FSTM: Bachelor of Mathematics

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Percolation

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Abstract

In the following, we will take a look at a number of problems appearing in percolation theory. More precisely, we will investigate site and bond percolation and examine corresponding random systems, as well as random variables connected to them. Our main goal is to estimate the dependence on parameters of those random variables in order to predict their behaviour for parameters that cannot be handled well computationally.

We are also going to see that there are some questions about percolation theory that are even computationally hard to grasp and that we were therefore not able to answer well.

Note that even though our main goal is to obtain experimental results, we take our time to define the objects we are working with rigorously. This allows us to formulate the questions we are interested in in a formal and precise way.

Contents

1 Site percolation

In this chapter, we will take a look at site percolation. Let us define the base objects we are going to be working with. For this, fix $n \in \mathbb{N}_{\geq 1}$.

Definition 1. A *system (of sites)* is defined to be a matrix $A = (a_{i,j}) \in \mathcal{M}_{n\times n}(\{0,2\})$. We say that n is the *size* of A.

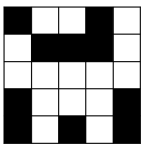
Remark 2. For simplicity, we will write "system" instead of "system of sites" throughout this chapter.

Interpretation 3. A system $A = (a_{i,j})$ of size n can be graphically interpreted: Draw a grid of size n by n. Each square of the grid is situated in some row i and some column j. If $a_{i,j} = 0$, leave the square blank. If $a_{i,j} = 2$, fill it black.

Take for instance the system

$$A = \begin{pmatrix} 2 & 0 & 0 & 2 & 0 \\ 0 & 2 & 2 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 2 \\ 2 & 0 & 2 & 0 & 2 \end{pmatrix}$$

of size $n = 5$. We can interpret A graphically as follows:



Definition 4. Let A be a system of size n. We will now define $F(A) = (b_{i,j}) \in \mathcal{M}_{n\times n}(\{0,1,2\})$ by the following rules:

(i) $\forall\, 1 \leq i,j \leq n : a_{i,j} = 2 \iff b_{i,j} = 2$,

(ii) $\forall\, 1 \leq j \leq n : a_{1,j} = 0 \iff b_{1,j} = 1$,

(iii) $\forall\, 2 \leq i \leq n,\ 1 \leq j \leq n,\ a_{i,j} = 0 : b_{i,j} = 1 \iff (b_{i-1,j} = 1 \text{ or } b_{i,j-1} = 1 \text{ or } b_{i,j+1} = 1)$,

(iv) $\#\{(i,j) \in \{1,\dots,n\}^2 : b_{i,j} = 1\}$ is minimal.

A *filled system (of sites)* is defined to be a matrix $F(A)$ for some system A.

The elements of A and $F(A)$ are called *sites*. A site is *open* if it equals 0, *closed* if it equals 2, and $filled$ if it equals 1.

Remark 5. The condition "$b_{i,j-1} = 1$" in (iii) is interpreted as "false" if $j = 1$. A similar remark holds for the last condition when $j = n$.

Interpretation 6. Let $B = (b_{i,j})$ be a filled system of size n. Reconsider a square in an n by n grid situated in row i and column j. If $b_{i,j} = 0$, leave the square blank. If $b_{i,j} = 1$, fill it blue. If $b_{i,j} = 2$, fill it black.

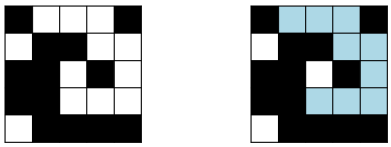
We shall consider the following system of size $n = 5$:

$$A = \begin{pmatrix} 2 & 0 & 0 & 0 & 2 \\ 0 & 2 & 2 & 0 & 0 \\ 2 & 2 & 0 & 2 & 0 \\ 2 & 2 & 0 & 0 & 0 \\ 0 & 2 & 2 & 2 & 2 \end{pmatrix}.$$

Then

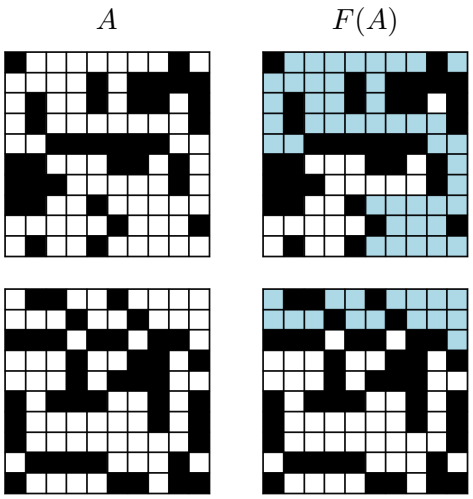
$$F(A) = \begin{pmatrix} 2 & 1 & 1 & 1 & 2 \\ 0 & 2 & 2 & 1 & 1 \\ 2 & 2 & 0 & 2 & 1 \\ 2 & 2 & 1 & 1 & 1 \\ 0 & 2 & 2 & 2 & 2 \end{pmatrix}.$$

Graphically, as described above, we can interpret A (left) and $F(A)$ (right) as follows:



We can think of $F(A)$ as the result of A being filled with water from the top, and flowing laterally and downwards through open sites.

Examples 7. To clarify the above interpretation of a filled system, we will take a look at two more examples of systems A of size $n = 10$ and the corresponding filled systems $F(A)$:



Definition 8. Let A be a system of size n and $F(A) = (b_{i,j})$ the corresponding filled system. A and $F(A)$ are said to *percolate*, if $b_{n,j} = 1$ for some $1 \leq j \leq n$.

Interpretation 9. Graphically, a system A percolates iff. one of the bottom squares is coloured blue in the graphical representation of $F(A)$. Hence, if A is filled with water from the top, it percolates iff. the water reaches the bottom.

Examples 10. In the examples 7, the first system percolates, while the second one doesn't.

Let us now consider random systems.

Definition 11. For a fixed probability $0 \leq p \leq 1$, let $a_{i,j}(p)$, $1 \leq i, j \leq n$, be independent random variables satisfying

$$\mathbb{P}\{a_{i,j} = 0\} = p = 1 - \mathbb{P}\{a_{i,j} = 2\}.$$

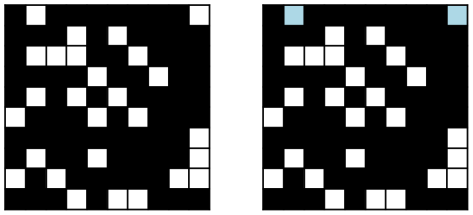
Then

$$A_n(p) := \begin{pmatrix} a_{1,1}(p) & \dots & a_{1,n}(p) \\ \vdots & \ddots & \vdots \\ a_{n,1}(p) & \cdots & a_{n,n}(p) \end{pmatrix}$$

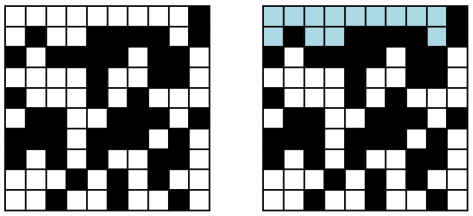
is called a *random system (of sites)*. We say that n is the *size* of $A_n(p)$.

Examples 12. We shall take a look at some random systems of size $n = 10$.

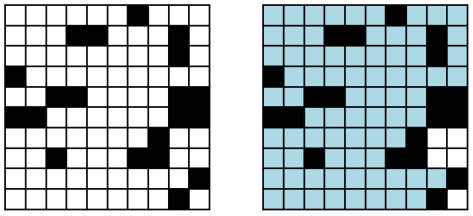
$A_{10}\left(\frac{1}{4}\right)$ $F\left(A_{10}\left(\frac{1}{4}\right)\right)$



$A_{10}\left(\frac{1}{2}\right)$ $F\left(A_{10}\left(\frac{1}{2}\right)\right)$



$A_{10}\left(\frac{3}{4}\right)$ $F\left(A_{10}\left(\frac{3}{4}\right)\right)$



Before focusing on our first problem, we will restate the Strong Law of Large Numbers (SLLN) that will repeatedly be used to get experimental results to our questions.

Theorem 13 (SLLN). *Let $(X_k)_{k\geq 1}$ be independent and identically distributed random variables with expected value $\mu \in \mathbb{R}$. For $n \geq 1$, let $\bar{X}_n := \frac{1}{n}\sum_{k=1}^{n} X_k$. Then*

$$\mathbb{P}\left\{\lim_{n\to+\infty} \bar{X}_n = \mu\right\} = 1.$$

1.1 Passage time

Definition 14. Let $F(A) = (b_{i,j})$ be a percolating system of size n. A *passage* through A (or $F(A)$) of *length* $m \in \mathbb{N}$ is a family $((i_1, j_1), \ldots, (i_m, j_m))$, such that

(i) $\forall\, 1 \leq k \leq m : i_k, j_k \in \{1, \ldots, n\}$,

(ii) $\forall\, 1 \leq k \leq m-1 : |i_{k+1} - i_k| + |j_{k+1} - j_k| = 1$,

(iii) $\forall 1 \leq k \leq m-1 : i_k \leq i_{k+1}$,

(iv) $\forall\, 1 \leq k \leq m : b_{i_k, j_k} = 1$,

(v) $i_1 = 1$ and $i_m = n$.

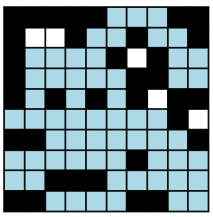
We call $\mathcal{P}(A) := \min\{m \in \mathbb{N} : \exists$ a passage of length m through $A\}$ the *passage time* of A (or $F(A)$).

Remark 15. The condition (ii) means that (i_k, j_k) and (i_{k+1}, j_{k+1}) are neighbouring vertices of $\mathbb{N}^2$. As $F(A)$ is percolating, the passage time of A exists. Moreover, conditions (ii) and (v) imply that $n \leq \mathcal{P}(A) \leq n^2$.

Interpretation 16. Graphically, the passage time of a percolation system $F(A)$ is the minimum number of filled sites you need to traverse to get from the top to the bottom row of $F(A)$.

Examples 17. We will take a look at passages through systems $F(A)$.

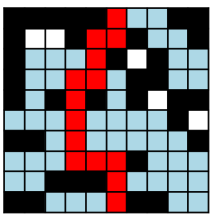
(i) Let us consider the following percolating system $F(A)$ of size $n = 10$, graphically given by



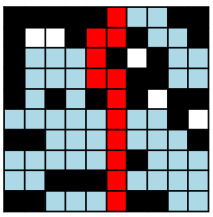
One passage through $F(A)$ is the family

$$((1,6),(2,6),(2,5),(3,5),(4,5),(4,4),(5,4),(6,4),(7,4),(8,4),(8,5),(8.6),(9,6),(10,6))$$

of length 14, graphically given by the following red-coloured sites:

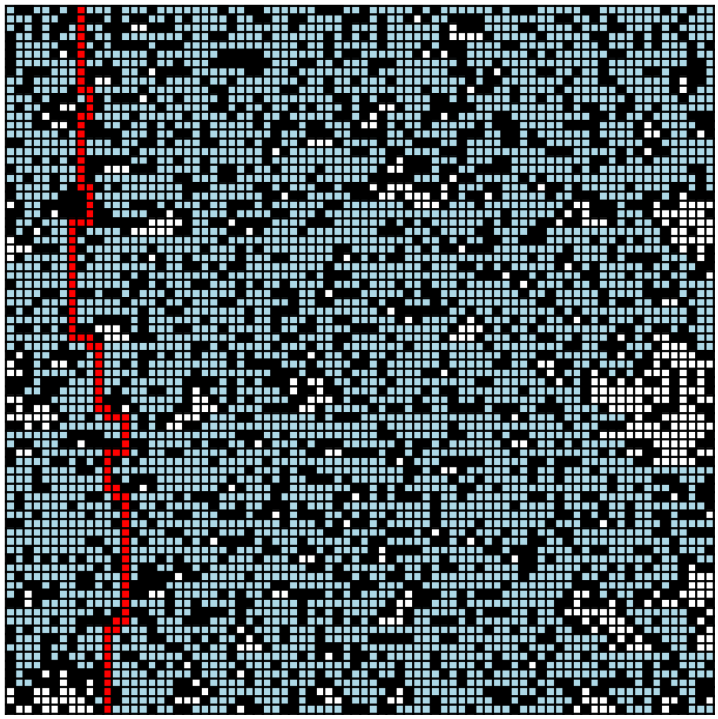


A shorter passage is given by



whose length equals 12. One easily checks that there is no strictly shorter passage through A. Hence, the passage time of A equals $\mathcal{P}(A) = 12$.

(ii) Here is an example of a percolating system $F(A)$ of size $n = 80$, where one of the passages with shortest length has again been marked in red:



The passage time of this system equals $\mathcal{P}(A) = 97$.

Question. Let $n \geq 1$ and $0 \leq p \leq 1$. Knowing that a random system $A_n(p)$ percolates, what is the average value of its passage time?

Mathematically, if the probability $\mathbb{P}$ in definition 11 is defined on a σ-algebra of some probability space Ω, we set $\Omega' := \{\omega \in \Omega : A_n(p)(\omega) \text{ percolates}\}$. For the rest of this section, let us replace $\mathbb{P}$ by the conditional probability $\mathbb{P}(\,\cdot \,|\, \Omega')$. In that case, we are interested in the behaviour of the expected value of the passage time $A_n(p)$, i.e. in

$$P_n(p) := \mathbb{E}(\mathcal{P}(A_n(p)).$$

Answer. We have

$$P_n(p) = \sum_{k \geq 0} k \cdot \mathbb{P}\left\{\mathcal{P}(A_n(p)) = k\right\}.$$

By remark 15, we can reduce this sum as follows:

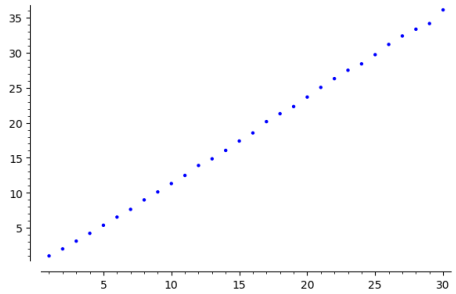
$$P_n(p) = \sum_{n \leq k \leq n^2} k \cdot \mathbb{P}\left\{\mathcal{P}(A_n(p)) = k\right\}.$$

However, determining the exact probabilities that appear in this sum is difficult for n great.

Thus, we will estimate $P_n(p)$ using Theorem 13: We compute, independently, a large number k of random systems $A_n(p)$, calculate their passage time, then take the corresponding average. The obtained result will be a good approximation of $P_n(p)$.

Using Sage, we are able to estimate $P_n(p)$ for $1 \leq n \leq 30$, p fixed, and represent the results graphically: The values on the x-axis stand for n, the values on the y-axis represent the approximated value of $P_n(p)$.

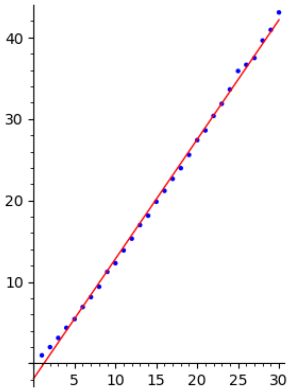
Here is an example for $p = 0.6$ and $k = 100$:



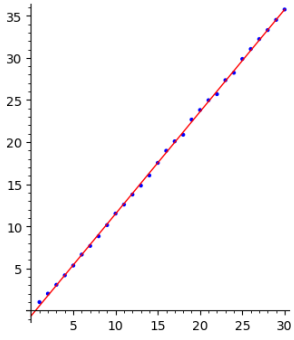
Graphically, we observe that $P_n(p)$ can be approximated by $a_p n + b_p$ for some $a_p, b_p \in \mathbb{R}$ depending on p. Using the "method of least squares," we can estimate, again using Sage, such a_p, b_p based on the obtained approximations for $P_1(p)$, ..., $P_{30}(p)$.

In the following, we will give some examples for such estimates. We will only list the value of a_p, as b_n has no asymptotic influence. Note that in all 4 cases, we choose $k = 100$.

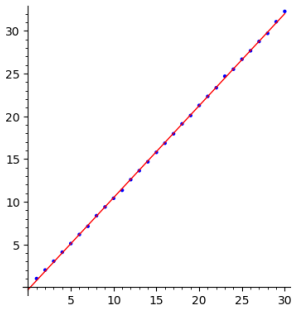
$p = 0.6, a_p \approx 1.45$:



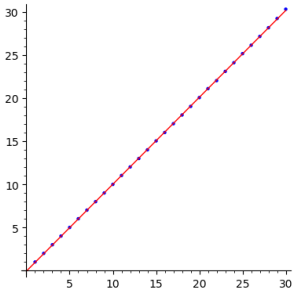
$p = 0.7, a_p \approx 1.22$:



$p = 0.8, a_p \approx 1.08$:



$p = 0.9, a_p \approx 1.01$:



Remark 18. We can make a number of remarks and observations concerning our experimental results.

(i) Due to computational difficulty, we are not able to give the corresponding graph for $p \leq 0.5$. The next section will deal in more detail with the cause of this problem.

(ii) Observe that

$$\forall\, 0 \leq p \leq 1 : a_p \geq 1.$$

This makes sense, because for n great, we have

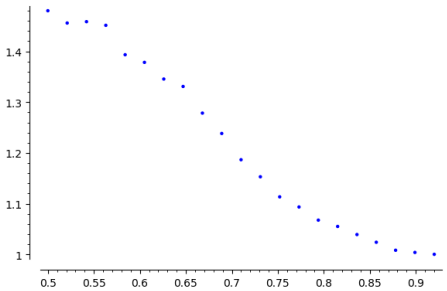
$$n \leq P_n(p) \approx a_p n + b_p \approx a_p n,$$

where the first inequality is due to $\mathcal{P}(A_n(p)) \geq n$ (see remark 15).

(iii) Moreover, notice that $P_n(1) = n = 1 \cdot n + 0$, hence $a_1 = 1$. Thus, it makes sense that $a_p \to 1$ for $p \to 1$.

(iv) The approximation $P_n(p) \approx a_p n + b_p$ is useful to estimate the passage time for percolating systems of large size n without explicitly computing it. As we can graphically deduce, the approximation is better for p closer to 1.

(v) Lastly, it is natural to wonder about a clearer dependence of a_p on p. Unfortunately, as the estimation of a_p is already very computationally heavy, it is even harder to approximate a_p for a great number of different values for p. Nonetheless, we shall present a graph depicting a rough estimate of a_p in function of $0.5 \leq p \leq 0.92$.



Every approximation of a_p has been computed similarly to above: First, estimate $P_1(p)$, ..., $P_{20}(p)$ by calculating the average passage time of $k = 50$ independent random systems respectively, then use the "method of least squares" to approximate a_p.

One could delve further into this estimation and find a function $f : [0,1] \to \mathbb{R}$ satisfying $f(p) \approx a_p$ for $0 \leq p \leq 1$, for example $x \mapsto f(x) = \alpha e^{-\beta x^2} + 1$ for some $\alpha, \beta \in \mathbb{R}, \beta > 0$. Another question arises then: Do we have the symmetric behaviour

$$a_p = a_{1-p}$$

for $0 \leq p \leq 1$? This would imply $a_p \approx 1$ for $0 < p \approx 0$, hence $P_n(p) \approx n$ for $0 < p \approx 0$. This would make sense, as for p very small, we would expect the length of the shortest passage through $A_n(p)$ to be close to n (otherwise a great number of sites would be filled, which is improbable for $p \approx 0$).

The equality $a_p = a_{1-p}$ would also imply that the average value of the passage time satisfies

$$P_n(p) \approx P_n(1-p) \text{ for } n \geq 1,\ p \in [0,1].$$

A good first step to investigate this guess is to get exact results for small n. We might want to return to this at a later point in time.

1.2 Percolation probability

In this section, we will analyse the behaviour of the probability that a random system $A_n(p)$ percolates, called the percolation probability, in dependence of its size n and the probability p. For n small, we can find exact expressions for this probability.

Definition 19. For $n \geq 1$ and $0 \leq p \leq 1$, we call

$$q_n(p) := \mathbb{P}\{A_n(p) \text{ is percolating}\}$$

the *percolation probability* of the random system $A_n(p)$.

Proposition 20. *The percolation probability $q_n(p)$ for $1 \leq n \leq 4$ and $0 \leq p \leq 1$ is given by the following table:*

n	$q_n(p)$
1	p
2	$-p^4 + 2p^2$
3	$p^9 - 6p^8 + 14p^7 - 9p^6 - 6p^5 + 4p^4 + 3p^3$
4	$p^{16} - 20p^{14} + 44p^{13} + 10p^{12} - 108p^{11} + 66p^{10} + 48p^9 - 22p^8 - 28p^7 - 6p^6 + 12p^5 + 4p^4$

Proof. For $n \geq 1$ and $0 \leq p \leq 1$, we can rewrite the percolation probability as follows:

$$\begin{aligned} q_n(p) &\overset{\text{def.}}{=} \mathbb{P}\{A_n(p) \text{ is percolating}\} \\ &= \sum_{\substack{A \in \mathcal{M}_{n\times n}(\{0,2\}) \\ A \text{ is percolating}}} \mathbb{P}(A_n(p) = A). \end{aligned} \tag{1.1}$$

Thus, if we generate all the percolating systems A of size n, compute the respective probabilities for $A_n(p) = A$, then sum them up, we end up with $q_n(p)$. Those tasks will be given to a computer program.

Note that in total, there are

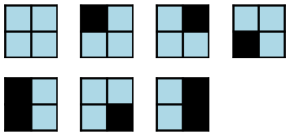
$$\#\mathcal{M}_{n\times n}(\{0,2\}) = 2^{n^2}$$

systems to consider. The number of filled systems is the same (as there is a 1-to-1-correspondence between the set of systems and the set of filled systems).

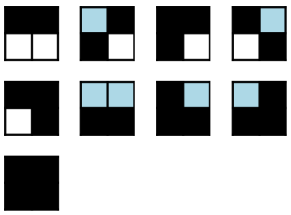
Because of this high number of systems to analyse, we shall give the proof for $n = 2$ only. The cases $n = 3, 4$ are treated analogously, and the case $n = 1$ is trivial (as there is only one percolating system of size 1).

Hence, let us fix $n = 2$. We can graphically give the $2^{n^2} = 2^{2^2} = 16$ filled systems $F(A)$:

Percolating systems



Non-percolating systems



For a fixed percolating system A of size n with $m(A)$ open sites, we have $n^2 - m(A)$ closed sites. Remember that p is the probability that a given site is open, and $1 - p$ is the probability that a given site is closed. Hence

$$\mathbb{P}\{A_n(p) = A\} = p^{m(A)} \cdot (1-p)^{n^2-m(A)}. \tag{1.2}$$

Finally, we obtain

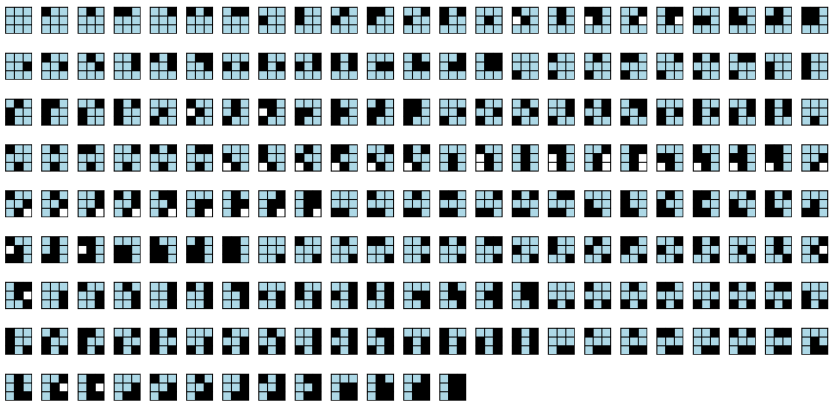
$$\begin{aligned}
q_2(p) &\overset{(1.1)}{=} \sum_{\substack{A\in\mathcal{M}_{2\times 2}(\{0,2\}) \\ A \text{ is percolating}}} \mathbb{P}(A_2(p) = A) \\
&\overset{(1.2)}{=} \sum_{\substack{A\in\mathcal{M}_{2\times 2}(\{0,2\}) \\ A \text{ is percolating}}} p^{m(A)} \cdot (1-p)^{2^2-m(A)} \\
&\overset{\text{graph}}{=} p^4 + p^3(1-p)^1 + p^3(1-p)^1 + p^3(1-p)^1 + p^2(1-p)^2 + p^3(1-p)^1 + p^2(1-p)^2 \\
&= -p^4 + 2p^2,
\end{aligned}$$

as was stated in the table above. □

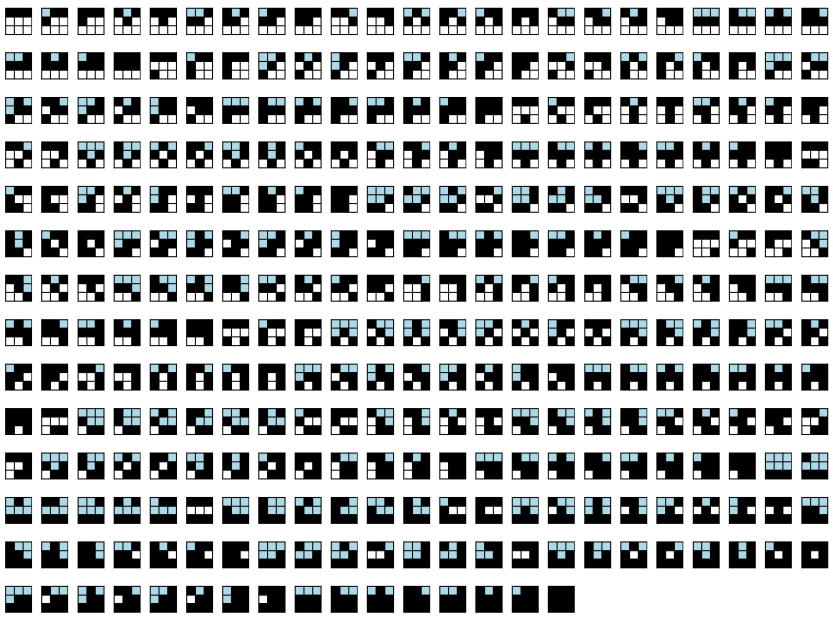
Remark 21. We can give some remarks and observations concerning the previous proposition.

(i) Similarly to what we did for $n = 2$ in above proof, we can give all the $2^{2^3} = 256$ filled systems of size $n = 3$:

Percolating systems



Non-percolating systems



(ii) For $n = 4$, one would already need to consider $2^{2^4} > 65\,000$ systems, that we will therefore not depict.

(iii) For $n \geq 5$, the time needed to compute an exact expression for $q_n(p)$ is elevated. Therefore, we decided to stop at $n = 4$.

(iv) By 1.2, $\mathbb{P}\{A_n(p) = A\}$ is a polynomial in p of degree n^2. Therefore, $q_n(p)$ is by 1.1 a sum of polynomials in p of degree n^2, hence again a polynomial in p (of degree less than or equal to n^2).

(v) The table in the proposition 20 suggests that the degree of the polynomial $q_n(p)$ equals n^2 and that the coefficient of p^{n^2} equals ± 1. However, we were not able to prove this claim in general.

Our next goal is to find $0 \leq p \leq 1$ such that the probability that a system $A_n(p)$ percolates is exactly one half.

Proposition 22. *For $n \geq 1$, there exists a unique $\tau_n \in]0, 1[$ such that $q_n(\tau_n) = \frac{1}{2}$.*

Proof. The function $q_n : [0,1] \to \mathbb{R}$ satisfies the following properties:

- q_n is continuous (as it is a polynomial by (iv) of the previous remark),
- $q_n(0) = 0$ (a system with no open sites cannot percolate),
- $q_n(1) = 1$ (a system with no closed sites always percolates),
- q_n is injective (if $0 \leq p_1 < p_2 \leq 1$, then we *expect* $q_n(p_1) < q_n(p_2)$, as a system with more open sites should be more likely to percolate).

By a direct consequence of the Intermediate Value Theorem, q_n must attain the value $\frac{1}{2}$ for some $\tau_n \in]0,1[$. Additionally, τ_n is unique, because q_n is injective. □

Definition 23. For $n \geq 1$, the unique probability τ_n of proposition 22 will be called the *percolation border* of $A_n(\cdot)$.

Examples 24. We shall examine τ_n , $n = 1, 2, 3, 4$, using proposition 20:

(i) $n = 1$: We have $q_1(p) = p$ for $0 \leq p \leq 1$. Hence $\tau_1 = \frac{1}{2} = 0.5$.

(ii) $n = 2$: We have $q_2(p) = -p^4 + 2p^2$, thus we are interested in solving

$$-p^4 + 2p^2 = \frac{1}{2}$$

for $p \in]0,1[$. We claim that $p = \sqrt{1 - \frac{1}{\sqrt{2}}} \approx 0.541196100$ is a solution. Indeed:

$$-\sqrt{1 - \frac{1}{\sqrt{2}}}^4 + 2\sqrt{1 - \frac{1}{\sqrt{2}}}^2 = -\left(1 - \frac{1}{\sqrt{2}}\right)^2 + 2\left(1 - \frac{1}{\sqrt{2}}\right) = -1 + \frac{2}{\sqrt{2}} - \frac{1}{2} + 2 - \frac{2}{\sqrt{2}} = \frac{1}{2}.$$

By proposition 22, this $p \in]0,1[$ is unique. Hence $\tau_2 = \sqrt{1 - \frac{1}{\sqrt{2}}} \approx 0.541196100$.

(iii) $n = 3$: In this case, $q_3(p)$ is a polynomial in p of degree $9 > 4$. As there is no general formula to solve equations of degree greater than 4, we shall approximate the solution $p \in]0,1[$ to the equation $q_3(p) = \frac{1}{2}$. Using Sage, we obtain the value $p \approx 0.559296316$. This is our estimation for the value of τ_3.

(iv) $n = 4$: Similar to the case $n = 3$, we find $\tau_4 \approx 0.569724134$.

Remark 25. Considering the examples above, we can make the following observations:

(i) $\tau_1 < \tau_2 < \tau_3 < \tau_4$. Hence, we expect $(\tau_n)_{n\geq 1}$ to be an increasing sequence of real numbers. This is only an *assumption*. We were not able to prove this claim.

(ii) $(\tau_n)_{n\geq 1}$ is bounded from above (by 1). Hence, if we assume that $(\tau_n)_{n\geq 1}$ is an increasing sequence, we can immediately conclude that $(\tau_n)_{n\geq 1}$ must be converging to some $\tau \in [0,1]$.

Definition 26. It it exists, we call

$$\tau := \lim_{n \to +\infty} \tau_n$$

the *percolation threshold (of site percolation).*

Question. Can we get experimental indications for the existence of the percolation threshold τ? If so, how can it be estimated?

Answer. Firstly, let us take a look at how we can estimate $q_n(p)$. For this, fix $n, k \geq 1$ and $p \in [0,1]$. Let $A_n^l(p)$, $1 \leq l \leq k$, be k independent random systems of size n. Let

$$X_l := \begin{cases} 1, & \text{if } A_n^l(p) \text{ percolates} \\ 0, & \text{otherwise.} \end{cases}$$

Then the expected value of X_l is given by

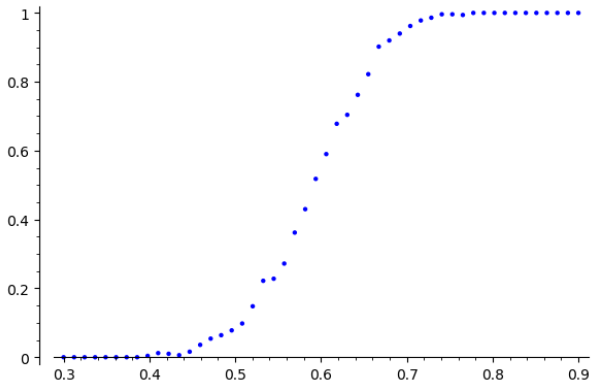
$$\mathbb{E}(X_l) \overset{\text{def.}}{=} \mathbb{E}\left(\mathbb{1}_{\{A_n^l(p) \text{ percolates}\}}\right) = \mathbb{P}\{A_n^l(p) \text{ percolates}\} \overset{\text{def.}}{=} q_n(p),$$

where "$\mathbb{1}$" denotes the indicator function.

By theorem 13, $\frac{1}{k}\sum_{l=1}^{k} X_l$ is a good estimation for $q_n(p)$ for k great. Based on this, we will compute k random systems $A_n(p)$ independently; if k_0 of them percolate, then $\frac{k_0}{k}$ is a good estimation for $q_n(p)$.

Now, this estimation for $q_n(p)$ can be done for varying p. In what follows, we will consider $m \geq 2$ different values of p, uniformly distributed in the interval $[0.3, 0.9]$.

Here is an example for $n = 15$, $k = 500$ and $m = 50$. The values on the x-axis represent the values for p, those on the y-axis stand for our estimations of $q_n(p)$ that have been computed as explained above.

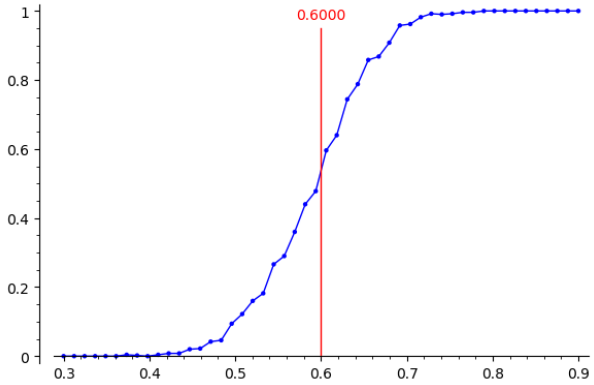


An imprecise observation suggests that the percolation border τ_n lies around 0.6. As we assume that the sequence $(\tau_n)_{n\geq 1}$ converges, this would already be a rough estimate for the percolation threshold τ.

Next, we will consider the same kind of graph, with two additions:

- We connect the points of the graph to get a better feeling for the curve,
- We consider the greatest considered p such that our estimation for $q_n(p)$ lies below $\frac{1}{2}$, as well as the smallest considered p such that $q_n(p)$ lies above $\frac{1}{2}$. Then we take the average value of both, to estimate τ_n.

This yields the following graph, again using $n = 15$, $k = 500$ and $m = 50$, where the vertical red line is given by the approximated value for τ_n:



Unfortunately, the precision of this method directly depends on m, since the obtained estimation of τ_n is the average of two consecutive probabilities, hence of the form

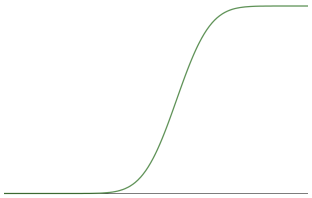
$$\frac{\left(0.3+\frac{i}{m-1}\right)+\left(0.3+\frac{i+1}{m-1}\right)}{2}=0.3+\frac{1}{2m-2}+\frac{i}{m-1}.$$

Thus, even if our estimations for $q_n(p)$ were *perfect* (which is clearly not the case), we would still systematically commit an average mistake of around $\frac{1}{2m}$. Hence, in above case, we expect an average error of at least $\frac{1}{2\cdot 50}=0.01$.

To get a better estimation, we will take a look at the method of curve fitting. Because of its graph, a first choice would be the cumulative distribution function for a normally distributed random variable, which in general has the form

$$G_{\mu,\sigma}:\left\{\begin{array}{ccc}\mathbb{R} & \to & \mathbb{R}\\ x & \mapsto & \frac{1}{2}\left[1+\operatorname{erf}\left(\frac{x-\mu}{\sigma\sqrt{2}}\right)\right]\end{array}\right.$$

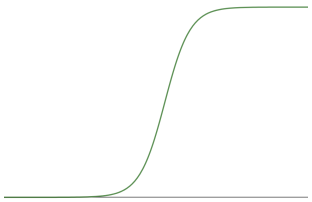
for $\mu\in\mathbb{R}$ and $\sigma>0$, as well as the graph



However, it is hard to work with this family of functions, since it is based on the error function erf. Therefore, we decided to consider a different family of functions, namely

$$F_{r,a}:\left\{\begin{array}{ccc}\mathbb{R} & \to & \mathbb{R}\\ x & \mapsto & \frac{1}{1+\mathrm{e}^{r(x-a)}}\end{array}\right.$$

for $r,a\in\mathbb{R}$. A graph of such a function is given directly below, similar to the one above:



Note that a function that would perfectly fit into our situation needed to satisfy $F(1) = q_n(1) = 1$. Unfortunately, we have $G_{\mu,\sigma}, F_{r,a} < 1$, so in particular $G_{\mu,\sigma}(1), F_{r,a}(1) < 1$. Nonetheless, we will see that choosing the family of curves $F_{r,a}$ will yield good estimates for τ_n and τ.

We should keep in mind the reason why we try to estimate our data points by a smooth curve: We want to approximate $p \in [0,1]$ such that $q_n(p) = \frac{1}{2}$. Therefore, after determination of the parameters $r, a \in \mathbb{R}$, we are interested in $x \in [0,1]$ such that $F_{r,a}(x) = \frac{1}{2}$:

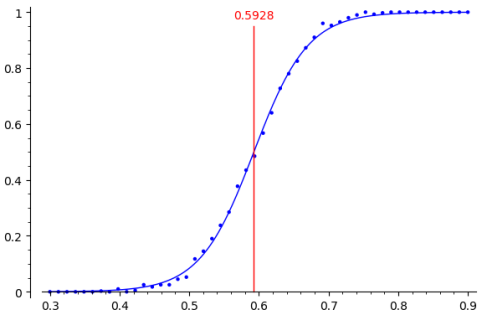
$$\begin{aligned} F_{r,a}(x) = \frac{1}{2} &\overset{\text{def. } F_{r,a}}{\iff} \frac{1}{1+\mathrm{e}^{r(x-a)}} = \frac{1}{2} \\ &\iff 1+\mathrm{e}^{r(x-a)} = 2 \\ &\iff \mathrm{e}^{r(x-a)} = 1 \\ &\iff r = 0 \text{ or } x = a. \end{aligned}$$

Choosing $r = 0$ would give us the constant function $F_{r,a} = \frac{1}{2}$. This case is clearly to be excluded, as it would fit our data points very poorly. Therefore, our estimation for τ_n is given by the parameter a. If n is great, the percolation threshold τ is close to τ_n (as we assume that the sequence of percolation borders converges to τ). This gives us the following estimation:

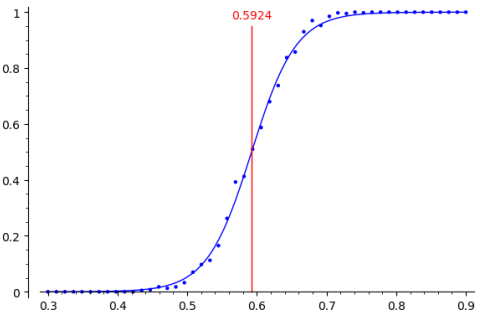
$$\tau \approx a.$$

In the graphs below, the points' x-coordinates are probabilities p, while their y-coordinates are estimates for $q_n(p)$, found as described at the beginning of this answer. The drawn curve is the graph of the function $F_{r,a}$, where the values for $r, a \in \mathbb{R}$ were found by using the method of curve fitting ("least squares"). The red line is given by the points $(a, y), y \in \mathbb{R}$. The given values for n, k and m have the same meaning as for the previous graphs.

$n = 15, k = 400, m = 50$:



$n = 20, k = 400, m = 50$:



Seeing that both approximations are close to another even though they correspond to different choices of n, we assume that the percolation threshold also lies in this range, which yields the approximation

$$0.592 \leq \tau \leq 0.593.$$

A comparison with other experiments that also estimated τ found that $\tau \approx 0.5927$, showing that our approximation is acceptable.

2 Bond percolation

In this chapter, we will consider bond percolation. Note that to avoid confusion, we will use the word "conduct" instead of "percolate" for the systems that we examine in this chapter (see definition 36). Let us now define the base objects we are going to be working with. Again, $n \geq 1$ will always denote a natural number.

Notation. (i) We use the notation $[n]_2 := \{0, \dots, n\}^2$. An element $V \in [n]_2$ is called a *vertex*.

(ii) $\|\cdot\|$ shall denote the Euclidean norm of $\mathbb{R}^2$.

Definition 27. A *system (of bonds)* is a set $A \subseteq [n]_2^2$ such that $\forall (V_1, V_2) \in A$:

(i) $\|V_1 - V_2\| = 1$,

(ii) $\|V_1\| < \|V_2\|$.

We say that n is the *size* of A. The elements of A are called *bonds* of A .

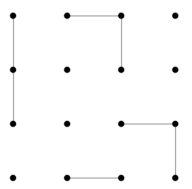
Remark 28. For simplicity, we will write "system" instead of "system of bonds" throughout this chapter.

Interpretation 29. As usual, the objects of the previous definition can easily be interpreted graphically. Let A be a system of size n. A bond (V_1, V_2) of A shall be interpreted as a line segment from V_1 to V_2. Condition (i) ensures that the points V_1 and V_2 are neighbouring vertices of $\mathbb{N}^2$. Condition (ii) implies that a line segment does not appear twice in A (because $(V_1, V_2) \in A \overset{\text{(ii)}}{\Longrightarrow} (V_2, V_1) \notin A$).

Examples 30. Here is an example of a system of bonds A of size $n = 3$, given by

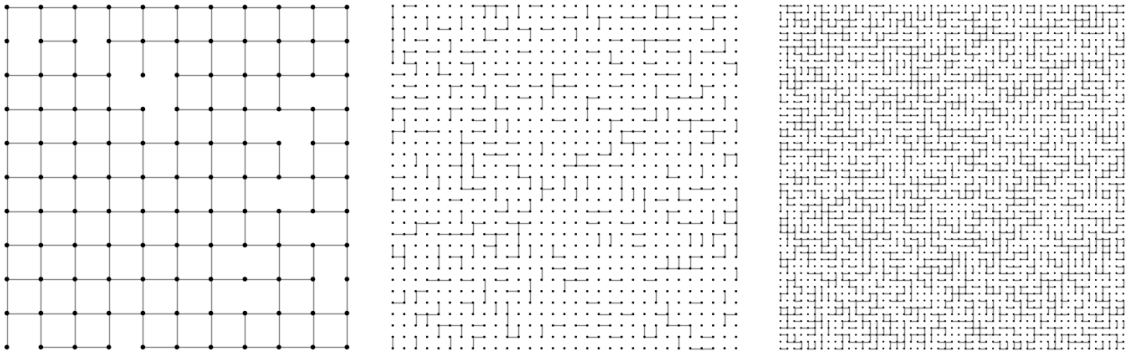
$$A=\{((0,0),(0,1)),((0,1),(0,2)),((1,0),(2,0)),((2,0),(2,1)),((2,2),(3,2)),((3,2),(3,3)),((1,3),(2,3))\}.$$

Graphically, it can be depicted by marking the vertices of $[n]_2^2 = \{0, 1, 2, 3\}^2$; then, for all the bonds (V_1, V_2) of A, one draws a line segment from V_1 to V_2 as shown in the following graph:



Note that we will always depict the systems of bonds in such a way that the positive direction of the y-axis is downwards. The origin $0 \in \mathbb{R}^2$ is therefore always in the upper left corner.

Different systems of respective sizes $n = 10, 30, 50$ are shown below:



Definition 31. Let A be a system of size n. A *chain of bonds* of A of *length* $m \in \mathbb{N}$ is an m-tuple $(V_1, \dots, V_m)$ such that

(i) $\forall\, 1 \leq i \leq m-1 : (V_i, V_{i+1})$ is a bond of A or (V_{i+1}, V_i) is a bond of A,

(ii) $\#\{V_1, \dots, V_m\} = m$.

Remark 32. Condition (ii) ensures that no vertex V_i is contained twice in the m-tuple.

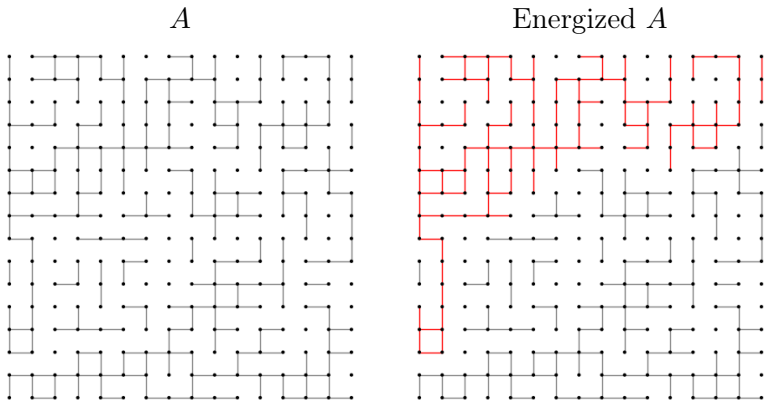
Definition 33. Let A be a system of size n and $V_1 = (a, b) \in [n]_2$ a vertex. Then V_1 is said to be *energized* via A if there exists a vertex $V_2 = (c, 0) \in [n]_2$ and a chain of bonds of A that contains both V_1 and V_2. Moreover, a bond $(W_1, W_2) \in A$ is said to be *energized* via A if W_1 is energized via A or W_2 is energized via A.

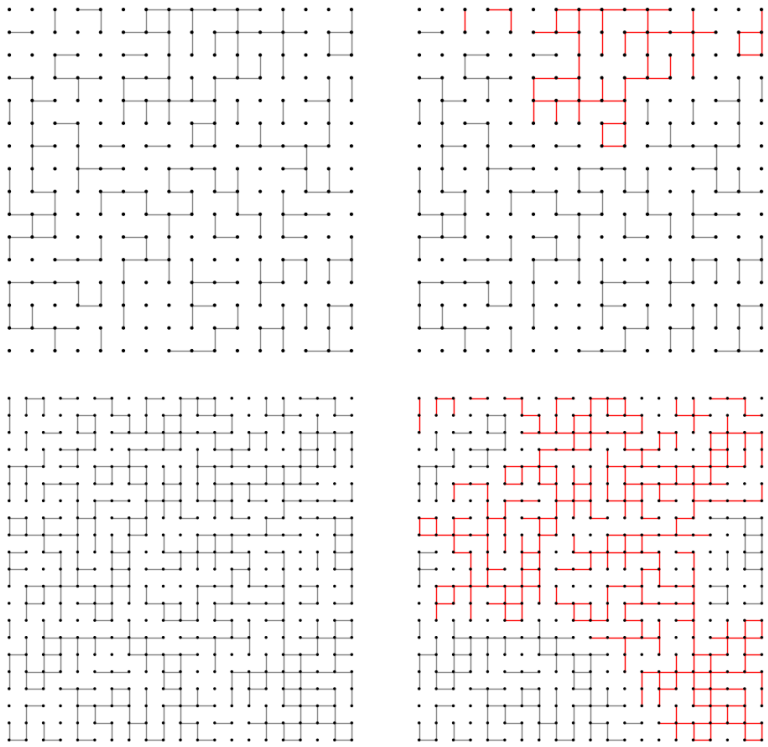
Interpretation 34. The previous definition can easily be understood graphically. Informally speaking, if we depict a system of bonds A, a bond of A (respectively a vertex) is energized iff. it can be connected to a vertex of the top row via drawn lines (i.e. via the bonds of A).

In the following, energized bonds of a system A will always be represented in the colour red. We say that this is the representation of the energized A.

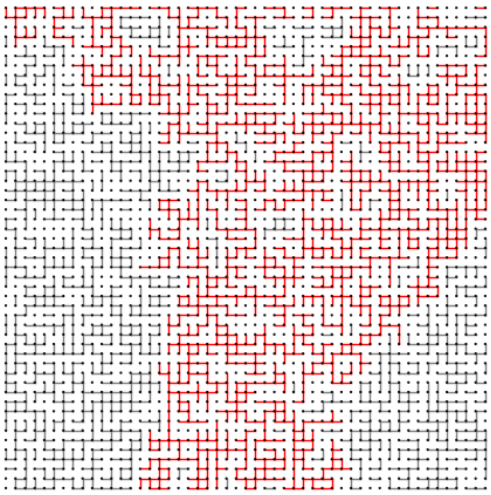
The idea behind this is the following: All the vertices $(0, 0), \dots, (n, 0)$ of the first row are connected to a power source. The bonds of a system A of size n are interpreted as wire. A vertex (respectively a bond) is energized if it can, via wire, be connected to the power source.

Examples 35. Below, we show some systems of bonds A of respective sizes $n = 15, 15, 20$ on the left, and the corresponding representation of the energized A on the right.





Lastly, below is a graph of an energized system of size $n = 50$:



Definition 36. Let A be a system of size n. The *conduction height* of A is defined as

$$h(A) := \max\{0 \leq b \leq n \,|\, \exists\, 0 \leq a \leq n : (a, b) \text{ is energized via } A\}.$$

A is said to *conduct* if $h(A) = n$.

Examples 37. In the examples 35, we have respective conduction heights of $h(A) = 13, 6, 20, 50$. The first two systems do not conduct, the last two do.

Definition 38. Fix $n \geq 1$ and $p \in [0, 1]$. Let

$$B_n := \left\{(V_1, V_2) \in [n]_2^2 : \|V_1 - V_2\| = 1 \text{ and } \|V_1\| < \|V_2\|\right\}$$

be the set of all possible bonds that can appear in a system of bonds of size n. Moreover, let a_W, $W \in B_n$, be independent random variables satisfying

$$\mathbb{P}\{a_W = 1\} = p = 1 - \mathbb{P}\{a_W = 0\}.$$

Lastly, let b_W, $W \in B_n$, be sets defined by

$$b_W := \begin{cases} \{W\}, & \text{if } a_W = 1 \\ \varnothing, & \text{otherwise.} \end{cases}$$

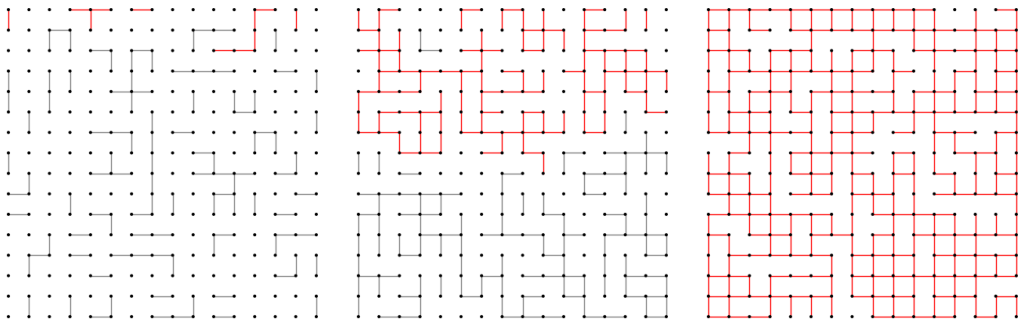
Then

$$A_n(p) := \bigcup_{W \in B_n} b_W$$

is called a *random system (of bonds)* of *size* n.

Remark 39. If the random variables a_W are defined on some probability space Ω, then by definition, $A_n(p)(\omega)$ is indeed a system of bonds of size n for all $\omega \in \Omega$. Informally speaking, we can graphically think of $A_n(p)$ as a system of size n, where the probability that a given bond is drawn equals p.

Examples 40. For clarification, we shall give some examples for random systems $A_n(p)$. In the following, we fix $n = 15$ and draw some energized systems $A_n(p)$ for $p = \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ respectively. Notice that the greater p is, the more bonds the system has (as expected).



2.1 Conduction height

Definition 41. For $n \geq 1$ and $0 \leq p \leq 1$, we call

$$h_n(p) := \mathbb{E}\{h(A_n(p))\}$$

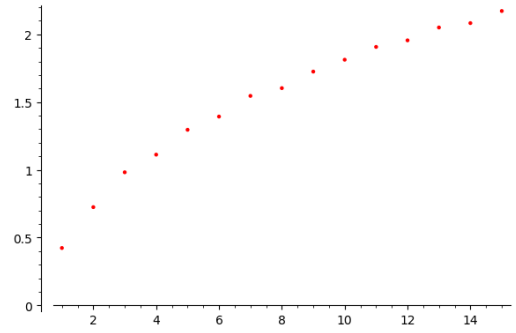
the *average conduction height* of $A_n(p)$.

Question. How does the average conduction height $h_n(p)$ depend on n and p?

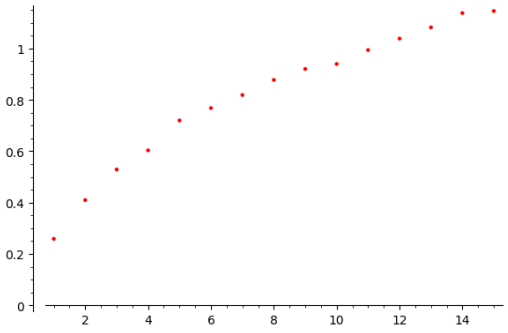
Answer. We can approximate $h_n(p)$ as follows: Generate an elevated number $k \geq 1$ of independent random systems $A_n(p)$, calculate their conduction height, then take the corresponding average of those k values. Theorem 13 ensures that the result will be a good estimation for $h_n(p)$.

In the following graphs, we represent the approximated points $(p, h_1(p))$, ..., $(p, h_n(p))$ for fixed $0 \leq p \leq 1, n \geq 1$ (i.e. represent $h_m(p)$ in dependence of m for $1 \leq m \leq n$).

$n = 15, k = 3\,000, p = 0.25$:



$n = 15, k = 3\,000, p = 0.15$:



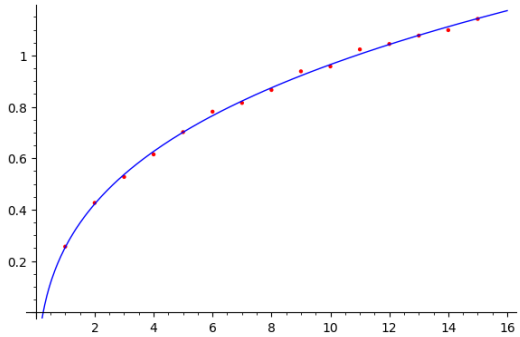
As we can see, the curves have a high slope for k small. The slope then gets smaller as k increases. Based on this observation, we try to find a fitting curve, corresponding to a map

$$f_{\alpha,\beta,\gamma} : \begin{cases} \mathbb{R} & \to & \mathbb{R} \\ x & \mapsto & \alpha x^{\beta} + \gamma \end{cases}$$

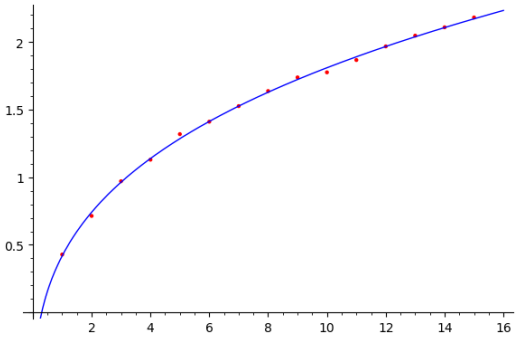
for $\alpha, \beta, \gamma \in \mathbb{R}$. The following graphs depict estimated points $(p, h_1(p)), \ldots, (p, h_n(p))$ for fixed p and n, but additionally represent the curve of a function $f_{\alpha_p,\beta_p,\gamma_p}$, where the three parameters have been determined using the "method of least squares."

In addition to the values of n, k, p, we will also list the corresponding determined value of β_p as it is, asymptotically speaking, the most relevant parameter for $f_{\alpha_p,\beta_p,\gamma_p}$.

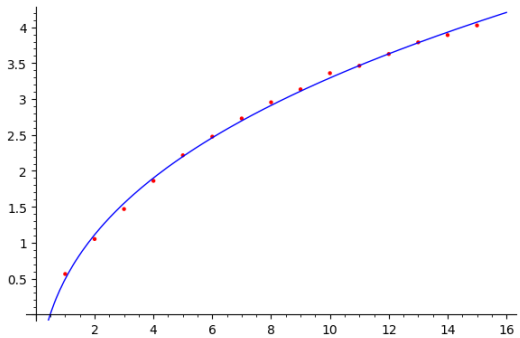
$n = 15, k = 3\,000, p = 0.15, \beta_p \approx 0.2766$:



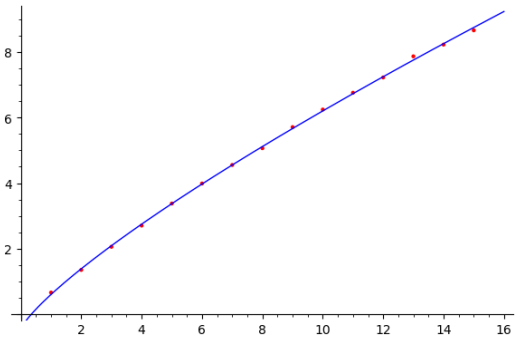
$n = 15, k = 3\,000, p = 0.25, \beta_p \approx 0.3027$:



$n = 15, k = 3\,000, p = 0.35, \beta_p \approx 0.3559$:



$n = 15, k = 3\,000, p = 0.45, \beta_p \approx 0.7985$:



Remark 42. We can make a number of observations and remarks concerning the above graphs.

(i) $A_n(1)$ is a conducting system, hence its conduction height equals n. Thus we have $h_n(1) = n = 1 \cdot n^1 + 0$, so $\beta_1 = 1$.

(ii) For all $0 \leq p \leq 1$, we have $\beta_p \leq 1$. This makes sense, otherwise we have for n great:

$$1 \overset{\text{(ii)}}{=} \frac{h_n(1)}{n} \geq \frac{h_n(p)}{n} \approx \alpha_p n^{\beta_p - 1} + \frac{\gamma_p}{n} \to +\infty, \text{ as } n \to +\infty,$$

which is a contradiction. We have used that $\alpha_p > 0$.

(iii) The approximation $h_n(p) \approx \alpha_p n^{\beta_p} + \gamma_p$ is useful to estimate the conduction height of a system $A_n(p)$ for n great, without explicitly computing it.

(iv) One might be interested in the dependence of β_p on the probability p. Unfortunately, the estimations of β_p have already been computationally heavy. Therefore, approximating β_p for a greater number of different values for p will take a long time. We tried estimating the values of β_p by computing fewer random systems (i.e. choosing k smaller). However, this yielded very rough approximations. The graph of the estimated points (p, β_p) was therefore not insightful. We did not include it.

2.2 Conduction probability

This section covers questions similar to those in section 1.2. We will give less explanations, as most ideas are analogous to the mentioned section above. Moreover, as the systems of this chapter are more complicated to work with, the results we give are often less precise to those of the previous chapter.

Definition 43. For $n \geq 1$ and $0 \leq p \leq 1$, we call

$$q_n(p) := \mathbb{P}\{A_n(p) \text{ conducts}\}$$

the *conduction probability* of the random system $A_n(p)$.

Proposition 44. *For $0 \leq p \leq 1$, we have*

$$q_1(p) = -p^2 + 2p$$

and

$$q_2(p) = 4p^8 - 18p^7 + 27p^6 - 10p^5 - 9p^4 + 4p^3 + 3p^2.$$

Proof. The idea is the same as in the proof of proposition 20. □

Remark 45. One can easily argue, as done in remark 21, that $q_n(p)$ is a polynomial in p whose degree is is less than or equal to $2n(n+1)$. The previous proposition shows that equality already fails for $n = 2$. This is different to what we saw in section 1.2.

Moreover, the computation time for $q_3(p)$ was already very high. We were therefore not able to give exact results for $\tau_n, n \geq 3$.

Proposition 46. *For $n \geq 1$, there exists a unique $\tau_n \in]0, 1[$ such that $q_n(\tau_n) = \frac{1}{2}$.*

Proof. Similar to the proof of proposition 22. □

Definition 47. For $n \geq 1$, the unique probability τ_n of proposition 46 will be called the *conduction border* of $A_n(\cdot)$.

Examples 48. We shall estimate the conduction borders τ_1, τ_2 using proposition 44:

(i) $n = 1$: As in the previous chapter, one can show $\tau_1 = 1 - \frac{1}{\sqrt{2}} \approx 0.292893219$.

(ii) $n = 2$: One can estimate $\tau_2 \approx 0.406779457$.

Definition 49. If it exists, we call

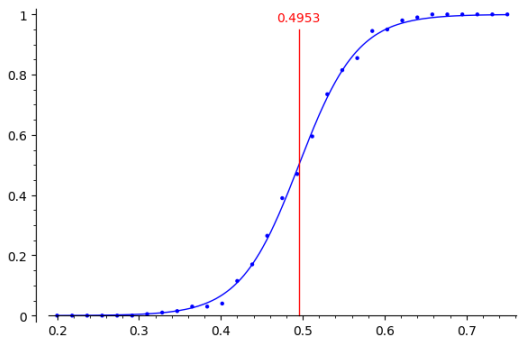
$$\tau := \lim_{n \to +\infty} \tau_n$$

the *conduction threshold*.

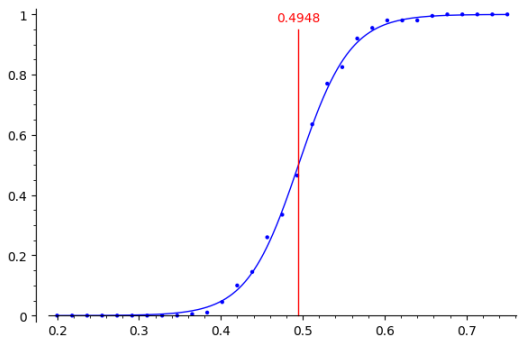
Question. Can we get experimental indications for the existence of the conduction threshold τ? If so, how can it be estimated?

Answer. We can estimate τ_n by using the method of curve fitting, similar to what we did in the previous chapter. We choose the family of functions $F_{r,a} : \mathbb{R} \to \mathbb{R}$ again, and obtain the following graphs.

$n = 12, k = 200, m = 30$:



$n = 15, k = 200, m = 30$:



Other values for n yielded similar results. We therefore approximate

$$0.494 \leq \tau \leq 0.496.$$

Bibliography

[1] G. Grimmett, *Percolation*. Grundlehren der mathematischen Wissenschaften 321, Springer-Verlag Berlin Heidelberg, 2nd ed., 1999.

[2] D. Stauffer and A. Aharony, *Introduction to percolation theory*. CRC Press, 2nd ed., 1994.