Percolation, Potts Model and Polymers on lattices

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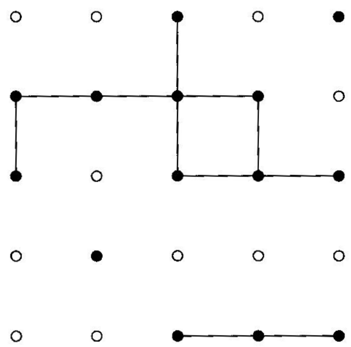
Abstract

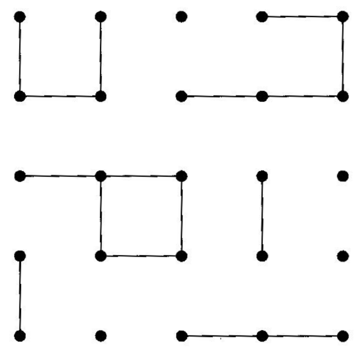
Percolation arises as a natural problem in the study of porous materials in a statistical manner. On a lattice two possible models are considered - site percolation and bond percolation. Both are based on similar ideas and are very suitable to understand phase transitions. Throughout the talk we discuss the one-dimensional percolation model and percolation on the Bethe lattice. Both can be solved analytically and are easy to handle on a statistical basis. Critical exponents close to the phase transition are calculated and follow naturally from the purely mathematical description. Additonally, results for two-dimensional lattices are stated. The second topic of this talk is the Potts Model as a generalization of the Ising Model. We discuss an analytic solution on the Bethe lattice, which can be generalised to study phase transitions once more. Lastly, we consider connections of the Potts Model to percolation and polymers.

Contents

I Percolation



(a) Parts of the open subgraph in site percolation. The open circles correspond to closed lattice points and the filled to open lattice points. The depictured subgraph in black shows the clusters from next-neighbour connections of two open lattice points.



(b) Parts of the open subgraph in bond percolation. The points show the lattice points. The black connections correspond to open bonds between next neighbours in the lattice and form the clusters.

Figure 1: An example of percolation on the square lattice $\mathbb{Z}^2$ for a finite part of the lattice. If, for a given point, we have an infinite cluster, we say we have percolation for this point. [BR06]

In the study of porous materials a description on a lattice is very fruitful. In the following we want to study such a lattice and construct a statistical model to describe the randomness of channels in such materials. In site percolation, as in figure 1a, we assign a probability p to the statistically independent lattice points to be open and consider connections between to open points. Connected points are called a cluster and we say we have percolation, if an arbitrary point is part of a cluster of infinite size (i.e. infinite number of lattice points). We make similar definitions for bond percolation, as in figure 1b, and assign p to an open bond between lattice points. In the following disccusion, which mainly follows [SA95], we concentrate on site percolation if not stated otherwise.

Definition (Probabilities in Percolation Theory)**.**

$$
\begin{aligned}
p &:= \text{Probability for open lattice site,} \qquad p \in [0,1],\\
n_s(p) &:= \text{Number of s-clusters (i.e. clusters with s points) per point,}\\
w_s(p) &= \frac{n_s s}{\sum_s n_s s} := \text{Probability that cluster to arbitrary open point is an s-cluster,}\\
S(p) &= \sum_s w_s s = \sum_s \frac{n_s s^2}{\sum_s n_s s} := \text{Mean cluster size for random clusterpoint,}\\
P(p) &:= \text{Percolation Probability (i.e. probability that arbitrary point is part of } \infty\text{-cluster).}
\end{aligned}
$$

(1) 1D percolation

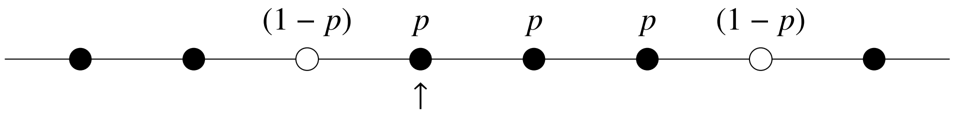


Figure 2: We consider a one-dimensional lattice. Filled circles are open sites and open circles are closed sites.

Definition (One-dimensional lattice)**.** We consider a one-dimensional lattice of N lattice sites as depicted in figure 2. The probability that the site ↑ is part of a 3-cluster is $p^3(1-p)^2$ for $N \gg 1$. This generalises to

$$n_s(p) = p^s(1-p)^2. \tag{1}$$

Since we have s points in the cluster, the probability that a random point is part of the s-cluster is $\frac{n_s s}{N}$. Thus, the percolation probability follows as

$$P(p) = \lim_{s\to\infty} \frac{n_s s}{N} \overset{s=N}{=} \lim_{s\to\infty} p^s(1-p)^2 = \begin{cases} 1 & p = 1 \\ 0 & p < 1 \end{cases}. \tag{2}$$

This reminds us of phase transitions for a critical probability $p_c \equiv 1$. Next, we consider the mean cluster size.

Proposition (Mean Cluster Size)**.**

$$S(p) = \frac{1+p}{1-p}, \qquad \textit{for } p < p_c.$$

Proof. (i) $$\sum_{s=1}^{\infty} n_s s = \sum_{s=1}^{\infty} p^s(1-p)^2 s = (1-p)^2 \sum_{s=1}^{\infty} p \frac{\mathrm{d}p^s}{\mathrm{d}p} = (1-p)^2 \left(p\frac{\mathrm{d}}{\mathrm{d}p}\right) \sum_{s=1}^{\infty} p^s$$

$$\overset{geom.sum}{=} (1-p)^2 \left(p\frac{\mathrm{d}}{\mathrm{d}p}\right)\left(\frac{p}{1-p}\right) = p(1-p) + p^2 = p.$$

(ii) $$S(p) = \frac{1}{p}\sum_{s=1}^{\infty} n_s s^2 = \frac{(1-p)^2}{p} \sum_{s=1}^{\infty} p^s s^2 = \frac{(1-p)^2}{p} \left(p\frac{\mathrm{d}}{\mathrm{d}p}\right)^2 \sum_{s=1}^{\infty} p^s = \ldots = \frac{1+p}{1-p}.$$

□

Remark. We found for $p \approx p_c$ that $S(p) \propto \dfrac{1}{p_c - p}$. In general one defines a critical exponent γ, which in our case is $\gamma = 1$.

$$S(p) \propto |p - p_c|^{-\gamma}, \qquad \text{for} \qquad p \lesssim p_c. \tag{3}$$

Definition (Correlation function and length)**.**

$g(r) :=$ probability that point at distance r from open point is part of the same cluster.

$$\Rightarrow g(r) = p^r = \exp\Big(\ln(p)\,r\Big) = \exp\left(-\frac{r}{\xi}\right) \qquad \text{with:} \quad \xi = -\frac{1}{\ln(p)} \text{ correlation length}$$

Taylor: $\ln(1-x) \cong -x \quad x \approx 0 \quad \Rightarrow \quad \ln\Big(p_c - (p_c - p)\Big) \cong p - p_c$

$$\Rightarrow \xi \cong \frac{1}{p_c - p} \propto S \qquad \text{for} \qquad p \approx p_c.$$

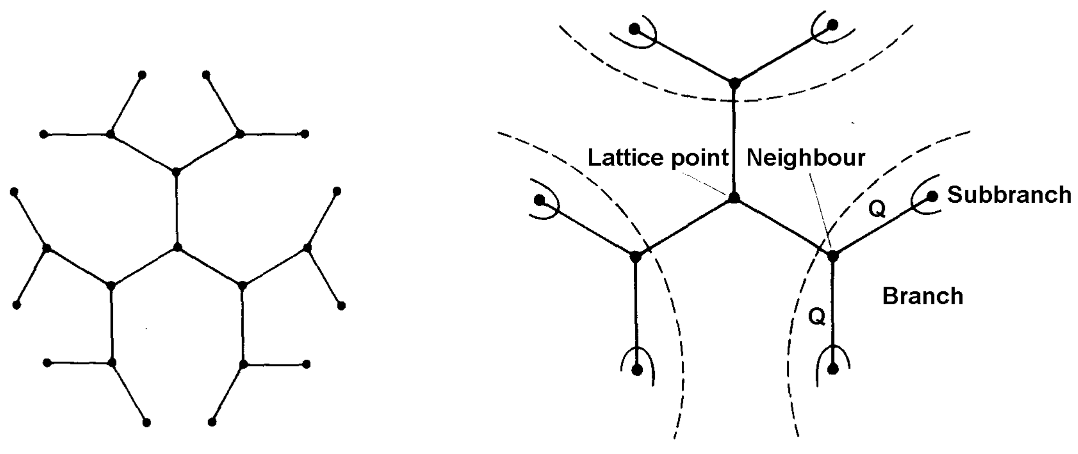
Remark.

- In general we define the critical exponent ν via $\xi = |p - p_c|^{-\nu}$, which in our 1D case is $\nu = 1$.

- We have divergencies at the critical probability, which follow simple power laws.
- This behaviour is typical of phase transitions. We will see that this behaviour also occurs for percolation on different lattices and thus, this is a good example to study phase transtions.
- This is much more complicated in higher dimensions, because of different shapes of clusters and the possibility of percolation despite of closed lattice points.

(2) Percolation on the Bethe lattice

We now want to consider the infinite Bethe lattice, as depicted in figure 3a. Percolation on the Bethe lattice is a good model to model polymerization and gelation and was first studied by Flory in 1941. [SA95]



(a) The Bethe lattice for coordination number $z = 3$. This lattice is a tree in which every point (in the infinite lattice) has three connections to nearest neighbours and no loops.

(b) The Bethe lattice seen from a central lattice point. This defines the terms neighbour, branch and subbranch in our derivation.

Figure 3: The Bethe lattice. [SA95]

Theorem (Critical probability Bethe lattice)**.**

(i) Let $\mathbb{P}_p(E)$ *be the probability that there exists a* ∞*-cluster.*
Then it follows $\left\{ \begin{array}{l} P(p) > 0 \;\Rightarrow\; \mathbb{P}_p(E) = 1 \\ P(p) = 0 \;\Rightarrow\; \mathbb{P}_p(E) = 0 \end{array} \right\}.$

(ii) $\exists\, p_c \in [0, 1] :\; P(p < p_c) = 0,\; P(p > p_c) > 0.$

(iii) For the Bethe lattice with coordination number $z \in \mathbb{N}\backslash\{1\}$ *follows* $p_c = \dfrac{1}{z-1}.$

Proof. (i) follows from probability theory, (ii) from monotonicity. For (iii) consider the central lattice point (figure 3b). After a step to the neighbour we have $(z - 1)$ new subbranches, thus $(z - 1)p$ open neighbours after every step. This means we have $(z - 1)p_c = 1$ or else the open neighbours decrease exponentially. □

This defines the critical probability for percolation. Also, we see that if the percolation probability does not vanish, there must exist an infinite subgraph (i.e. cluster). This makes sense on an infinite lattice.

Theorem (Flory, 1941)**.**
For the Bethe lattice with $z = 3$ *it holds that*

$$\frac{P}{p} = 1 - \left[\frac{1-p}{p}\right]^3, \quad for \quad p > p_c. \tag{4}$$

Proof. Let Q := Probability that arbitrary lattice site is not connected to ∞ via (sub)branch. (figure 3b) Thus, the probability that arbitrary neighbour is not connected with ∞ is Q^2.
The probability that the neighbour of (arbitrary) lattice point is open but not connected with ∞ is pQ^2. The probability that neighbour is not open (subbranch not relevant) is $(1 - p)$.

$$\Rightarrow \quad Q = (1-p) + pQ^2 \quad Solutions: \quad Q_1 = 1,\; Q_2 = \frac{1-p}{p}$$

The result Q_1 is clear and corresponds to $p < p_c$. For Q_2 we will see $p > p_c$. For the probability that a (arbitrary) lattice point is open, but not connected with ∞, we obtain

$$\begin{aligned} (p - P) = pQ^3 \quad &\Rightarrow \quad P = p\,(1 - Q^3), \\ For\ Q = 1 \quad &\Rightarrow \quad P = 0 \quad (p < p_c), \\ For\ Q = \frac{1-p}{p} \quad &\Rightarrow \quad P(p) = p\left[1 - \left(\frac{1-p}{p}\right)^3\right], \quad for \quad p > p_c. \end{aligned}$$

□

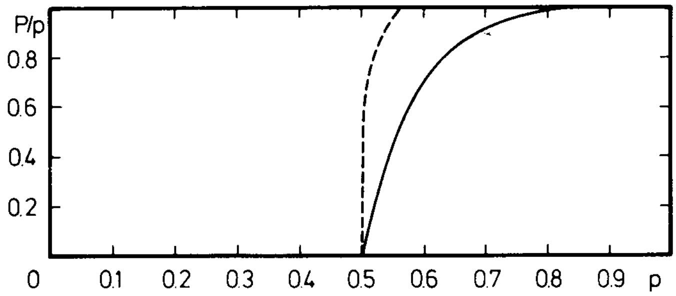


Figure 4: The order parameter P(p) (to be more specific P/p) plotted as a function of p for the Bethe lattice with $z = 3$. The solid line corresponds to equation (4) and the dashed line to numerical calculations for site percolation on the triangular lattice. [SA95]

Corollary. *For the Bethe lattice with $z = 3$ it holds for the mean cluster size:*

$$S(p) = \frac{1+p}{1-2p} = \frac{1}{2}\frac{1+p}{\frac{1}{2}-p} \propto \frac{1}{p_c - p}. \tag{5}$$

Thus, the critical exponent is $\gamma = 1$ as in one dimension.

Proof. Let $T :=$ mean clustersize of (arbitrary) (sub)branch. It holds for $z = 3$, because every (sub)branch contributes by T to the mean clustersize, $T = (1-p) \cdot 0 + p \cdot (1 + 2T)$. It follows $T = \frac{p}{1-2p}$ for $p < \frac{1}{2}$. For the central (open) lattice point we have the contribution of 1 and the size of the three independent branches

$$S(p) = 1 + 3T = \frac{1+p}{1-2p}.$$

□

Corollary. $P(\frac{1}{2}) = 0$ *and* $P(p) \propto (p - pc)$, *for* $p \gtrsim p_c$.

Proof. Taylor expansion yields: $P(p) \cong P(\frac{1}{2}) + P'(\frac{1}{2})(p - \frac{1}{2}) = 3(p - p_c)$. □

Remark.

- In general, we define the critical exponent β via $P(p) = (p - p_c)^{-\beta}$ for $p \gtrsim p_c$, which in the Bethe lattice is $\beta = -1$.

- We have seen a phase transition, which strongly resembles continuous thermal phase transitions in statistical physics. The order parameter in percolation is the percolation probability and the analogy to the temperature is the probability p.

- The theory of percolation can be used for the description of branched polymers.[Van98]

(3) 2D percolation

Finally, we want to state a few results for percolation on two dimensional lattices without proofs. The proofs are mathematically involved and can be studied in [BR06] with the rigorous mathematical background using probability and graph theory.

Theorem (Harris-Kasten-Theorem)**.**
For bond percolation on the square lattice $\mathbb{Z}^2$ it holds $p_c = \frac{1}{2}$.

Theorem (Critical probability triangular lattice)**.**
For site percolation on the triangular lattice it holds $p_c = \frac{1}{2}$.

Theorem (Critical exponents triangular lattice)**.**
For site percolation on the triangular lattice we find

$$\begin{aligned} \beta = \frac{5}{36} \quad &\Rightarrow \quad P(p) = (p - p_c)^{-\frac{5}{36}}, \quad \textit{for } p \searrow p_c, \\ \gamma = \frac{43}{18} \quad &\Rightarrow \quad S(p) = |p - p_c|^{-\frac{43}{18}}, \quad \textit{for } p \nearrow p_c, \\ \nu = \frac{4}{3} \quad &\Rightarrow \quad \xi(p) = |p - p_c|^{-\frac{4}{3}}, \quad \textit{for } p \approx p_c,\ p \neq p_c. \end{aligned}$$

II The Potts Model

Remark (Reminder Ising Model)**.**

$$\mathcal{H} = \underbrace{J}_{\substack{\text{next}\\ \text{neighbour}\\ \text{coupling}}} \cdot \sum_{<i,j>} s_i s_j - \underbrace{B}_{\substack{\text{ext.}\\ \text{field}}} \cdot \underbrace{\mu}_{\substack{\text{magn.}\\ \text{mom.}}} \cdot \sum_i s_i, \qquad s_i \in \{1, -1\}. \tag{6}$$

We now want to study the Potts Model as a generalisation of the Ising Model in (6). This disccusion follows [Wu82].

Definition (Standard Potts Model)**.**

$$\mathcal{H} = -\epsilon_1 \sum_i \delta_{Kr}(\sigma_i, 0) - \epsilon_2 \sum_{<i,j>} \delta_{Kr}(\sigma_i, \sigma_j) - \mathcal{O}(\sigma^3),$$

$$\sigma_i \in \{0, \ldots n-1\}, \qquad \delta_{Kr}(\sigma_i, \ldots, \sigma_k) = \begin{cases} 1 & \sigma_i = \ldots = \sigma_k \\ 0 & else \end{cases}.$$

Remark.

- For $q = 2$ we have the rescaled Ising model as a special case. The Potts Model is a generalisation of the Ising model.
- We have an external field ϵ_1 that only couples to the 0-spins and next-neighbour (and higher) coupling in the Hamiltonian.
- We will see that statistical physics in the context of the Potts Model can be used to study percolation.
- Polymers in a dense phase can be described by the Potts Model.[Van98]

(1) Solution on the Bethe lattice

On the Bethe lattice an analytic solution can be derived in an easy fashion. Following the ideas from [WW76], we define the Hamiltonian $\mathcal{H}$ of the Potts Model on the finite Bethe lattice with N points (as in figure 3a) and $\epsilon_1 = 0$ and find as the partition function Z

$$\mathcal{H} = -\epsilon \sum_{<i,j>} \delta_{Kr}(\sigma_i, \sigma_j),$$

$$Z = \sum_{\sigma_1=0}^{q-1} \cdots \sum_{\sigma_N=0}^{q-1} \exp(-\beta\mathcal{H}) = \sum_{\{\sigma\}} \prod_{<i,j>} \exp\left[\epsilon\, \beta\, \delta_{Kr}(\sigma_i, \sigma_j)\right].$$

If we look at one isolated spin σ and calculate the next neighbour contribution with σ', we observe

$$\sum_{\sigma'=0}^{q-1} \exp\left[\epsilon\, \beta\, \delta_{Kr}(\sigma, \sigma')\right] = (q-1) + \mathrm{e}^{\epsilon\beta} \equiv w.$$

We can evaluate the partition function Z from the outer lattice points going inwards, recursively summing the contributions and find for Z and the free energy f per lattice point (in the thermodynamic limit $N \to \infty$)

$$Z = w^{N-1} \sum_{\sigma=0}^{q-1} 1 = q \cdot w^{N-1},$$

$$f = -\mathrm{k_B} T \lim_{N\to\infty} \frac{\ln(Z)}{N} = -\mathrm{k_B} T \ln(w).$$

Remark.

- f is analytical in the temperature T and no phase transition occurs. For $\epsilon \neq 0$ one can find a phase transition.[WW76]
- In general, the Potts Model can be adressed similarly to the Ising model, i.e. Mean Field approaches and Renormalisation.

(2) Percolation as $q \to 1$ limit

To address the problem of percolation using the Potts Model [Wu82] we define the Hamiltonian $\mathcal{H}(q; K, L, M)$ accordingly and calculate the free energy per lattice site $f(q; K, L, M)$. Taking the $q \to 1$ limit gives a function, which gives access to the percolation probability $P(p)$ and the mean cluster size $S(p)$. For example, in bond correlation, we consider

$$-\beta\mathcal{H} = K \sum_{<i,j>} \delta_{Kr}(\sigma_i, \sigma_j) + L \sum_i \delta_{Kr}(\sigma_i, 0) + M \sum_{<i,j>} \delta_{Kr}(\sigma_i, 0)\, \delta_{Kr}(\sigma_j, 0),$$

$$h(K, L, M) = \left[\frac{\partial}{\partial q} f(q; K, L, M)\right]_{q=1},$$

$$P(p) = 1 + h'(K, 0+, 0) \equiv 1 + \lim_{L\searrow 0} \frac{\partial}{\partial L} h(K, L, 0),$$

$$S(p) = h''(K, 0+, 0).$$

III Closing Remarks

- We have seen a close relationship between percolation, the Potts Model and polymers on lattices.
- The talk only scratched the surface of the plethora of results in the descriptions of polymers on lattices. Common approaches to lattice polymer models are Random Walks and Self Avoiding Random Walks. Additionally, percolation is used for the description of branched polymers and the Potts Model for dense polymers. For further results see [Van98].
- We have studied percolation in this talk from the starting point of porous materials. We have looked at phase transitions and critical exponents, based on the one-dimensional model and percolation on the Bethe lattice. Two dimensional lattices were mentioned, albeit their difficult description.
- The Potts Model as a generalization of the Ising Model was discussed. The approaches to solve the model are similar to the Ising model with Mean Field approaches and Renormalisation. We considered the analytical solution on the Bethe lattice and have described a method to solve percolation problems using the Potts Model.

- To summarise, we saw that percolation is a good model to understand phase transitions and critical exponents. The Potts Model is a generalization of the Ising model and can be, for example, used to study percolation.

References

[BR06] Bela Bollobás and Oliver Riordan. *Percolation*. Cambridge University Press, 2006.

[SA95] Dietrich Stauffer and Amnôn Aharonî. *Perkolationstheorie*. VCH, Weinheim, 1995.

[Van98] Carlo Vanderzande. *Lattice models of polymers*. Cambridge lecture notes in physics. Cambridge University Press, Cambridge, 1. publ. edition, 1998.

[Wu82] F. Y. Wu. *The Potts model*. Reviews of Modern Physics, 54:235–268, Jan 1982.

[WW76] Y. K. Wang and F. Y. Wu. *Multi-component spin model on a Cayley tree*. Journal of Physics A: Mathematical and General, 9(4):593–604, 1976.