that for any two p_1 and p_2 such that $p_1 < p_2$, for all edges e in our lattice, $\eta_{p_1}(e) \leq \eta_{p_2}(e)$. Therefore, we cannot increase p yet realize a smaller number of open edges in our overall lattice, thus $\theta(p)$ can never decrease in value as p increases.

3.1 Bounds for p_c on $\mathbb{L}^d$

One of the most important problems in the history of percolation theory was finding the critical probability of $\mathbb{L}^2$. In order to first approximate it, early theorems focused on establishing upper and lower bounds for p_c. We now provide an overview of such a proof.

Theorem 3.1. *For all natural numbers $d \geq 2$, the critical probability $p_c(d)$ for bond percolation on the lattice $\mathbb{L}^d$ satisfies $0 < p_c(d) < 1$.* [Gri99]

Proof. Fix $d \geq 2$ in $\mathbb{N}$. First, consider that the critical probability at which an infinite cluster occurs in $\mathbb{L}^d$ must be greater than or equal to the critical probability in $\mathbb{L}^{d+1}$. Notice since each vertex in $\mathbb{L}^{d+1}$ has $d + 1$ coordinates, for any vertex v in $\mathbb{L}^d$ there exists a coordinate u in $\mathbb{L}^{d+1}$ where the first i coordinates of v and u are the same, and u's $(i+1)^{th}$ coordinate is 0 (or some other constant value). Through this mapping, we can embed both the vertex and edge set of $\mathbb{L}^d$ into $\mathbb{L}^{d+1}$ (similar to how we can embed a copy of the i^{th}-dimensional hypercube into the $(i+1)^{th}$-dimensional hypercube). Therefore, $p_c(d+1)$ is clearly at most $p_c(1)$, as if an infinite open component exists in $\mathbb{L}^d$ it would also exist in $\mathbb{L}^{d+1}$ where the $(i + 1)^{th}$ vertex coordinate is fixed through this mapping. Thus,

$$p_c(d + 1) \leq p_c(d) \text{ [Gri99}, Eq.\ 1.9]. \tag{4}$$

Therefore, to prove the remaining inequality we must show that $p_c(d)$ is bounded below by zero and $p_c(2)$ is bounded above by one. Then, for all natural numbers $d \geq 3$, we would have $0 < p_c(d) \leq p_c(2) < 1$.

To prove the lower bound, we will consider how $\theta(p)$ behaves as p approaches zero. Define $\sigma(n)$ to be the number of paths in $\mathbb{L}^d$ that begin at the origin 0^d and contain n edges, and let $N(n)$ be the number of such paths that are open. Since each of these path contain n edges that are individually open with probability p, any full path is open with probability p^n. Therefore, $E_p(N(n)) = p^n\sigma(n)$ can be used to represent the expected number of open walks for a given configuration at p. However, if there exists an infinite open cluster C in $\mathbb{L}^d$, there must exist open paths of length n for all $n \in \mathbb{N}$ starting at any vertex inside the cluster. This is because all vertices in C are connected through open edges, and C contains a path of infinite length.

Without loss of generality, assume that the origin is a vertex reachable in C. If such a C exists, then

$$\theta(p) \leq P_p(N(n) > 1) \leq E_p(N(n)) = p^n \sigma(n), \tag{5}$$

for every n, as there must be at least one reachable path of length n from the origin for all values of n if $|C| = \infty$. Next, consider the connective constant $\lambda(d) = \lim_{n\to\infty}(\sigma(n)^{1/n})$ where $\sigma(n)$ is the number of self-avoiding walks (that never repeat vertices) of $\mathbb{L}^d$ that begin at the origin and have length n. If $p\lambda(d) < 1$, then the right hand side of this equation must go to 0 as n increases, so $0 < \frac{1}{\lambda(d)} \leq p_c(d)$ as a result. Therefore, $p_c(d)$ must be bounded below by 0.

Finally, consider the upper bound of the critical probability in $\mathbb{L}^2$ (i.e., $p_c(2)$). In Section 2, we showed that $\mathbb{L}^2$ was self-dual. The idea behind proving this upper bound relies on the fact that if the open cluster C containing the origin is finite, then we can form a closed cycle (and hence circuit) around it using edges in the dual of $\mathbb{L}^2$, as there will exist no infinite path crossing this surrounding cycle. Therefore, $|C| < \infty$ if and only if the origin of $\mathbb{L}^2$ lies in the interior of a closed circuit formed from its dual. Now, we proceed by counting such circuits and bound the probability that any of them exist to determine an upper bound for p_c. Let $\rho(n)$ be the number of such closed circuits with length n around a finite open cluster containing the origin of $\mathbb{L}^2$. Consider that if these circuits surround the open cluster, they must pass through a vertex of the form $(k + \frac{1}{2}, \frac{1}{2})$ for some $0 \leq k < n$, but cannot pass through vertices if $k \geq n$. If they did, then the circuit would be too long as it would need to wrap around the origin and return to this vertex (which would be impossible as the circuit has max length n). Based on these constraints, the number of self-avoiding walks can be estimated to be at most $\rho(n) \leq n\sigma(n-1)$.

Let γ be a circuit in the dual that surrounds an open component containing the origin, $M(n)$ be the number of such closed circuits with length n, and let $q = 1 - p$. We can bound the number of these circuits using the number of self-avoiding walks using $\rho(n) \leq n\sigma(n-1)$, to get an upper bound on the total probability that any circuit γ is closed [Gri99, pg. 18].

Specifically, this sum converges to $\frac{1}{2}$ if p is sufficiently large ($p > \pi$, $0 < \pi < 1$) implying that the probability that any such closed circuit surrounds the origin approaches 0. Hence, if no circuit surrounds the origin, $|C|$ must be infinite. Thus $P_p(|C| = \infty) = P_p(M(n) = 0 \text{ for all } n) \geq \frac{1}{2}$ if $p > \pi$, so the probability an infinite cluster exits can be nonzero when $p < 1$. $\square$

While it has been proven that $p_c(0) = 1$ and $p_c(2) = \frac{1}{2}$ [Kes80], finding the exact critical values for higher dimensional square lattices is still an open problem. For example, we have shown that for for $\mathbb{L}^3$, the value of $p_c(3)$ must be between $\frac{1}{6}$ and $\frac{1}{2}$, and through simulations it is estimated to be roughly around 0.2488 to 0.25 [LZ98, Gri99].

3.2 Exact Values of p_c In Different Lattices

In order to find the exact value of $p_c(2)$, duality arguments were used based on the function $\chi(p)$, which represents the mean size of an open cluster containing the origin of a lattice. A new critical probability

$$p_T(d) = \sup\{p \mid \chi(p) < \infty\} \text{ [Gri99, } Eq. \text{ 5.3]} \tag{6}$$

was defined, where p_T is the value at which $\chi(p)$ goes from finite to infinite in $\mathbb{L}^2$. However, notice that this is related to the critical probability in the dual lattice of $\mathbb{L}^2$, as a finite open cluster C can only exist in $\mathbb{L}^2$ if there exists a closed circuit of closed edges surrounding C (and hence an open circuit in the dual).

Lattice	Critical Probability	Simulated Critical Probability
Square	0.5	0.4853
Triangle	$2\sin(\pi/18) \approx 0.3472$	0.3287
Cube	$\approx 02488^{+}$	0.2549
K_{50}	$\frac{1}{150} = 0.02$	0.0274
K_{100}	$\frac{1}{100} = 0.01$	0.0127
K_{150}	$\frac{1}{150} \approx 0.00667$	0.0076

$^{+}$Signifies estimated p_c.

Table 1: Comparison of known/estimated critical probabilities and simulated critical probabilities across different graphs.

Using this new critical probability and the dual argument idea, Russo, Seymour, and Welsh proved results for $\mathbb{L}^2$ which culminated in showing $p_T + p_c = 1$ by using certain crossing rectangles, and by arguing that p_T is related to the dual of $\mathbb{L}^2$ as above [Gri99]. Finally, Kesten proved that $p_T = p_c$ for $\mathbb{L}^2$, thus proving that $p_c(2) = \frac{1}{2}$ by combining this result with the previous equality [Kes80].

Using the structure of this dual argument the critical probabilities of other 2-dimensional lattices were found. These arguments utilized similar equalities by showing that p_c of a lattice $\mathcal{L}$ was equal to $1 - p_c(\mathcal{L}_d)$ (where $p_c(\mathcal{L}_d)$ is the critical probability of $\mathcal{L}$'s dual), even for graphs that were not self-dual [Gri99, pg. 53]. These include the 2-dimensional triangle and hexagonal lattices, whose critical probabilities were proven to be $2\sin(\frac{\pi}{18})$ and $1 - 2\sin(\frac{\pi}{18})$, respectively.

4 Simulations of Critical Probabilities

While duality arguments were useful in proving the critical probabilities of 2-dimensional lattices, similar techniques could not be generalized to lattices in higher dimensions [Gri99]. For many lattices, including special lattices like $\mathbb{L}^3$ that could be used to closer model percolation in the real-world, finding p_c remains an open problem. Due to the complexity that would be required for proving such results, many have turned to computer simulations to get a better understanding of how bond percolation behaves in such lattices [LZ98, Gri99].

For this project, finite 2-dimensional square, triangle, and complete graphs were simulated alongside a finite 3-dimensional cube graph using Python. To simulate bond percolation in these graphs, the size of the connected component containing the origin was recorded as p was varied between 0 and 1 (since we have shown that p_c must be within these bounds). This was done across multiple seeded values so the average size of this component for each value of p could be calculated. From the resulting graphs, the critical probability could be approximated by finding regions where the slope of the graph rapidly increased. By increasing the size of these simulations, we could better estimate the true probability value of p_c for infinite lattices. Additionally, interactive simulations were also created to visually demonstrate how varying p even slightly above the critical probability leads to the sudden emergence of large connected components (which can be seen in Figure 1. The results of the estimated critical probabilities from these simulations is recorded in Table 1.

In particular, it should be noted that the simulation of bond percolation on a complete graph is similar to the structure of Erdős–Rényi random graphs. A Erdős–Rényi random graph over n vertices is a subgraph of a complete graph where each of the $\binom{n}{2}$ is individually included with probability p (denoted by denoted by $G(n,p)$) [AS08]. From this definition, it is clear that this random graph is similar to bond percolation on a finite complete graph. Similar to the critical probability in a bond percolation graph, Erdős–Rényi graphs are

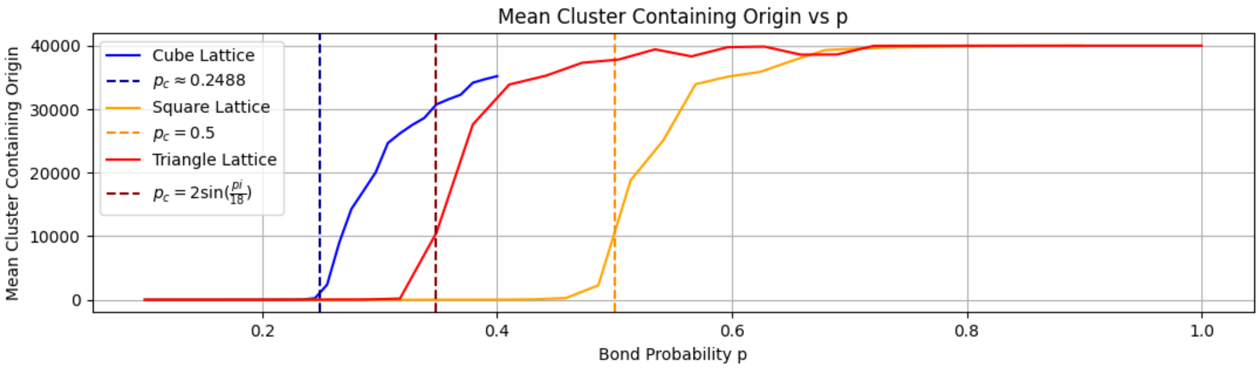

Figure 2: Simulations of multiple lattices and their estimated critical probabilities.

concerned with studying a phase transition at which certain values of p a random graph will go from being sparse with small independent components to containing a large component, similar to the sub and super critical phases of bond percolation. It is known that for $G(n, p)$, $\frac{1}{n}$ acts as the critical threshold where a large component is likely to exist if $p > \frac{1}{n}$ [AS08]. Table 1 shows the simulated results of bond percolation on three complete graphs, which found critical values similar to the phase transition of the equivalent Erdős–Rényi graphs over n vertices.

5 Conclusion

In conclusion, while the critical probability for some infinite lattices such as the 2-dimensional square and triangle lattices have been proven, p_c for higher dimensional lattices remains an open problem that can be estimated through simulations. From our own estimations, we found values for p_c that were relatively close to accepted values, however it is clear that much more precise estimations would require an intense amount of computation.

Acknowledgment

The code that was created to estimate the critical values and create the interactive simulations can be found at https://github.com/notred27/GraphTheory.

References

[AS08] Noga Alon and Joel H. Spencer. *The Probabilistic Method*. Wiley-Interscience, 3rd edition, 2008.

[Gri99] Geoffrey Grimmett. *Percolation*. Springer, 2 edition, 1999.

[Kes80] Harry Kesten. The critical probability of bond percolation on the square lattice equals 1/2. 1980.

[LZ98] Christian D Lorenz and Robert M Ziff. Precise determination of the bond percolation thresholds and finite-size scaling corrections for the sc, fcc, and bcc lattices. *Physical Review E*, 57(1):230, 1998.

[W+01] Douglas Brent West et al. *Introduction to graph theory*, volume 2. Prentice hall Upper Saddle River, 2 edition, 2001.