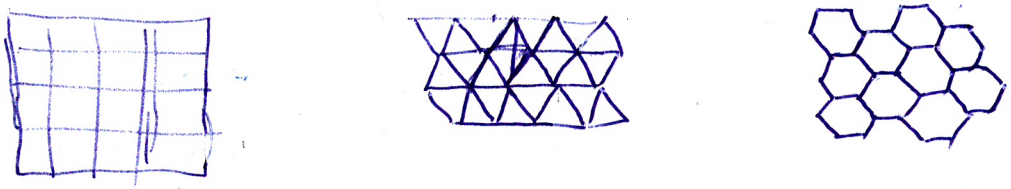
Percolation – MC simulations

- percolation theory studies the number and properties of clusters in „random" structures and phenomena occurring in these systems
- typically, we model some real system (surface of a solid, forest, polymers etc.) on a specific lattice in the d-dimensional space

  e.g. in the 2-dim. space we can consider

  square lattice triangular l. honeycomb l.



  or in the 3d cubic, diamond, bcc, fcc etc.

- depending on the modelled system one can study site-occupied lattices (site percolation) or bond-occupied lattices (bond perc.)

  e.g.

  sites are occupied bonds are occupied

- number of occupied sites or bonds depends on some parameter of the system (such as concentration or density of trees etc.)

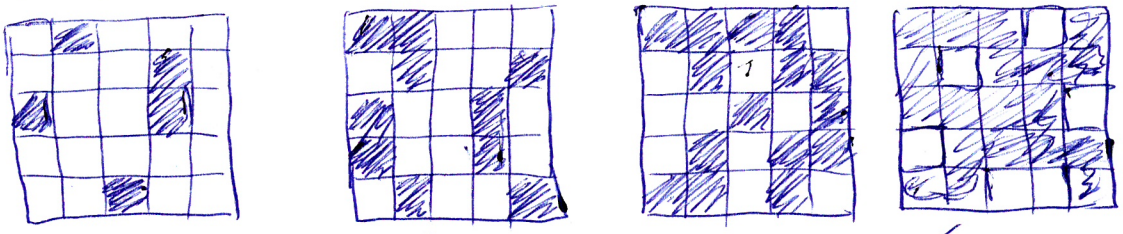
in percolation theory we work with a parameter

p = probability that a site or a bond is occupied

this probability p is usually considered to be independent for each site or bond but one can construct also models where occupation of sites depends on the neighborhood

- percolation theory studies distribution of clusters of various sizes in such lattices and particularly appearance of an „infinite" cluster or a spanning cluster for finite lattices depending on the probability p (or a corresponding physical parameter)

e.g. p = 0,2 p = 0,4 p = 0,6 p = 0,8



smaller separated clusters

large „spanning" clusters + a few small

- for each type of lattices there is a critical value of the parameter p - usually called the threshold p_c - for which there appears to be a transition from smaller clusters for $p < p_c$ to a large „spanning" cluster for $p > p_c$

e.g. for the square lattice above $p_c = 0,59275$

for the triangular lattice $p_c = 0,5$

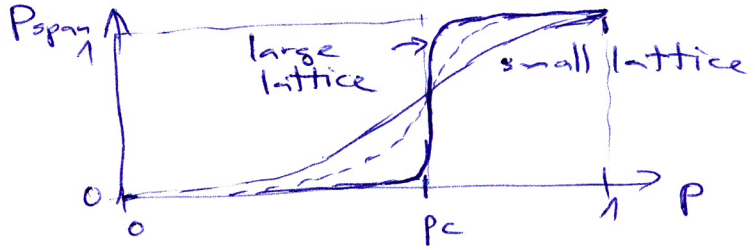
3d cubic $p_c = 0,3117$

if sites are occupied

thresholds are different for bond percolation

e.g. for the square lattice $p_c = 0,5$

- for finite lattices there is non-zero probability that a spanning cluster appears for any $p > 0$ but for $p \ll p_c$ it is very small
- as the size of the lattice increases the propability that the spanning cluster appears goes to zero for $p < p_c$ and goes to one for $p > p_c$



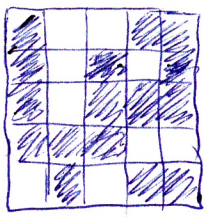
Exercise: We can use Monte-Carlo simulation to determine the threshold (at least approximately) from the point where curves $P_{span}(p)$ cross
- see the Mathematica notebook for the example for the square lattice

- we need somehow to determine whether there is a spanning cluster in a random lattice
- we can do that in two steps:
  1) use Hoshen-Kopelman algorithm to label clusters in the lattice
  2) compare labels in the first and last rows (this step is more or less trivial) (or columns)

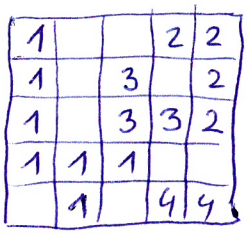
• Hoshen-Kopelman algorithm (Phys. Rev B 14 (1976) 3438)

basic structure: 1) go through all sites systematicly
2) assign labels (numbers) to occupied sites according to neighbours which are also occupied and which were already labelled
3) resolve conflicts of labels from two (or more) neighbours using an auxiliary array of labels

exaple:



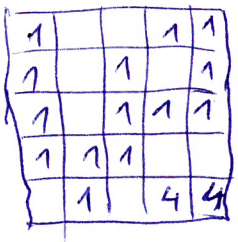
→



with an array of labelAssignments

1 → 1
2 → 1
3 → 1
4 → 4

after relabelling



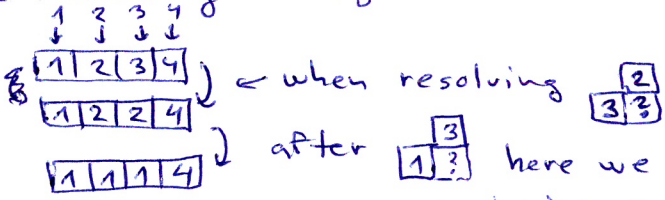
→ by counting 1's and 4's we set cluster sizes

and we can easily check that cluster 1 is a spanning cluster

notes: 1) always assign smaller labels to greater ones

2) it is necessary to relabel all label assignments whenever there is a conflict

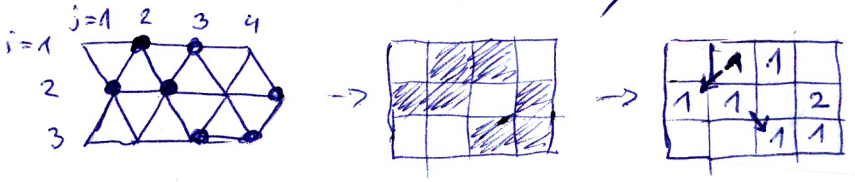
in the example above we have subsequently the following assignments:



here we changed both 2's assigning 2 → 1 and 3 → 1

3) it is not necessary to do relabelling to count sites belonging to the same cluster or for finding a spanning cluster but we have to keep and work with an auxiliary array „labelAssignments"

4) slight modifications are necessary for other types of lattices; e.g. for the triangular lattice we can still use a 2d array



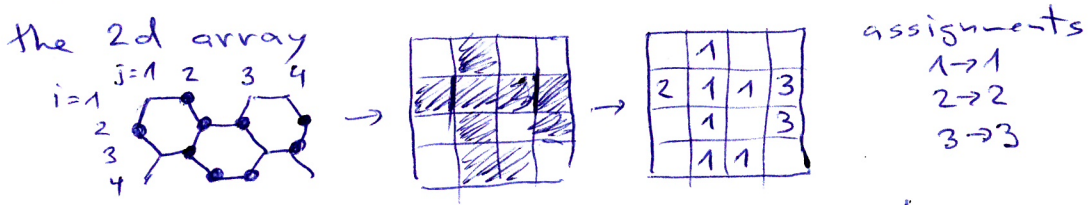
assignments
1 → 1
2 → 1

here the element (2,1) has two neighbour sites above (1,1) and (1,2) and we have to check both (1,2) is occupied ⇒ in (2,1) is 1

on the other hand, the element (3,3) has two neighbour sites (2,2) and (2,3) and because (2,2) is occupied we get (3,3) → 1 even though in the „square" array they are not closest neighbours

(notice that „neighbours above" are changing from row to row, they depend on whether i is odd or even)

- honeycomb lattice can be also arranged into the 2d array



but! here element (2,1) and (2,2) are not neighbours

[(2,2) and (2,3) are neighbours] and the same is true for (2,3) and (2,4)!

thus we have three clusters (not one)

- we see that number of neighbours increases when we go from ⬡ → □ → △

and that is why $p_c(⬡) > p_c(□) > p_c(△)$

- once we have labelled clusters using the H-K algorithm we can easily determine the cluster sizes and by repeating this process for many randomly occupied lattices, we can find the probabilities of finding a cluster of size s in a lattice occupied with probability p for each site (normalized per site)

these probabilities are called <u>cluster numbers</u> $n_s(p)$

from them other quantities of interest can be determined, such as the average cluster size S at a randomly chosen site which is occupied $S(p) = \sum_s n_s(p) s^2 \Big/ \sum_s n_s(p) s = \frac{M_2(p)}{M_1(p)}$

in 1D:

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

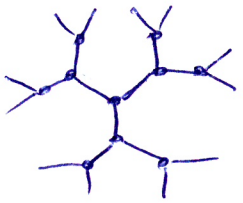
$p = \sum_{s=1}^{\infty} s\, n_s(p)$

prob. that occupied site is a part of the s cluster

$S = \frac{1+p}{1-p}$

where $M_k(p) = \sum_s n_s(p) s^k$ are k-th moments of the cluster size distribution $n_s(p)$

- such quantities can be determined in a closed form only for a few special lattices (one-dimensional, Bethe lattice)



or only asymptotic behaviour is known for $p \to p_c$ and large s

and for $p \to p_c$ and large s the cluster numbers assume the form

$$n_s(p) = s^{-\tau} f[(p-p_c) s^{\sigma}]$$

"scaling assumption" works for $d \leq 6$

where τ and σ do not depend on p but they and the function f depend on the lattice type and dimension and in general they must be determined from MC simulations

but e.g. for the square lattice $\tau = \frac{187}{91}$ and $\sigma = \frac{36}{91}$

(see D. Stauffer: Introduction to Percolation Theory, 1985 for details)

- many quantities have abrupt change in behaviour at the threshold p_c (as we have seen for $P_{span}(p)$) similar to phase transitions in thermodynamics

e.g. $$S \propto |p-p_c|^{\frac{t-3}{\sigma}} = |p-p_c|^{-\gamma} \qquad \gamma = \frac{3-\tau}{\sigma}$$

or termination time of fire in the forest simulated in the square lattice