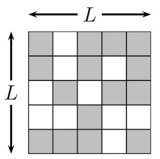
Percolation

Aim: Study connections between macroscopic quantities and the underlying microscopic world in the simplest not exactly solved model displaying a phase transition.

Objective: Gain qualitative and quantitative understanding of the phenomenon of phase transition and associated concepts such as scale-free behaviour, scaling theory, and universality.



Each site in a lattice is occupied randomly and independently with occupation probability p, $0 \leq p \leq 1$. A cluster is a group of nearest-neighbour occupied sites. The size s of a cluster is the number of sites in the cluster. The critical occupation probability p_c is the occupation probability p above which a percolating infinite cluster appears for the first time in an infinite lattice $L = \infty$.

Quantities of interest

- Onset of percolation – critical occupation probability, p_c.
- Probability that a site belongs to the infinite cluster, $P_\infty(p)$.
- Geometry of the infinite cluster and the finite clusters.

Excluding the infinite cluster:

- Average cluster size, $\chi(p)$.
- Typical size of the largest cluster, $s_\xi(p)$.
- Typical radius of the largest cluster, $\xi(p)$.

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Introduced the cluster number density $n(s,p)$ as the number of s-clusters per lattice site implying that the probability for a site to belong to any finite cluster is $\sum_{s=1}^{\infty} sn(s,p)$. The probability that a site belongs to the infinite cluster

$$P_\infty(p) = \begin{cases} 0 & \text{for } p \leq p_c \\ \text{nonzero} & \text{for } p > p_c, \end{cases}$$

such that

$$P_\infty(p) + \sum_{s=1}^{\infty} sn(s,p) = p \quad \text{valid for all } p.$$

The average cluster size

$$\chi(p) = \frac{\sum_{s=1}^{\infty} s^2 n(s,p)}{\sum_{s=1}^{\infty} sn(s,p)}.$$

Percolation in $d = 1$ has onset of percolation at $p_c = 1$ and

$$n(s,p) = (1-p)^2 p^s = (1-p)^2 \exp(-s/s_\xi)$$

where the characteristic cluster size (typical largest cluster)

$$s_\xi(p) = -\frac{1}{\ln p} \propto (p_c - p)^{-1} \quad \text{for } p \to p_c^-$$

and the average cluster size

$$\chi(p) = \frac{1+p}{1-p} \propto (p_c - p)^{-1} \quad \text{for } p \to p_c^-.$$

The quantities $s_\xi(p)$ and $\chi(p)$ diverge as a power laws in terms of $(p_c - p)$, the distance of p away from p_c.

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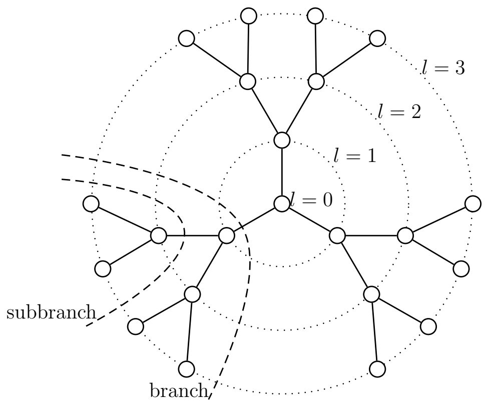

Considered the Bethe lattice with coordination number z. Lattice contains no loops.

Critical occupation probability $p_c = \frac{1}{z-1}$.

The average cluster size

$$\chi(p) = \frac{p_c(1+p)}{p_c - p} \propto (p_c - p)^{-1} \quad \text{for } p \longrightarrow p_c^-.$$

The probability that a site belongs to the infinite cluster

$$P_\infty(p) = \begin{cases} 0 & \text{for } p \leq p_c \\ p\left[1 - \left(\frac{1-p}{p}\right)^3\right] & \text{for } p > p_c \end{cases}$$
$$= \begin{cases} 0 & \text{for } p \leq p_c \\ 6(p - p_c) & \text{for } p \longrightarrow p_c^+. \end{cases}$$

Picks up abruptly at $p = p_c$ signalling the onset of percolation.

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Introducing

$$\begin{aligned} t &= \text{perimeter} = \text{number of empty neighbours of a cluster} \\ g(s,t) &= \text{number of different clusters with size } s \text{ and perimeter } t. \end{aligned}$$

the general form of the cluster number density

$$n(s,p) = \sum_{t=1}^{\infty} g(s,t)(1-p)^t p^s.$$

In a Bethe lattice $t = s(z-2) + 2$ and

$$\begin{aligned} n(s,p) &\propto n(s,p_c)\exp(-s/s_\xi) \\ &\propto s^{-\tau}\exp(-s/s_\xi) \quad \text{for } s \gg 1 \end{aligned}$$

where the characteristic cluster size

$$s_\xi \propto |p_c - p|^{-2} \quad \text{for } p \longrightarrow p_c.$$

Note that

$$n(s,p) = \begin{cases} s^{-\tau} & \text{for } 1 \ll s \ll s_\xi \\ \text{decays rapidly} & \text{for } s \gg s_\xi. \end{cases}$$

Using the ansatz above, the average cluster size

$$\begin{aligned} \chi(p) &\propto \int_1^\infty s^{2-\tau}\exp(-s/s_\xi)ds \\ &\propto s_\xi^{3-\tau} && \text{for } p \longrightarrow p_c \\ &\propto |p_c - p|^{-1} && \text{for } p \longrightarrow p_c \end{aligned}$$

implying that the cluster number density exponent $\tau = 5/2$ in the Bethe lattice. Hence, the cluster number density

$$\begin{aligned} n(s,p) &\propto s^{-5/2}\exp(-s/s_\xi) \quad \text{for } s \gg 1 \\ s_\xi &\propto |p_c - p|^{-2} \quad \text{for } p \longrightarrow p_c. \end{aligned}$$

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We introduced the critical exponents characterising the percolation phase transition at $p = p_c$.

The exponent β characterises the abrupt pick up of the order parameter

$$P_\infty(p) = \begin{cases} 0 & \text{for } p \le p_c \\ (p - p_c)^\beta & \text{for } p \to p_c^+. \end{cases}$$

The exponent γ characterises how the average cluster size diverges

$$\chi(p) \propto |p - p_c|^{-\gamma} \quad \text{for } p \to p_c.$$

The exponent σ characterises how the characteristic cluster size (typical size of largest cluster) diverges

$$s_\xi(p) \propto |p - p_c|^{-1/\sigma} \quad \text{for } p \to p_c.$$

The exponent τ characterises the cluster number density at $p = p_c$. Generally, in dimensions higher than one, the cluster number density

$$n(s,p) = \begin{cases} s^{-\tau} & \text{for } 1 \ll s \ll s_\xi \\ \text{decays rapidly} & \text{for } s \gg s_\xi. \end{cases}$$

Critical exponents depend only on dimensionality, not the details of the lattice. In this sense, they are universal.

Exponent:	Quantity	$d=1$	$d=2$	$d=3$	$d=4$	$d=5$	$d \geq 6$	Bethe
$\beta:$	$P_\infty(p) \propto (p-p_c)^\beta$	0 (dis)	5/36	0.4181(8)	0.657(9)	0.830(10)	1	1
$\gamma:$	$\chi(p) \propto \|p-p_c\|^{-\gamma}$	1	43/18	1.793(3)	1.442(16)	1.185(5)	1	1
$\nu:$	$\xi(p) \propto \|p-p_c\|^{-\nu}$	1	4/3	0.8765(16)	0.689(10)	0.569(5)	1/2	1/2
$\sigma:$	$s_\xi(p) \propto \|p-p_c\|^{-1/\sigma}$	1	36/91	0.4522(8)	0.476(5)	0.496(4)	1/2	1/2
$\tau:$	$n(s,p) \propto s^{-\tau}\mathcal{G}(s/s_\xi)$	2	187/91	2.18906(6)	2.313(3)	2.412(4)	5/2	5/2
$D:$	$s_\xi \propto \xi^D$	1	91/48	2.523(6)	3.05(5)	3.54(4)	4	4

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The general scaling ansatz

$$\begin{aligned} n(s,p) &\propto s^{-\tau}\mathcal{G}(s/s_\xi) && \text{for } s \gg 1 \\ s_\xi &\propto |p - p_c|^{-1/\sigma} && \text{for } p \to p_c. \end{aligned}$$

- E.g. $\mathcal{G}_{1d}(x) = x^2 \exp(-x)$ and $\mathcal{G}_{\text{Bethe}}(x) = \exp(-x)$.
  In general

  $$\mathcal{G}(s/s_\xi) = \begin{cases} \mathcal{G}(0) + \mathcal{G}'(0)s/s_\xi + \frac{1}{2}\mathcal{G}''(0)(s/s_\xi)^2 + \cdots & \text{for } s \ll s_\xi \\ \text{decays rapidly} & \text{for } s \gg s_\xi. \end{cases}$$

- At $p = p_c$, $s_\xi = \infty$ so the argument of $\mathcal{G}$ is zero. Therefore

  $$n(s, p_c) \propto s^{-\tau}\mathcal{G}(0) = \text{pure power-law decay} = \text{scale invariance}.$$

  except in $d = 1$ where $\mathcal{G}(0) = 0$.
- The critical occupation probability p_c depend on lattice details.
  Non-universal quantity.
- Critical exponents τ, σ and the scaling function $\mathcal{G}$ are independent of lattice details and depend only on dimensionality.
  Universal quantities.
- Plotting $s^\tau n(s,p)$ versus s/s_ξ all data fall on the graph of the universal scaling function $\mathcal{G}$. Concept of data collapse.

The scaling ansatz imply the scaling relations

$$\chi(p) \propto |p_c - p|^{-\frac{3-\tau}{\sigma}} \propto |p_c - p|^{-\gamma} \quad \text{for } p \to p_c \Rightarrow \gamma = \frac{3-\tau}{\sigma}$$

$$P_\infty(p) \propto |p_c - p|^{\frac{\tau-2}{\sigma}} \propto (p - p_c)^\beta \quad \text{for } p \to p_c^+ \Rightarrow \beta = \frac{\tau-2}{\sigma}$$

There are only two independent critical exponents.

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The infinite cluster at $p = p_c$ is fractal. It looks alike on all length scales ℓ. Mathematically, the concept of self-similarity is expressed by the mass of the infinite cluster in a window of size ℓ

$$M_\infty(p_c, \ell) \propto \ell^D \quad \text{for } \ell \gg 1.$$

To discuss geometry, we introduced the centre of mass, $\mathbf{r}_{cm}$, and the radius of gyration, R_s, of s-clusters, where

$$\mathbf{r}_{cm} = \frac{1}{s}\sum_{i=1}^{s} \mathbf{r}_i, \quad R^2(s) = \frac{1}{s}\sum_{i=1}^{s} |\mathbf{r}_{cm} - \mathbf{r}_i|^2, \quad R_s = \sqrt{\langle R^2(s)\rangle}.$$

The mass of large but finite cluster $1 \ll s < \infty$ at $p = p_c$

$$M(s, p_c, \ell) = \begin{cases} \ell^D & \text{for } \ell \ll R_s \text{ – fractal} \\ R_s^D & \text{for } \ell \gg R_s \text{ – non-fractal} \end{cases}$$
$$= \ell^D m(\ell/R_s)$$

where the crossover function

$$m(\ell/R_s) \propto \begin{cases} \text{constant} & \text{for } \ell/R_s \ll 1 \\ (\ell/R_s)^{-D} & \text{for } \ell/R_s \gg 1. \end{cases}$$

The correlation length, ξ, is the radius of gyration of the characteristic cluster size

$$\xi = R_{s_\xi}.$$

It it the typical radius of the largest cluster. For $p > p_c$, it is also the typical radius of the largest hole in the infinite cluster. Since s_ξ diverges for $p \to p_c$, so does the correlation length and

$$\xi \propto |p - p_c|^{-\nu} \quad \text{for } p \to p_c.$$

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The correlation length, ξ, is the typical largest cluster radius:

$$\xi \propto |p - p_c|^{-\nu} \quad \text{for } p \to p_c.$$

Typical largest cluster size at occupation probability p

$$s_\xi \propto \xi^D \propto |p - p_c|^{-\nu D} \propto |p - p_c|^{-1/\sigma} \quad \text{for } p \to p_c.$$

Mass of the infinite cluster for $p \geq p_c$:

$$M_\infty(\xi, \ell) = \begin{cases} \ell^D & \text{for } \ell \ll \xi \\ \xi^D(\ell/\xi)^d & \text{for } \ell \gg \xi \end{cases}$$
$$= \begin{cases} \ell^D & \text{for } \ell \ll \xi \text{ – fractal} \\ P_\infty(p, \ell)\ell^d = \xi^{-\beta/\nu}\ell^d & \text{for } \ell \gg \xi \text{ – homogeneous} \end{cases}$$

Thus we have two additional scaling relations

$$D = 1/(\sigma\nu) \quad \text{and} \quad D - d = -\beta/\nu \quad (\text{valid for } d \leq 6).$$

The mass of the infinite cluster for $p \geq p_c$

$$M_\infty(\xi, \ell) = \ell^D m_\infty(\ell/\xi)$$

with the crossover function

$$m_\infty(\ell/\xi) = \begin{cases} \text{constant} & \text{for } \ell \ll \xi \\ (\ell/\xi)^{d-D} & \text{for } \ell \gg \xi. \end{cases}$$

Alternatively,

$$M_\infty(\xi, \ell) = b^D M_\infty(\xi/b, \ell/b)$$
$$= \begin{cases} \ell^D M_\infty(\xi/\ell, 1) & \text{for } \ell \ll \xi \\ \xi^D M_\infty(1, \ell/\xi) & \text{for } \ell \gg \xi \end{cases}$$
$$= \begin{cases} \ell^D & \text{for } \ell \ll \xi \text{ – fractal} \\ \xi^D(\ell/\xi)^d & \text{for } \ell \gg \xi \text{ – homogeneous.} \end{cases}$$

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Finite-size scaling

Assuming $p \neq p_c$, then $|p-p_c| \propto \xi^{-1/\nu}$, implying for $L=\infty$

$$
\begin{aligned}
P_\infty(p) &\propto (p-p_c)^\beta && \propto \xi^{-\beta/\nu} && \text{for } p \to p_c^+ \\
\chi(p) &\propto |p-p_c|^{-\gamma} && \propto \xi^{\gamma/\nu} && \text{for } p \to p_c \\
M_k &\propto |p-p_c|^{(\tau-k-1)/\sigma} && \propto \xi^{D(1+k-\tau)} && \text{for } p \to p_c, D = 1/(\sigma\nu) \\
n(s,p) &\propto s^{-\tau}\mathcal{G}(s/s_\xi) && \propto s^{-\tau}\mathcal{G}(s/\xi^D) && \text{for } p \to p_c, s \gg 1.
\end{aligned}
$$

For finite system sizes L we find

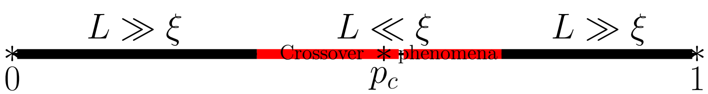
$$P_\infty(\xi,L) \propto \begin{cases} \xi^{-\beta/\nu} & \text{for } L \gg \xi \text{ – constant} \\ L^{-\beta/\nu} & \text{for } L \ll \xi \text{ – decaying.} \end{cases}$$

$$\chi(\xi,L) \propto \begin{cases} \xi^{\gamma/\nu} & \text{for } L \gg \xi \text{ – constant} \\ L^{\gamma/\nu} & \text{for } L \ll \xi \text{ – increasing.} \end{cases}$$

$$M_k(\xi,L) \propto \begin{cases} \xi^{D(1+k-\tau)} & \text{for } L \gg \xi \text{ – constant} \\ L^{D(1+k-\tau)} & \text{for } L \ll \xi \text{ – increasing.} \end{cases}$$

$$n(s,\xi) \propto \begin{cases} s^{-\tau}\mathcal{G}(s/\xi^D) & \text{for } L \gg \xi, s \gg 1 \text{ – cutoff constant} \\ s^{-\tau}\mathcal{G}(s/L^D) & \text{for } L \ll \xi, s \gg 1 \text{ – cutoff increasing.} \end{cases}$$

At $p = p_c$, the correlation length $\xi = \infty$, i.e., ALWAYS $L \ll \xi$. Measure critical exponents by investigating how the quantities scale with system size at $p = p_c$.



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The fixed point equation for the rescaling transformation $\xi = \xi/b$ has two solutions only: $\xi = 0, \infty$. These are associated with the solutions to the fixed point equation in p-space, $T_b(p) = p$, that is, $p = 0, 1, p_c$, representing the trivially self-similar states of the empty and fully occupied lattice and the nontrivial self-similar state at $p = p_c$, respectively. The critical exponent

$$\nu = \frac{\log(b)}{\left(\left.\frac{dT_b(p)}{dp}\right|_{p_c}\right)} \approx \frac{\log(b)}{\left(\left.\frac{dR_b(p)}{dp}\right|_{p^\star}\right)}$$

where the rescaling transformation T_b has been substituted with a real-space renormalisation transformation R_b incorporating coarsening with rescaling. We identify p_c with $p^\star$, the nontrivial solution to the fixed point equation

$$R_b(p^\star) = p^\star.$$

Often, the real-space renormalisation transformation chosen

$$R_b(p) = \begin{cases} \text{prob. of having a spanning cluster in block} \\ \text{prob. of having a majority of sites occupied in block.} \end{cases}$$

Real-space renormalisation transformation procedure:

1. Divide the lattice into blocks of linear size b.
2. Replace all sites in a block by a single block of size b occupied with probability $R_b(p)$ according to the real-space renormalisation transformation (coarse graining procedure).
3. Rescale all length scales by the factor b.

As critical exponents are determined by the large scale behaviour, they are insensitive to lattice details. They are universal.