

Percolation Theory

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This essay describes percolation theory. Once percolation theory is defined, we explore applications to the renormalization group, computer simulations of potts models, and randomly punctured conducting sheets.

Lattice	# nn	Site percolation	Bond percolation
1d	2	1	1
2d Honeycomb	3	0.6962	$1 - 2 \sin(\pi/18) \approx 0.65271$
2d Square	4	0.592746	1/2
2d Triangular	6	1/2	$2 \sin(\pi/18) \approx 0.34729$
3d Diamond	4	0.43	0.388
3d Simple cubic	6	0.3116	0.2488
3d BCC	8	0.246	0.1803
3d FCC	12	0.198	0.119
4d Hypercubic	8	0.197	0.1601
5d Hypercubic	10	0.141	0.1182
6d Hypercubic	12	0.107	0.0942
7d Hypercubic	14	0.089	0.0787
Bethe lattice	z	$1/(z-1)$	$1/(z-1)$

Imagine a very large lattice of empty sites. At random, a site could be occupied with probability p or unoccupied with probability $1-p$. If we define a cluster as a set of occupied sites that can be traversed by jumping from neighbor to occupied neighbor, then site percolation theory is the study of such clusters. Two sites may also be attached with a bond with probability b or unattached with probability $1-b$. Bond percolation is the study of clusters formed by such a procedure, where analogously a cluster is defined as a collection of points that can be traversed by only travelling across occupied bonds. Finally, site-bond percolation theory has both sites and bonds that are filled at random, with bonds only permitted to be between occupied sites.

It is intuitively clear that the larger p and b are, the larger the average cluster is. At a certain threshold called p_c (or b_c), an infinite cluster forms. These critical thresholds are listed in the table above for various lattices. Note that analytic expressions for p_c are only known for a few cases. Above p_c , the infinite cluster takes up an increasingly greater share of the lattice points, and the remaining finite clusters shrink. The infinite cluster obviously contains every site when $p=1$. Near p_c , several quantities characterizing the system obey power laws, and exhibit universal behavior. It should be no surprise therefore that some of the machinery used for phase transitions can be applied to percolation theory.

The history of percolation theory goes back to the 1940s, to the work of Flory and Stockmayer who attempted to understand the process of small molecules with random bonds forming larger macromolecules, in a process called gelation. A seminal paper in 1957 by Broadbent and Hammersely could alternatively be called the start of percolation theory, where many of the terms such as p_c were defined, and "percolation" was coined.

One Dimensional Percolation

The first illustrative model we investigate is 1D percolation, which is simple enough to be solved exactly. We will see that many of the concepts introduced here generalize to more complicated cases. In this dimension, site and bond percolation are very similar, so we will restrict ourselves to

site percolation. In 1D, there is only one possible infinite cluster, that which extends from -infinity to infinity. Clearly $p_c=1$ is a necessity, for p^L goes to 0 for $p<1$ as L goes to infinity, and we cannot have a single empty site. Let's now calculate $n_s(p)$, the number of clusters of size s per lattice site. We require two boundary sites to be empty with probability $(1-p)$ each, and s consecutive occupied sites in between the boundary points, so

$$n_s(p) = p^s (1-p)^2 .$$

Note

$n_s(p) = (1-p)^2 \exp(s \ln(p)) = (p_c - p)^2 \exp(-s/s_\xi)$, where $s_\xi = -1/\ln(p) \propto (p_c - p)^{-1}$
 This expression begs us to define a critical exponent for the cutoff cluster size s_ξ , so we define

$$s_\xi \propto (p_c - p)^{-1/\sigma}$$

, where $\sigma=1$ for 1D percolation. Another critical exponent is associated with $S(p)$, the mean cluster size. The probability that an arbitrary site belongs to an s -cluster is given by $s n_s(p)$, and by Bayes' Theorem the probability a site belongs to an s -cluster given that is occupied is

$$w_s = \frac{s n_s(p)}{\sum_{s=1}^{\infty} s n_s(p)} .$$

Thus the mean cluster size is

$$S(p) = \sum_{s=1}^{\infty} s w_s = \frac{1+p}{1-p} = \frac{p_c + p}{p_c - p} \propto (p_c - p)^{-\gamma} ,$$

where $\gamma=1$, defining the critical exponent γ .

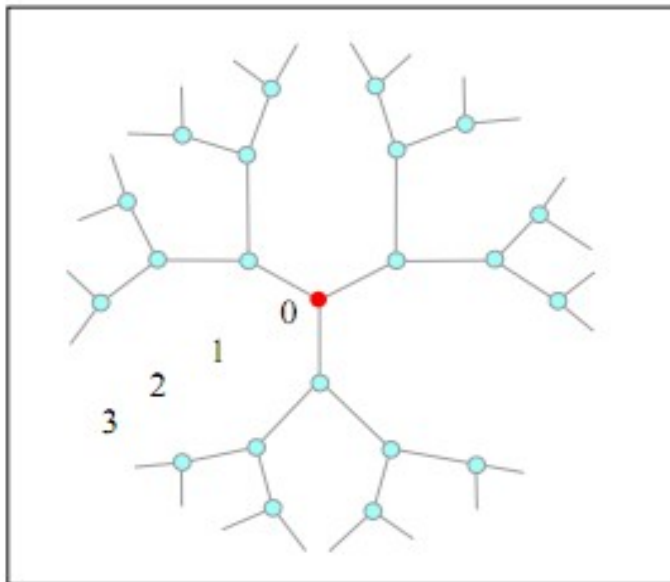
Another system that can be solved exactly to give us more critical exponents is percolation on a Bethe lattice, or Cayley tree. In a Bethe lattice, every point has z neighbors, the first 4 generations of a $z=3$ Bethe lattice is pictured to the right. For a Bethe lattice, $p_c=1/(z-1)$. Let $P(p)$ be the probability that an arbitrary site belongs to the infinite cluster. It can be shown via consideration that all lattice sites are equivalent that for $z=3$,

$$P(p) = \begin{cases} 0 & \text{for } p < p_c \\ p \left(1 - \left(\frac{1-p}{p} \right)^3 \right) & \text{for } p > p_c \end{cases} .$$

Thus

$$P(p) \propto (p - p_c)^\beta ,$$

where $\beta=1$ for the $z=3$ Bethe lattice. Note $P(p)$ is an order parameter of the system.



As we did so for $d=1$, we now calculate $n_s(p)$ for the Bethe lattice.

$$n_s(p) = \sum_t g_{s,t} p^s (1-p)^t ,$$

where $g_{s,t}$ is a sort of density of states telling us the number of clusters of s sites with t neighbors. For a Bethe lattice, it turns out that $t=2+s*(z-2)$, giving

$$n_s(p) = g_{s, 2+s(z-2)} p^s (1-p)^{2+s(z-2)} .$$

We specialize again to $z=3$, We compute

$$\frac{n_s(p)}{n_s(p_c)} = \left(\frac{1-p}{1-p_c}\right)^2 \left(\frac{p(1-p)}{p_c(1-p_c)}\right)^s = \left(\frac{1-p}{1-p_c}\right)^2 \exp\left(\frac{-s}{s_\xi}\right)$$

, where $s_\xi \propto (p_c - p)^{-1/\sigma}$ for $\sigma=1/2$. It is also possible to show, albeit with some difficulty, that $n_s p_c \propto s^{(-\tau)}$.

So we have a scaling relation

$$n_s(p) \propto s^{(-\tau)} * \exp(-s/s_\xi)$$

If we use our scaling $n_s(p)$ to calculate $P(p)$, we get

$$\beta = \frac{\tau - 2}{\sigma}$$

Similarly, If we use our scaling form to calculate the mean cluster size $S(p)$, we get $\gamma = (3 - \tau)/\sigma$. Finally consider the kth moment of the cluster size distribution. By using the scaling ansatz once more we obtain

$$M_k \propto (p - p_c)^{((\tau - 1 - k)/\sigma)}$$

For $k=0$, we define α such that

$$2 - \alpha = \frac{(\tau - 1)}{\sigma} = 2\beta + \gamma$$

and thus we recover by design the Rushbrooke scaling law.

Fractal Dimension of Clusters

On the right we have a graph where the y axis is the size of the largest cluster in site percolation at the critical threshold and the x axis the dimension of the $L \times L$ grid of lattice points. We see there is strong evidence that the fractal dimension of the cluster is well defined and not equal to 2. We now derive a relationship between this fractal dimension and the critical exponents. First define the radius of gyration of a cluster as

$$R_s^2 = 1/s \sum_{i=1}^s (r_i - r_{cm})^2$$

It can be shown that

$$R_s^2 = 1/2 * 1/s^2 * \sum_{ij} (r_i - r_j)^2$$

Let $g(r)$, the correlation function, be the probability that a site at relative position r from an occupied site belongs to the same finite cluster.

Then

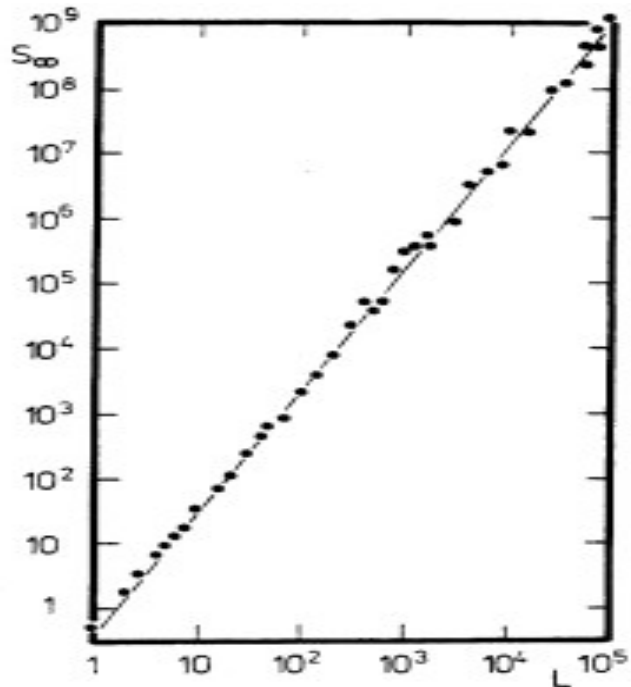
$$\sum_r g(r) = S(p)$$

So if we define the correlation length as

$$\xi^2 = \frac{\sum_r r^2 g(r)}{\sum_r g(r)}$$

, then as the probability that a site belongs to a cluster of size s is $n_s(p)$, we obtain

$$\xi^2 = \frac{\sum_s 2R_s^2 s^2 n_s(p)}{\sum_s s^2 n_s(p)}$$



Inserting previous scaling results for $n_s(p)$ into this expression, and assuming that $s \propto R_s^D$ defines the fractal dimension, then if $\xi \propto (p - p_c)^{-\nu}$, then we derive the fact that $D = \frac{1}{\nu \sigma}$.

We can derive another relation involving the fractal dimension by using the fact that the mass of the infinite cluster is given by both $L^d (p - p_c)^\beta$ and also by $L^d * \xi^{(-\beta/\nu)}$. Substituting ξ for L turns the latter expression into $M(L) = \xi^{(d - \beta/\nu)}$, so we thus have the hyperscaling relation $D = d - \beta/\nu$

Renormalization Group Methods

The renormalization group is a theoretically beautiful and powerful tool that also applies to this problem. In general, we reduce the scale of the problem, and then we define renormalized bonds and renormalized sites in a well defined way. It is best to illustrate this concept by way of example.

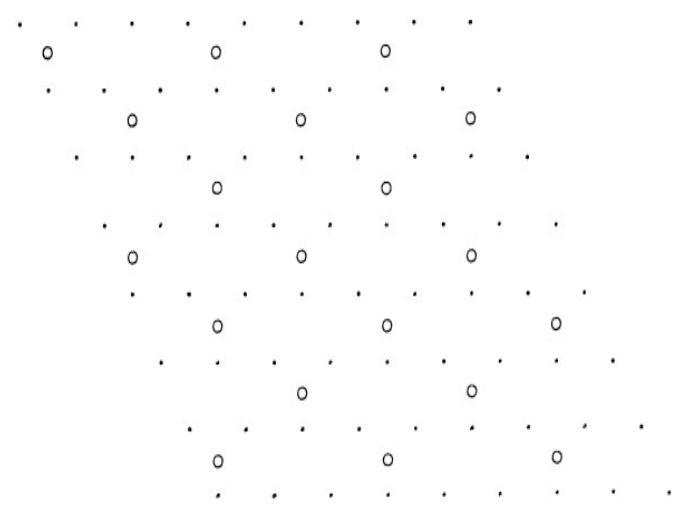
Our first example of applying the renormalization group technique will be site percolation on the triangular lattice. We coarse grain according to the diagram with three sites per coarse grained site. We declare that a cell is occupied if at least two out of three sites are occupied. Thus

$$p' = p^3 + 3p^2(1 - p)$$

The fixed points of this transformation are 0, 1/2, and 1. 0 and 1 are trivial fixed points, $p^* = 1/2$ is the interesting unstable fixed point. The exponent

$$\nu = \frac{\ln(b)}{\ln(\frac{dp'}{dp})} = \frac{\ln(\sqrt{3})}{\ln(3/2)} = 1.355$$

These numbers compare well with the exact results of $p_c = 1/2$ and $\nu = 4/3$.

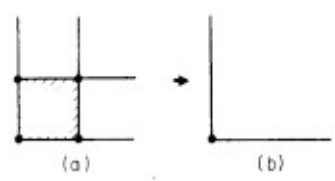


A more complicated example comes from site-bond percolation. Here both p and b must change under the renormalization group transformation. For calculating p' , using the figure as our guide requires us to define the coarse grained site as occupied if there is a connected path either vertically or horizontally spanning the cell. Therefore

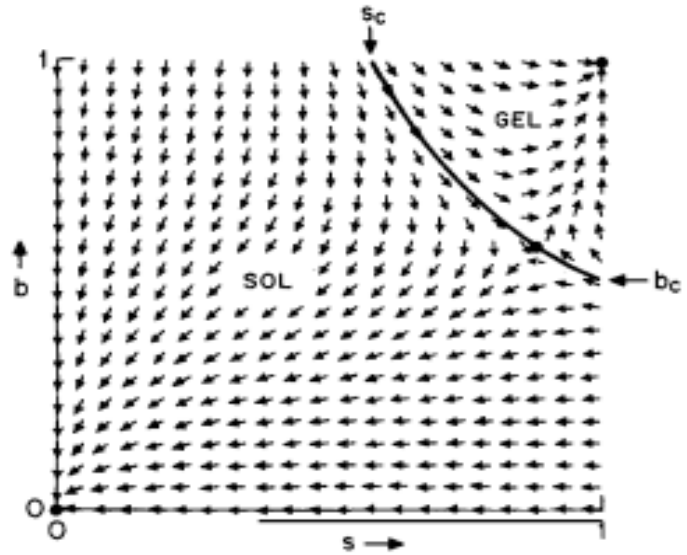
$$p' = p^4(1 - (1 - b)^4) + 4p^3(1 - p)(1 - (1 - b)^2) + 4p^2(1 - p)^2 b$$

It is useful to remember when interpreting this equation that the b factors represent the probability that at least one of a certain number of bonds is filled. As for b' , we need to enter the cell from a particular direction, and traverse sites and bonds to connect to the opposing end. We get

$$p' b' = (1 - (1 - b)^2)(p^4(b^4 + 4b^3(1 - b) + 3b^2(1 - b)^2) + 2p^3(1 - p)b^2) + b(p^4(2b^2(1 - b)^2 + 2b(1 - b)^3) + p^3(1 - p)(2b(1 - b) + 2b) + 2p^2(1 - p)^2 b)$$



. The flow diagram is given below. It is seen that there are two trivial fixed points at (0,0) and (1,1). There is also a critical fixed point at (.879,.586). The critical surface consists of the points which flow into the critical fixed point, which is also drawn on the diagram. The intersection of this surface with the axes gives $p_c=.570$, $b_c=.506$, which compares favorably with the exact answers $p_c=.593$, $b_c=.5$. After linearizing the renormalization group transformation and diagonalizing it, we get $\nu=1.47$, which is an OK approximation to the exact $\nu=1.354$. The source of the error is that the probabilities of having bonds between coarse-grained sites are no longer independent. A nearest neighbor interaction must be included, and the renormalization group flow occurs in a higher dimensional space. This is why analyzing pure site or pure bond percolation via the renormalization group is more accurate when we allow flows in (p,b) space instead of p or b space alone.



A Relationship between percolation and the Potts Model

We closely follow (6). Consider a lattice

$\Lambda \subset L^d$, let $S=\{1,\dots,q\}$ denote the set of possible spin states at each site $x \in \Lambda$. The partition function is $Z(\beta) = \sum_{\sigma} \exp(-\beta H(\sigma))$ where $H(\sigma) = \sum_{ij} J_{i,j} (\delta_{\sigma_i, \sigma_j} - 1) - h \sum_i \delta_{\sigma_i, 1}$

To map this onto a percolation problem, we use the method of Fortuyn and Kasteleyen. Define

$K_d = \{(i, j) \in \Lambda : J_{i,j} \neq 0\}$. For a subset $K \subset K_d$, the definition of configuration space is given by $\Omega_K = \{0,1\}^K$. Ω_K represents bond configurations, where 1 denotes the existence of a bond, and 0 the nonexistence of a bond. We define $p_{i,j} = 1 - \exp(-\beta J_{i,j})$ and specialize to the case where $h=0$.

Then
$$Z(\beta) = \sum_{\sigma} \exp(-\beta H(\sigma)) = \sum_{\sigma} \prod_{K_d} \exp(-\beta J_{i,j} (\delta_{\sigma_i, \sigma_j} - 1))$$

$$Z(\beta) = \sum_{\sigma} \prod_{(i,j) \in K_d} \{(1 - p_{i,j}) + p_{i,j} \delta_{\sigma_i, \sigma_j}\}$$

Now every term in this expression is associated with a configuration $\omega \in \Omega_K$

where there is a bond for the factor $p_{i,j} \delta_{\sigma_i, \sigma_j}$ and there is no bond for the factor $1 - p_{i,j}$. Thus

$$Z(\beta) = \sum_{\sigma} \sum_{\omega \in \Omega_K} \prod_{\text{empty bonds}} (1 - p_{i,j}) \prod_{\text{present bonds}} p_{i,j} \prod_{\text{present bonds}} \delta_{\sigma_i, \sigma_j}$$

$$Z(\beta) = \sum_{\omega \in \Omega_K} \prod_{\text{empty bonds}} (1 - p_{i,j}) \prod_{\text{present bonds}} p_{i,j} \sum_{\sigma} \prod_{\text{present bonds}} \delta_{\sigma_i, \sigma_j}$$

The $\sum_{\sigma} \prod_{\text{present bonds}} \delta_{\sigma_i, \sigma_j}$ acts as a big delta function which divides the spins into clusters, each with the same spin. Thus at last we have

$$Z(\beta) = \sum_{\omega \in \Omega_K} \prod_{\text{empty bonds}} (1 - p_{i,j}) \prod_{\text{filled bonds}} p_{i,j} q^{N_c}$$

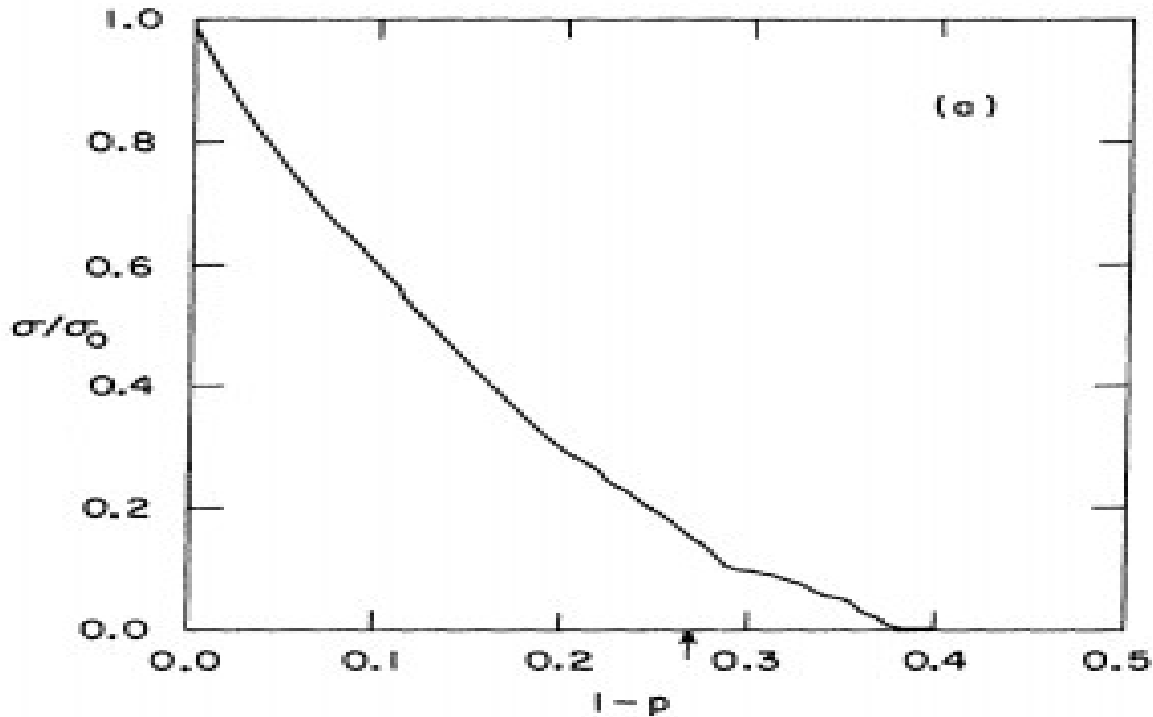
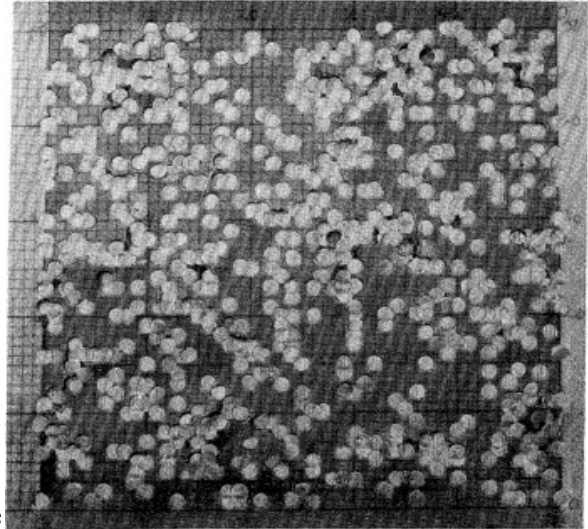
where N_c is the number of clusters in the bond configuration ω .

The Swendsen-Wang uses this formula to simulate Potts models. The algorithm consists of initially generating a random lattice of spins, then iterating the following procedure: If two spins are identical, create a bond between them with probability $p_{i,j}$. Then flip each cluster of bonds to a

random q . This algorithm typically converges much faster than the Metropolis algorithm, as it is similar to the Metropolis algorithm but involves flipping clusters instead of individual spins. This speedup is especially important when the phenomenon of critical slowing down is considered.

Conductivity of Randomly Punctured Sheets

A final application is conductivity of randomly punctured sheets. Last and Thouless (4) randomly punctured graphite sheets. A picture of the experiment is to the right. Below there is a graph of $1-p$ versus the conductivity. Notice how the conductivity is only nonzero for p approximately .60, indicating that percolation has at least limited success modeling this system. Unfortunately, percolation fails to model the conductivity or predict its critical behavior. This is because the conductivity only depends on the “backbone” of a percolation cluster, and not on arms that don't connect to the sides of the sheet of graphite.



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