Extremal and Probabilistic Bootstrap Percolation

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This dissertation is the result of my own work and includes nothing that is the outcome of work done in collaboration except where specifically indicated in the text. Chapters 1 and 2 are based on joint work with Fabricio S. Benevides, then of University of Memphis, USA, but now of Universidade Federal do Ceará, Fortaleza, Brazil, and my contribution was about 50%. Chapters 4 and 5 are based on joint work with Béla Bollobás of University of Cambridge and University of Memphis, Karen Gunderson of University of Bristol, Cecilia Holmgren, then of University of Cambridge, but now of Stockholm University, Sweden, and Svante Janson of Uppsala University, Sweden, and my contribution was about 30%. No part of this dissertation has been submitted for any other qualification.

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ABSTRACT

In this dissertation we consider several extremal and probabilistic problems in bootstrap percolation on various families of graphs, including grids, hypercubes and trees. Bootstrap percolation is one of the simplest cellular automata. The most widely studied model is the so-called r-neighbour bootstrap percolation, in which we consider the spread of infection on a graph G according to the following deterministic rule: infected vertices of G remain infected forever and in successive rounds healthy vertices with at least r already infected neighbours become infected. Percolation is said to occur if eventually every vertex is infected.

In Chapter 1 we consider a particular extremal problem in 2-neighbour bootstrap percolation on the $n \times n$ square grid. We show that the maximum time an infection process started from an initially infected set of size n can take to infect the entire vertex set is equal to the integer nearest to $(5n^2 - 2n)/8$. In Chapter 2 we relax the condition on the size of the initially infected sets and show that the maximum time for sets of arbitrary size is $13n^2/18 + O(n)$.

In Chapter 3 we consider a similar problem, namely the maximum percolation time for 2-neighbour bootstrap percolation on the hypercube. We give an exact answer to this question showing that this time is $\lfloor n^2/3 \rfloor$.

In Chapter 4 we consider the following probabilistic problem in bootstrap percolation: let T be an infinite tree with branching number $\mathrm{br}(T) = b$. Initially, infect every vertex of T independently with probability $p > 0$. Given r, define the critical probability, $p_c(T, r)$, to be the value of p at which percolation becomes likely to occur. Answering a problem posed by Balogh, Peres and Pete, we show that if $b \geq r$ then the value of b itself does not yield any non-trivial lower bound on $p_c(T, r)$. In other words, for any $\varepsilon > 0$ there exists a tree T with branching number $\mathrm{br}(T) = b$ and critical probability $p_c(T, r) < \varepsilon$.

However, in Chapter 5 we prove that this is false if we limit ourselves to the well-studied family of Galton–Watson trees. We show that for every $r \geq 2$ there exists a constant $c_r > 0$ such that if T is a Galton–Watson tree with branching number $\mathrm{br}(T) = b \geq r$ then

$$p_c(T, r) > \frac{c_r}{b} e^{-\frac{b}{r-1}}.$$

We also show that this bound is sharp up to a factor of $O(b)$ by describing an explicit family of Galton–Watson trees with critical probability bounded from above by $C_r e^{-\frac{b}{r-1}}$ for some constant $C_r > 0$.

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Contents

Introduction

In this dissertation, we consider the following process known as r-neighbour bootstrap percolation on a graph G. Initially a subset A of the set of vertices (often called sites when we consider bootstrap percolation) of $G = (V, E)$ is infected and the remaining vertices are healthy. Infected vertices of G remain infected forever and in consecutive rounds healthy vertices with at least r already infected neighbours become infected. More precisely, we set $A_0 = A$ and for $t = 1, 2, 3, \dots$, we let

$$A_t = A_{t-1} \cup \{v \in V(G) : |N(v) \cap A_{t-1}| \geq r\}.$$

In this process we think of t as time and of A_t as the set of sites whose state at time t is 'infected', so that $A_{t-1} \cap N(v)$ is the set of neighbours of v which are infected at time $t-1$. By $\langle A \rangle = \bigcup_{t=0}^{\infty} A_t$ we denote the set of all eventually infected vertices which we call the *closure* of A. We say that A *percolates* if $\langle A \rangle = V(G)$.

Bootstrap percolation, suggested in 1979 by Chalupa, Leath, and Reich [**27**], is a particularly simple cellular automaton. As is well known, cellular automata were introduced by von Neumann in the 1940s and 1950s after a suggestion of Ulam (see [**45**] and [**52**]). Bootstrap percolation has been used to model various phenomena: the behaviour of ferromagnetic materials [**44**], water flowing through cracks in rocks [**3**], the impact of failures of individual nodes in computer networks on the connectivity of the entire system [**39**], the spread of opinion and voting preferences [**32, 54**], information processing in neural networks [**40**] and thermal annealing of damaged regions in diamonds [**49**]. Originally the behaviour of the process under the assumption that the set A of initially infected sites is random–like attracted most attention, since the infected vertices in our model can reflect particles of some ferromagnetic material with a particular value of their magnetic spin. (For more on the various physical motivations and applications of bootstrap percolation, we refer the reader to the survey articles of Adler, Stauffer and Aharony [**1**], Adler [**2**] and Adler and Lev [**4**].) Consequently, the most natural setup to consider was to assume that each site is initially infected (i.e., belongs to A) independently with some probability p. The natural setup was then to consider, given a particular graph G and a value r of the infection threshold, for what values of p percolation is likely to occur. It is clear that the probability of percolation is nondecreasing in p and therefore one of the fundamental first problems was to determine the critical probability, $p_c(G, r)$, defined as follows:

$$\begin{aligned} p_c(G,r) = \inf\{p : \mathbb{P}_p(A \text{ percolates in } r\text{-neighbour} \\ \text{bootstrap process on } G) \geq 1/2\}. \end{aligned} \tag{0.1}$$

Let $\mathbb{Z}^2$ denote the two-dimensional integer lattice, in which two sites (i_1, i_2) and (j_1, j_2) are neighbours if and only if $|i_1 - j_1| + |i_2 - j_2| = 1$. The first precise result in the field was the following theorem proved by van Enter [**53**].

Theorem 0.1. *The critical probability for 2-neighbour bootstrap percolation on the two-dimensional integer lattice is* $p_c(\mathbb{Z}^2, 2) = 0$.

□

The proof of this result actually shows that whatever value $p > 0$ we use to initially infect the sites in $\mathbb{Z}^2$, almost surely every site of the lattice will become infected at some point in time. Note that $r = 2$ is the only interesting value of the infection threshold in this problem. For $r = 1$ even a single initially infected site would cause percolation, while for $r \geq 3$ any initially healthy 2×2 square would remain healthy forever. Schonmann [**50**] generalized van Enter's result to all dimensions and values of the infection threshold: using much more sophisticated methods he proved the following result.

Theorem 0.2. *For all* $d, r \geq 2$ *we have*

$$p_c(\mathbb{Z}^d, r) = \begin{cases} 0, & \text{if } r \leq d, \\ 1, & \text{if } r > d. \end{cases}$$

□

It is worth noticing that results of this type are much easier for $r = 2$ and $r = d$, than for the interval $3 \leq r \leq d - 1$.

The next step to understand bootstrap percolation models was to consider finite graphs instead of infinite ones. Most work in bootstrap percolation has been focused on a particular case where, for some natural numbers n and d, the underlying graph G is the d-dimensional grid $[n]^d$ defined as follows: the set of sites of G is

$$V(G) = \{(i_1, i_2, \dots, i_d) : 1 \leq i_j \leq n \text{ for all } 1 \leq j \leq d\}$$

and two sites $v, w \in V(G)$ are neighbours if $\|v - w\|_1 = 1$, that is, v and w differ in exactly one coordinate and by one unit. The first important result for such graphs is found in the work of Aizenman and Lebowitz [**5**].

THEOREM 0.3. *For any $d \geq 2$, the critical probability in 2-neighbour bootstrap percolation on the d-dimensional cube $[n]^d$ is*

$$p_c([n]^d, 2) = \Theta\left(\left(\frac{1}{\log n}\right)^{d-1}\right).$$

$\square$

Surprisingly, even though the framework developed in [**5**] turned out to be useful in many other problems, it took ten more years before similar results were proved for higher infection thresholds. The groundbreaking work of Cerf and Cirillo [**25**] in the case $d = r = 3$ and the proof by Cerf and Manzo [**26**] which followed it, proved the following natural generalization to higher thresholds.

THEOREM 0.4. *For any $d \geq r \geq 2$, the critical probability for r-neighbour bootstrap percolation on the d-dimensional cube $[n]^d$ is*

$$p_c([n]^d, r) = \Theta\left(\left(\frac{1}{\log_{(r-1)} n}\right)^{d-r+1}\right),$$

where $\log_{(1)} n = \log n$ and, for all $k \geq 2$, $\log_{(k)} n = \log(\log_{(k-1)} n)$.

□

Again, considering $r > d$ is not interesting as any initially healthy subcube $[2]^d$ would then remain healthy forever.

Theorem 0.4 says that there exist constants $c_2 \geq c_1 > 0$ such that

$$\left(\frac{c_1}{\log_{(r-1)} n}\right)^{d-r+1} \leq p_c([n]^d, r) \leq \left(\frac{c_2}{\log_{(r-1)} n}\right)^{d-r+1}.$$

However, it was conjectured very early (and strongly supported by simulation results) that at least in the case $d = r = 2$ a much sharper formula holds, i.e., that

$$p_c([n]^2, 2) = \frac{c}{\log n} + o\left(\frac{1}{\log n}\right)$$

for some $c > 0$. This conjecture was finally confirmed by the following theorem of Holroyd [**36**] who also determined the value of the constant c.

THEOREM 0.5. *The critical probability for* 2*-neighbour bootstrap percolation on the square grid* $[n]^2$ *is*

$$p_c([n]^2, 2) = \frac{\pi^2}{18 \log n} + o\left(\frac{1}{\log n}\right).$$

□

The upper bound in Theorem 0.5 was “easy” since it can be obtained by analyzing one particular way of percolating $[n]^2$ and hoping that its probability “dominates” all other ways of infecting the grid. Holroyd showed that for $p = \frac{\pi^2+\varepsilon}{18 \log n}$ such a way can be found with high probability. Namely, he proved that somewhere in $[n]^2$ we will find a square of side length $\lfloor \log^3 n \rfloor$ (referred to as a “critical droplet” in the literature), such that the infection process limited to this square will fully infect it. Together with the fact that with high probability every stripe of sites of length $\lfloor \log^3 n \rfloor$ in $[n]^2$ will contain at least one infected site, this gave the result.

However, things were far from being that simple in the case of the lower bound on $p_c([n]^2, 2)$. This is because we now have to bound the probability of *all* possible ways of infecting $[n]^2$. Holroyd found a way of doing this by introducing a notion of a *hierarchy.* This tree–like structure describes the growth of the infected area and can be parameterized by an arbitrary level of “precision” of the description. Holroyd defined a family of *good hierarchies* by characterizing them as satisfying an explicitly given precision and showed that if percolation occurs in $[n]^2$ then at least one of those hierarchies must be a valid description of the infection process. By showing that there are only “few” good hierarchies and that for $p = \frac{\pi^2-\varepsilon}{18 \log n}$ each one of them is not satisfied with high probability, he finally obtained the lower bound on $p_c([n]^2, 2)$. It is worth noticing here that Holroyd’s result was surprising for at least two reasons. First, many researchers did not expect that such a precise result can in fact be obtained with analytic methods. Second, the value of the constant in Theorem 0.5 was highly unexpected, being more than twice as large as numerical simulations predicted.

Again, the results for higher infection thresholds did not follow easily after the result for $r = 2$ was announced. For a long time obtaining precise thresholds for $r \geq 3$ seemed like a hopeless task but again the case $d = r = 3$, solved by Balogh, Bollobás and Morris [**10**], turned out to be crucial. Finally, Balogh, Bollobás, Duminil-Copin and Morris [**9**] in the following theorem gave the asymptotic values of critical probabilities for all $d \geq r \geq 2$.

Theorem 0.6. *The critical probability for r-neighbour bootstrap percolation on the d-dimensional cube $[n]^d$ is*

$$p_c([n]^d, r) = \left(\frac{\lambda(d,r) + o(1)}{\log_{(r-1)} n} \right)^{d-r+1},$$

where $\lambda(d,r)$ are equal to the values of specific definite integrals.

□

The current research in this direction, motivated by the fact that the constants in the above theorems “contradict” the simulation results even for large values of n, focuses on finding the second terms in the formulae for $p_c([n]^d, r)$. For example, for $d = r = 2$ Gravner and Holroyd [**34**] and Gravner, Holroyd and Morris [**35**] obtained results explaining the slow convergence of the critical probability and estimating the second order term in the asymptotic formula for $p_c([n]^2, 2)$.

However, the value of the critical probability is not the only interesting probabilistic parameter of a bootstrap percolation model. Once we know for what values of p percolation is likely to occur, it is interesting to ask about the typical time that the infection process takes before it occupies the entire vertex set. These questions have recently been considered in $[n]^d$ by Bollobás, Holmgren, Smith and Uzzell [**21**] for $r = d$ and by Bollobás, Smith and Uzzell [**24**] for $r < d$.

The progress achieved for grid-like graphs (with a fixed dimension and side length tending to infinity) encouraged research on bootstrap percolation on other underlying graphs. Interesting results, some of them very sharp, were then obtained, e.g., by Balogh and Bollobás [**8**] and by Balogh, Bollobás and Morris [**11, 12**] for the hypercube graph, by Janson, Łuczak, Turova and Vallier [**38**] for the random graph $G_{n,p}$ and by Balogh and Pittel [**15**], and Janson [**37**], for the random regular graph. Bootstrap percolation on infinite trees and Cayley graphs was studied by Balogh, Peres and Pete [**13**] while Fontes and Schonmann [**30**] and Biskup and Schonmann [**18**] worked with infinite regular trees. It is worth mentioning that this particular model was introduced already in the early work of Chalupa, Leath and Reich [**27**]. This can be partially explained by the fact that bootstrap percolation is easier to analyze on trees than on other graphs.

Various modifications and generalizations of the r-neighbour bootstrap percolation models have also been considered. Let us mention here the work of Gravner and Griffeath [**33**] on more general update rules called *threshold dynamics*, the results of Bollobás, Smith and Uzzell [**23**] which generalize the bootstrap processes even further, and the work of Coker and Gunderson [**28**] who studied the bootstrap process on the square grid in which infected vertices with less than two infected neighbours recover from the infection.

Turning to extremal problems, the size of the smallest percolating sets in $[n]^d$ was studied by Pete who proved a general lower bound on this size for a fixed value of d and gave an exact or asymptotic value in a few simple cases. A summary of his results can be found in [**46**] and [**14**]. However, the case $d = r = 2$, which is now a famous coffee-time problem and a folklore puzzle for high-school students, was answered very early. In this case the answer is n, with a diagonal of the $n \times n$ square being an obvious example of such a percolating set. We present a full proof of this fact in Proposition 1.3 and Corollary 1.4. (The interested reader is encouraged to stop at this point and try to prove that a percolating set cannot have less than n elements.) The structure of the smallest percolating sets for $G = [n]^2$ and $r = 2$ has also been considered by Shapiro and Stephens [**51**]. A famous and still wide open problem in this area is the determination of the size of the smallest percolating sets for G being the n-dimensional hypercube ($[2]^n$) and $r = 3$. Balogh and Bollobás conjectured this size to be $n^2/6 + O(n)$ (percolating sets of that size can be constructed using Steiner triple systems) but the best lower bound on it so far is $n + 1$.

Recently, however, a first major extremal result in bootstrap percolation, as a partial answer to a question of Bollobás, was obtained by Morris [**43**]. Defining $E(n)$ to be the cardinality of the largest minimal percolating sets in $[n]^2$ under 2-neighbour bootstrap percolation (i.e, the largest percolating sets A such that for any $v \in A$ the sets $A \backslash \{v\}$ do not percolate, i.e., $\langle A \setminus \{v\} \rangle \neq [n]^2$) he proved the following theorem.

THEOREM 0.7. *For every $n \in \mathbb{N}$, we have*

$$\frac{4n^2}{33} + o(n^2) \leq E(n) \leq \frac{(n+2)^2}{6}.$$

$\square$

Following the steps of Morris, Riedl [**48**] proved that in 2-neighbour bootstrap percolation on the n-dimensional hypercube graph, the size $E^H(n)$ of the largest minimal percolating sets satisfies the following formula.

THEOREM 0.8. *Let* $1 \leq r \leq 4$ *be such that* $n = r \pmod 4$. *Then*

$$E^H(n) = \begin{cases} n+1, & 0 \leq n \leq 1 \\ n, & 2 \leq n \leq 10 \\ (1+2^{r-4})2^{\lfloor \frac{n+3}{4} \rfloor}, & n \geq 11. \end{cases}$$

□

In Chapters 1, 2 and 3 of this dissertation we contribute to this developing family of extremal results. Answering questions posed by Bollobás [**19**], we consider percolating sets of vertices for which the infection process under 2-neighbour bootstrap percolation is as slow as possible. In Chapter 1 we look at this problem for $G = [n]^2$ and show that for percolating sets of minimal size n percolation occurs after at most $\left\lfloor \frac{5n^2-2n}{8} \right\rceil$ time steps, where $\lfloor x \rceil$ denotes the integer nearest to x. In Chapter 2 we analyze all percolating sets in $[n]^2$ and prove that the maximum percolation time for arbitrary sets equals $\frac{13}{18}n^2 + O(n)$. Chapter 3 contains a solution to an analogous problem on the n-dimensional hypercube. We show that in this case the maximum percolation time is $\lfloor \frac{n^2}{3} \rfloor$. We should mention that despite strong similarities, the result in Chapter 2 is significantly harder than the ones in Chapters 1 and 3.

Chapters 4 and 5 contain probabilistic results in bootstrap percolation on infinite trees. This direction of research has already been initiated in the original work of Chalupa, Leath and Reich. Given an infinite tree T, let $\mathrm{br}(T)$ denote the branching number of T (the branching number is a measure of the "average" number of children of a vertex of T; we define it precisely is Section 4.2). Motivated by the work of Lyons [**41**], who showed that in the context of percolation (for background on percolation see Bollobás and Riordan, [**22**]), on any tree T we have $p_c(T) = 1/\mathrm{br}(T)$, Balogh, Peres and Pete [**13**] investigated the relation between the branching number of a tree T and the critical probability in bootstrap percolation on that tree. In [**13**] they proved the following theorem.

THEOREM 0.9. *For all* $r \geq 2$*, given an infinite tree* T*, if* $\mathrm{br}(T) < r$ *then* $p_c(T, r) = 1$.

□

The authors asked a question about the possible values of the critical probability of trees T with $\mathrm{br}(T) \geq r$. In Chapter 4 we answer that question, showing that for any $b \geq r$ and $\varepsilon > 0$ there exists a tree T with branching number $\mathrm{br}(T) = b$ and critical probability $p_c(T, r) < \varepsilon$. This shows that for $b \geq r$ no bounds on the critical probability follow from the value of the branching number.

In **[13]** the authors show that regular trees do not in general minimize the critical probability among all trees with a given branching number. In particular, they analyze the Galton–Watson tree T_ξ with offspring distribution ξ, such that $\mathbb{P}(\xi = 2) = \mathbb{P}(\xi = 4) = 1/2$ (which as shown in **[41]** almost surely has branching number equal to $\mathrm{br}(T_\xi) = \mathbb{E}(\xi) = 3$). They show that T_ξ has critical probability in 2-neighbour bootstrap percolation almost surely equal to $p_c(T_\xi, 2) = 0.10504\ldots < 1/9 = p_c(T_3, 2)$, where T_3 is the infinite 4-regular tree. In Chapter 5 we focus our attention on bootstrap percolation on Galton–Watson trees and show that for this family of trees non-trivial bounds based only on the branching number can be found. Namely, we prove that for every $r \geq 2$ a constant $c_r > 0$ exists, such that for any Galton–Watson tree T_ξ with branching number $\mathrm{br}(T_\xi) = \mathbb{E}(\xi) = b \geq r$ we have

$$p_c(T_\xi, r) > \frac{c_r}{b} e^{-\frac{b}{r-1}}.$$

We then construct a family of Galton–Watson trees with critical probability bounded from above by $C_r e^{-\frac{b}{r-1}}$ for some constant $C_r > 0$, which shows that our bound on $p_c(T_\xi, r)$ is sharp up to a $O(b)$ factor. We also give some additional upper and lower bounds on $p_c(T_\xi, r)$ based on higher moments of the offspring distribution ξ.

CHAPTER 1

Slowly percolating sets of minimal size in bootstrap percolation

1.1. Introduction

Let us recall the definition of r-neighbour bootstrap percolation on a graph G. In the context of percolation, the vertices of G are usually called *sites* and the edges of G *bonds*. For each $v \in V(G)$, we denote by $N(v)$ the set of neighbours of v. Each site $v \in V(G)$ is in one of the two *states*, say *healthy* or *infected*; we write A for the set of sites whose initial state is 'infected' and call A the set of *initially infected sites*.

Let $\mathbb{N} = \{1, 2, 3, \ldots\}$ and let $[n] = \{1, 2, \ldots, n\}$. Set $A_0 = A$ and, thinking of A_t as the set of sites infected at time t, for $t \in \mathbb{N}$ set

$$A_t = A_{t-1} \cup \{v \in V(G) : |N(v) \cap A_{t-1}| \geq r\}. \tag{1.1}$$

This means that sites of G become infected if they have at least r infected neighbours. Note that in bootstrap percolation once a site is infected it never becomes healthy.

The *closure* of $A \subset V(G)$ is the set $\langle A \rangle = \bigcup_{t=0}^{\infty} A_t$ of all sites that are eventually infected. We say that a set A *percolates* if all sites are eventually infected, that is, if $\langle A \rangle = V(G)$. We say that a set A is *closed* under percolation if $\langle A \rangle = A$. Furthermore, we say that A *takes time* T to percolate if $\langle A \rangle = V(G)$ and T is the smallest natural number such that $A_T = V(G)$.

In this chapter we are interested in a particular case where, for some natural number n, the graph G above is the grid $[n]^2$ defined as follows: the set of sites of G is $V(G) = \{(i, j) : 1 \leq i, j \leq n\}$, which we represent by an n by n square-grid where each site is a unit square whose centre has coordinates $(i - 1/2, j - 1/2)$ in the Cartesian plane. Two sites are adjacent if the corresponding squares share an edge. This particular model was introduced in 1979 by Chalupa, Leath and Reich [**27**], together with bootstrap percolation on regular trees.

In this chapter we answer an extremal question posed by Bollobás, that of bounding the time that a percolating subset A of the set of vertices of $G = [n]^2$, such that $|A| = n$, can take to percolate under 2-neighbour bootstrap percolation. For small values of n it is easy to answer our question computationally by an exhaustive search. But as a main result of this chapter we prove the following theorem. Let $T(A)$ denote the time that A takes to percolate in $[n]^2$. Moreover, let

$$M_0(n) = \max\{T(A) : \langle A\rangle = [n]^2 \text{ and } |A| = n\}.$$

THEOREM 1.1. *For every* $n \geq 4$,

$$M_0(n) = \left\lfloor \frac{5n^2 - 2n}{8} \right\rceil, \tag{1.2}$$

where $\lfloor x \rceil$ *denotes the integer nearest to* x.

It is clear that $M(1) = 0$, $M(2) = 1$, and it is easy to check that $M(3) = 4$.

This chapter is joint work with Fabricio S. Benevides. The chapter appeared in our paper, [**17**].

1.2. Preliminaries

Given natural numbers k and ℓ, a k by ℓ rectangle is a subset of $\mathbb{Z}^2$ of the form $\{a, a+1, \dots, a+k-1\} \times \{b, b+1, \dots, b+\ell-1\}$ for some choice of a and b. Let $\mathrm{Rec}(k,\ell)$ denote the set of all k by ℓ rectangles in $[n]^2$. We say that a rectangle R is *internally spanned* by a given set of infected sites A if $\langle A \cap R\rangle = R$.

Given a finite set $A \subset \mathbb{Z}^2$, we represent a site $(i,j) \in A$ as a shaded unit square on the grid so that its centre has coordinates $(i-1/2, j-1/2)$ in $\mathbb{R}^2$. We define the *boundary* of A as the set of bonds of $\mathbb{Z}^2$ having exactly one endpoint in A; in our pictures this corresponds to a side shared by a shaded and a non-shaded unit square. The *perimeter* of A is the number of bonds in its boundary. Its *semi-perimeter* is half of the perimeter; we denote it by $\Phi(A)$. In particular, if $R \in \mathrm{Rec}(k,\ell)$ is a k by ℓ rectangle then its semi-perimeter is $\Phi(R) = k + \ell$.

In our proofs we shall talk about distances between sites and rectangles. The distance we use is given by the usual l_1 norm, i.e., the distance between a pair of sites, say (i_1, j_1) and (i_2, j_2), is $|i_1 - i_2| + |j_1 - j_2|$. The *distance* between two sets A and B is the minimum distance between a site in A and a site in B; it is denoted by $\operatorname{dist}(A,B)$.

We remark that this definition of distance coincides with the length of the shortest path from A to B' when viewing $\mathbb{Z}^2$ as a graph. Note that two sets are at distance 0 from each other if and only if they intersect; and at distance 1 if and only if they are disjoint but their boundaries share at least one edge.

Fact 1.2. *For any two finite sets* $A, B \subset \mathbb{Z}^2$ *we have* $\Phi(A) + \Phi(B) \geq \Phi(A \cup B)$. *Equality occurs if and only if* $\operatorname{dist}(A,B) \geq 2$, *that is, if* A *and* B *do not intersect and have disjoint boundaries.*

Proof. Clearly, every bond in the boundary of $A \cup B$ is in the boundary of at least one of the sets A and B. If $\operatorname{dist}(A,B) \geq 2$ then every such bond is in the boundary of exactly one of A and B, and so $\Phi(A)+\Phi(B) = \Phi(A\cup B)$ holds. If $\operatorname{dist}(A,B) \leq 1$ then there exists a bond in the product of the boundaries of A and B and the inequality is strict. $\square$

From now on let us consider 2-neighbour bootstrap percolation on $[n]^2$ only. Let us start with the following simple proposition which follows from the fact that the perimeter of the infected set cannot grow when a new site becomes infected.

Proposition 1.3. *Let* A *be a set of infected sites and let* $\langle A \rangle$ *be its closure. Then* $\Phi(\langle A \rangle) \leq \Phi(A)$.

Proof. Let $A_0 = A$ and let A_t be the set of infected sites at time t. A healthy site becomes infected at time $t+1$ if at least two of its neighbours are in A_t. Additionally, every edge can transmit infection only once from a uniquely determined infected site to a uniqely determined healthy site. As a result, at least $2|A_{t+1} \setminus A_t|$ bonds in the boundary of A_t are not in the boundary of A_{t+1}.

Furthermore, each $v \in A_{t+1} \setminus A_t$, after using two bonds to become infected, contributes at most two new bonds to the boudary of the infected area. Thus there are at most $2|A_{t+1} \setminus A_t|$ bonds in the boundary of A_{t+1} which were not in the boundary of A_t.. Thus the perimeter cannot grow during the infection process. □

COROLLARY 1.4. *Given* $k, \ell \in \mathbb{N}$ *and a rectangle* $R \in \mathrm{Rec}(k, \ell)$*, if* $A \subset R$ *is a set that internally spans* R *then* $|A| \geq \lceil \Phi(R)/2 \rceil = \left\lceil \frac{k+\ell}{2} \right\rceil$. *In particular, if* $n \in \mathbb{N}$ *and* $A \subset [n]^2$ *percolates, then* $|A| \geq n$.

□

It is easy to show that the lower bounds in Corollary 1.4 are sharp. For example, a diagonal is a percolating set of size n in $[n]^2$.

As we mentioned before, we are interested in finding sets of size n in $[n]^2$ that do percolate but do so in the maximum possible time $M_0(n)$. To do this we build a family of sets that percolate in a particular way. In order to do so we shall need to use induction on the size of the underlying graph. Hence it is natural to extend the definition of $M_0(n)$ to percolation on rectangles.

Given natural numbers k and ℓ such that $k + \ell$ is even (the reason why we only look at even values of $k + \ell$ will become clear in our proof), let $T(A)$ again denote the time that A takes to percolate. We define $M_0(k, \ell)$ by

$$M_0(k, \ell) = \max\{T(A) : \langle A \rangle = [k] \times [\ell] \text{ and } |A| = (k + \ell)/2\}.$$

For a rectangle $R \in \mathrm{Rec}(k, \ell)$ define $M_0(R)$ to be the maximum time in which some set of order $\Phi(R)/2$ internally spans R. Of course, $M_0(R)$ is just another notation for $M_0(k, \ell)$.

Before trying to compute bounds on $M_0(n)$ we should also understand how the infection spreads on a broader scale. The first simple but important observation is the following.

FACT 1.5. *Given any set* A *of infected sites,* $\langle A \rangle$ *is a union of rectangles such that any distinct two of them are at distance at least* 3.

PROOF. The set A can be viewed as a union of 1 by 1 rectangles. Also, any two fully infected rectangles within distance at most 2 span the minimal rectangle containing them both. Thus, in this “rectangle process” in which we replace a union of two infected rectangles at distance at most 2 by the minimal rectangle containing them both, at each step we decrease the number of rectangles. Therefore, trying to write $\langle A\rangle$ as a union of rectangles with the minimal number of rectangles, in finitely many steps we obtain a union of rectangles such that any distinct two of them are at distance at least 3. $\square$

The next proposition (see Proposition 30 in [**36**]) is a much more precise result in this direction.

PROPOSITION 1.6. *Let R be a rectangle with area at least 2. Suppose that R is internally spanned by a set of sites A. Then there exist disjoint subsets of A, say A' and A'', and rectangles R' and R'' such that:*

(1) $R' \subsetneq R$ and $R'' \subsetneq R$,

(2) R' is internally spanned by A' and R'' is internally spanned by A'',

(3) $\langle R' \cup R''\rangle = R$; in particular, $\operatorname{dist}(R', R'') \leq 2$.

PROOF. The proposition follows from a similar argument as Fact 1.5. If A percolates then in the rectangle process we finally obtain one infected rectangle R. If we stop at the penultimate step of the process then we obtain two rectangles R' and R'' which together span R, being themselves spanned by two disjoint sets A' and A''. $\square$

Note that in Proposition 1.6 we cannot require the rectangles R' and R'' to be disjoint (see Figure 1.1).

Although Proposition 1.6 is sharp, it does not describe the percolation process in a step by step fashion (i.e., as the time t increases by one). In fact, it may happen that some sites in $R \setminus (R' \cup R'')$ become infected while some of $R' \cup R''$ are still healthy. Even though the problem we study is intrinsically time related, we shall be able to make heavy use of Proposition 1.6.

1.3. Slowly percolating sets with the minimal number of sites

In this section our aim is to compute the exact value of $M_0(n)$ for every $n \in \mathbb{N}$. Let us start by giving some intuitions about the solution to this

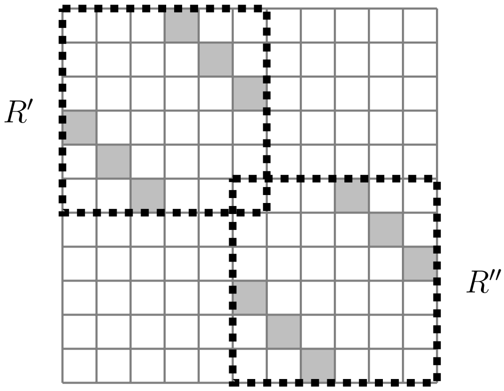


FIGURE 1.1. An example where the rectangles R' and R'' are uniquely determined by the initially infected sites and do overlap.

problem. First, we clearly have $M_0(n) \leq n^2 - n$, since at each time step we need to infect at least one of the initially healthy sites to continue the process. Also, without too much effort one can show that $M_0(n) \geq \frac{n^2}{2} + O(n)$. For example, consider the set of initially infected sites of the grid $[7]^2$ in Figure 1.2, which generalizes in a self-explanatory way to the grid $[n]^2$. It is clear that with this particular starting set at each time step, except the first one, at most two new sites become infected.

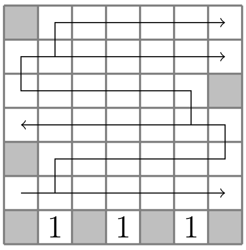


FIGURE 1.2. An initial set showing that $M_0(n) \geq \frac{n^2}{2} + O(n)$.

This shows that $M_0(n) = \Theta(n^2)$. As a main result of this chapter we prove that the structure of sets maximizing percolation time is actually more complicated. To be more precise, we show that to infect a $k \times \ell$ rectangle R in the maximum time we should use an initially infected set $A = A' \cup \{v\}$ such that the set A' first internally spans either a $(k-1) \times (\ell-1)$, $(k-2) \times \ell$ or $k \times (\ell - 2)$ rectangle in the maximum possible time, and then using "help" from the site v finishes the infection of R. It will turn out that, when $k = \ell = n$, the structure of a set $A(n)$ with $|A(n)| = n$ maximizing percolation time can be described as follows. We have $A(n) = B(n) \cup C(n) \cup D(n)$, where $|B(n)| \approx n/4$, $|C(n)| \approx n/2$ and $|D(n)| \approx n/4$, and such that

1. The set $B(n)$ internally spans a rectangle of size roughly $\frac{n}{2} \times 2$ in time $\frac{3n}{4} + O(1)$,
2. The set $C(n)$ extends the infected area to a rectangle of size roughly $n \times \frac{n}{2}$ in time $\frac{3n^2}{8} + O(n)$,
3. The set $D(n)$ finishes the infection of the $n \times n$ grid in time $\frac{n^2}{4} + O(n)$.

(See Figure 1.6.) Thus the set $A(n)$ percolates in time $5n^2/8 + O(n)$, significantly beating the simple construction presented in Figure 1.2. In fact, with a more precise analysis we shall show that the maximum percolation time in this case is equal to the integer nearest to $(5n^2 - 2n)/8$. We would like to emphasize that this value does not follow immediately from the recursive formula for maximum percolation time which we obtain first, but requires some additional work. What is more, in Chapter 2, where we work with percolating sets of arbitrary size, we also first obtain a recursive formula for percolation time. Even though it does not look that much more complicated, we are able to later find only an asymptotic formula for this value.

Now, let us return to Proposition 1.6. Given $A \subset [n]^2$, consider the sets A', A'', R' and R'', given by Proposition 1.6, and assume that A' takes at least as many time steps to internally span R' as A'' takes to internally span R''. Then clearly we can bound from above the time that A takes to percolate R by the time A' takes to infect R' plus the time to grow from $R' \cup R''$ to R, that is, to infect all sites in $R \setminus (R' \cup R'')$ given that all sites in R' and R'' are infected. Intuitively, the time to grow from $R' \cup R''$ to R does not change much if we only slightly change the sizes of R' and R'' while the infection time of R' might grow a lot if we increase the side lengths of R' even by some small quantities (this follows from our intuitions about the quadratic growth of M_0). It is then intuitive that, to maximize the time that A takes to percolate, R''

should probably be as small as possible, maybe even a single site. Let us now make our arguments formal.

First, we consider a family of sets of initially infected sites that internally span a rectangle in a particular way. The following definition is the most important concept of this chapter.

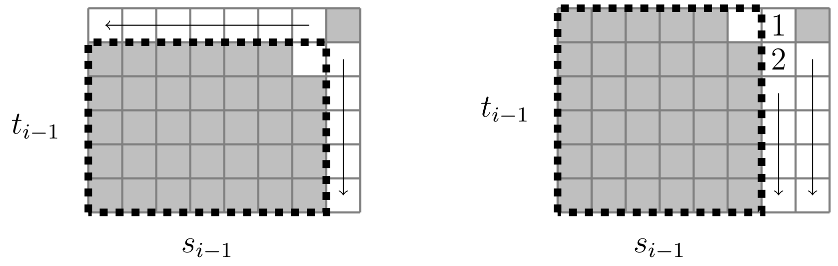
DEFINITION 1.7. *Let k and ℓ, with $k+\ell$ even, be given natural numbers. We say that a set A of initially infected sites is (k,ℓ)-*good *if it has cardinality $(k+\ell)/2$ and the 2-neighbour bootstrap percolation process starting from A can be described as follows. There exists a nested sequence of rectangles $P_0 \subset P_1 \subset \ldots \subset P_r \in \mathrm{Rec}(k,\ell)$, such that $P_i \in \mathrm{Rec}(s_i,t_i)$ where s_i, t_i satisfy the following properties:*

1. *either $s_0 \le 2$ or $t_0 \le 2$ or $s_0 = t_0 = 3$; and $s_1, t_1 \ge 3$ and $(s_1,t_1) \ne (3,3)$,*
2. *for every $1 \le i \le r$, the rectangle P_i is in*
$$\mathrm{Rec}(s_{i-1}+1, t_{i-1}+1) \cup \mathrm{Rec}(s_{i-1}+2, t_{i-1}) \cup \mathrm{Rec}(s_{i-1}, t_{i-1}+2),$$
3. *for all $0 \le i \le r$, the rectangles P_i are internally spanned by $A \cap P_i$ in the maximum possible time, that is, in time $M_0(P_i)$,*
4. *for every $0 \le i \le r$, if the rectangle P_i has no side of length 1 then among the sites which become infected last in P_i there is at least one of its corner sites,*
5. *for every $0 \le i < r$, there exists a site $v_i \in A$ such that $P_i \cup \{v_i\}$ internally spans P_{i+1} and v_i is at distance exactly 2 from one of the last sites to become infected in P_i and at distance at least 3 from any other site in P_i (see Figure 1.3).*

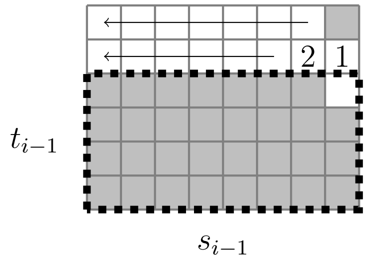
DEFINITION 1.8. *If A is (k,ℓ)-good we say that $P_0 \subset P_1 \subset \ldots \subset P_r \in \mathrm{Rec}(k,\ell)$ is a* good sequence *of rectangles associated with A if it satisfies conditions (1)-(5) above.*

From condition (2) it follows that for every $0 \leq i \leq r-1$ we have $\Phi(R_{i+1}) = \Phi(R_i) + 2$. From condition (3), taking $i = r$, it follows that any (k, ℓ)-good set infects a $k \times \ell$ rectangle in the maximum possible time. We shall show that for every $n \geq 4$ there exists an (n, n)-good set A.

For a (k, ℓ)-good set $A \subset [k] \times [\ell]$ and a good sequence $P_0 \subset P_1 \subset \ldots \subset P_r = [k] \times [\ell]$ associated with it, we say that we use *Move* 1 at moment i (to construct P_i from P_{i-1}) if $P_i \in \operatorname{Rec}(s_{i-1} + 1, t_{i-1} + 1)$, that we use *Move* 2 at moment i if $P_i \in \operatorname{Rec}(s_{i-1} + 2, t_{i-1})$ and that we use *Move* 3 at moment i if $P_i \in \operatorname{Rec}(s_{i-1}, t_{i-1} + 2)$.



Move 1 at moment i Move 2 at moment i



Move 3 at moment i

FIGURE 1.3. Moves 1, 2 and 3.

Figure 1.3 shows all possible alignments of subrectangles spanned by (k, ℓ)-good sets, which follows from condition (5) of the definition of (k, ℓ)-good sets.

We shall prove a recursive formula for $M_0(k, \ell)$ that works for all values of k and ℓ such that $k + \ell$ is even. The reader should keep in mind the description of (k, ℓ)-good initial sets as we are going to build such a set in our proof. In the next two lemmas we deal with some small cases which we will later use as base cases for the recursion. Since $M_0(k, \ell) = M_0(\ell, k)$, we shall omit some cases where $k < \ell$. Recall also that we only define $M_0(k, \ell)$ for $k + \ell$ even.

LEMMA 1.9. *We have* $M_0(1,1) = 0$*;* $M_0(k,1) = 1$ *for all odd* $k \geq 3$*; and* $M_0(3,3) = 4$*. Furthermore, in all these cases there exist* (k,ℓ)*-good sets.*

PROOF. The proof of this lemma is easy and we leave it as an exercise to the reader. In all these cases, in the definition of (k,ℓ)-good sets and good sequences of rectangles we have $r = 0$. ☐

LEMMA 1.10. *For any even* k *we have* $M_0(k,2) = (3k-4)/2$*. Furthermore, there is a* $(k,2)$*-good set,* $A^0(k,2)$*, which percolates* $[k] \times [2]$ *in time* $M_0(k,2)$*.*

PROOF. We define $A^0(k,2)$ to be the set of shaded sites in Figure 1.4. Clearly $|A^0(k,2)| = (k+2)/2$ and $A^0(k,2)$ percolates $[k] \times [2]$ in time $(3k-4)/2$. Thus we have $M_0(k,2) \geq (3k-4)/2$ for any k even. Note that, setting $P_0 = [k] \times [2]$, to prove that $A^0(k,2)$ is a $(k,2)$-good set we only need to show that in fact $M_0(k,2) = (3k-4)/2$.

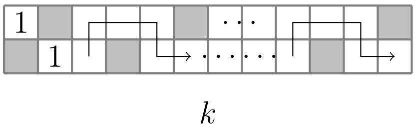


FIGURE 1.4. A set of initially infected sites which gives the maximum percolation time on $[k] \times [2]$ when k is even.

Now we prove by induction on k that for any k even we have $M_0(k,2) \leq (3k-4)/2$. Clearly, $M_0(2,2) = 1$. Assume that we are given some even $k \geq 4$ and that $M_0(k-2,2) = (3k-10)/2$. Let A, with $|A| = (k+2)/2$, be any set that percolates $[k] \times [2]$.

Since A percolates, any two consecutive columns of $[k] \times [2]$ contain at least one site of A. In particular, each of the 2 by 2 squares of the form $\{2i-1, 2i\} \times \{1,2\}$, $1 \leq i \leq k/2$, must contain at least one site of A. So only one such square can contain two sites of A. Therefore, either $\{1,2\} \times \{1,2\}$ or $\{k-1,k\} \times \{1,2\}$ contains exactly one site of A. Assume without loss of generality that the latter holds. Since A percolates, either $(k,1)$ or $(k,2)$ must be an initially infected site. Again without loss of generality we may assume that the latter holds. In this setting it is trivial to check that $A \cap ([k-2] \times [2])$ must internally span $[k-2] \times [2]$. Therefore A takes time at most $M_0(k-2, 2) + 3 = (3k-4)/2$ to percolate. This completes the proof. $\square$

Now, we state a lemma giving a recursive formula for $M_0(k, \ell)$. Let us note that in the formula we are about to prove the sum of the parameters that the function $M_0(\cdot, \cdot)$ depends on at each recursive step decreases by two. This is why, being interested in the value of $M_0(n, n)$, we only need to look at values of k and ℓ with even $k + \ell$.

THEOREM 1.11. *For $k, \ell \geq 3$ such that $(k, \ell) \neq (3, 3)$ and $k + \ell$ is even, we have*

$$M_0(k, \ell) = \max \begin{cases} M_0(k-1, \ell-1) + \max\{k, \ell\} - 1, \\ M_0(k-2, \ell) + \ell + 1, \\ M_0(k, \ell-2) + k + 1. \end{cases} \tag{1.3}$$

Furthermore, for all such k and ℓ there exists a (k, ℓ)-good set.

PROOF. We use Lemmas 1.9 and 1.10 as base cases for induction. We prove Theorem 1.11 by induction on $k + \ell$. Assume that we are given $k, \ell \geq 3$ such that $(k, \ell) \neq (3, 3)$ and $k + \ell$ is even. Our induction hypothesis is that for any k', ℓ' such that $k' + \ell'$ is even and $k' + \ell' < k + \ell$ there exists a (k', ℓ')-good set $A^0(k', \ell')$ which percolates in time $M_0(k', \ell')$, as in the statement of Theorem 1.11.

The fact that $k, \ell \geq 3$ guarantees that we have $k-1, \ell-1 \geq 2$. This will be important for us as in the constructions below we shall use property (4) of Definition 1.7 of (k, ℓ)-good sets a lot. We shall first prove that the following inequality holds for k and ℓ as above.

$$M_0(k, \ell) \geq \max \begin{cases} M_0(k-1, \ell-1) + \max\{k, \ell\} - 1, \\ M_0(k-2, \ell) + \ell + 1, \\ M_0(k, \ell-2) + k + 1. \end{cases} \tag{1.4}$$

Consider the following three particular ways of infecting $[k] \times [\ell]$ (see Figure 1.3).

(a) By the induction hypothesis there exists a $(k-1, \ell-1)$-good set $A^0(k-1, \ell-1)$ which internally spans the rectangle $[k-1] \times [\ell-1]$ in time $M_0(k-1, \ell-1)$. Without loss of generality, since $k-1, \ell-1 \geq 2$, we may assume that the site $(k-1, \ell-1)$ becomes infected at time $M_0(k-1, \ell-1)$. Let $A_1(k, \ell) = A^0(k-1, \ell-1) \cup \{(k, \ell)\}$. Then the infection of sites in $([k] \times [\ell]) \setminus ([k-1] \times [\ell-1])$ starts only after $(k-1, \ell-1)$ is infected and so $A_1(k, \ell)$ takes time $M_0(k-1, \ell-1) + \max\{k, \ell\} - 1$ to internally span $[k] \times [\ell]$. In addition, note that at least one of the corner sites $(k, 1), (1, \ell)$ becomes infected at time $M_0(k-1, \ell-1) + \max\{k, \ell\} - 1$.

(b) When $k \geq 4$, by the induction hypothesis there exists a $(k-2, \ell)$-good set $A^0(k-2, \ell)$, internally spanning the rectangle $[k-2] \times [\ell]$ in time $M_0(k-2, \ell)$, which infects the site $(k-2, \ell)$ at time $M_0(k-2, \ell)$ (this follows from the fact that $k-2, \ell \geq 2$). Let $A_2(k, \ell) = A^0(k-2, \ell) \cup \{(k, \ell)\}$. Then the infection of sites in $([k] \times [\ell]) \setminus ([k-2] \times [\ell])$ starts only after $(k-2, \ell)$ is infected and so $A_2(k, \ell)$ takes time $M_0(k-2, \ell) + \ell + 1$ to internally span $[k] \times [\ell]$. In addition, note that the corner site $(k, 1)$ becomes infected at time $M_0(k-2, \ell) + \ell + 1$.

(c) When $\ell \geq 4$, analogously to case b), by the induction hypothesis there exists a $(k, \ell-2)$-good set $A^0(k, \ell-2)$, internally spanning the rectangle $[k] \times [\ell-2]$ in time $M_0(k, \ell-2)$, which infects the site $(k, \ell-2)$ at time $M_0(k, \ell-2)$. Then the set $A_3(k, \ell) = A^0(k, \ell-2) \cup \{(k, \ell)\}$ internally spans $[k] \times [\ell]$ in time $M_0(k, \ell-2) + k + 1$, with the corner site $(1, \ell)$ becoming infected at the last time step.

The above constructions show that inequality (1.4) holds when $k, \ell \geq 4$. It remains to check that it also holds for $k = 3$ and $\ell \geq 5$, and for $\ell = 3$ and $k \geq 5$ (recall that $k + \ell$ is even so, e.g., when $k = 3$ we have $\ell \neq 4$). These cases are clearly symmetric so let us just show that $M_0(k, 3) \geq M_0(k, 1) + k + 1$

for $k \geq 5$. This is immediate as $M_0(k,1)+k+1 = k+2$ and we already know by construction (a) that

$$M_0(k,3) \geq M_0(k-1,2)+k-1 \geq M_0(4,2)+k-1 \geq k+3.$$

Thus the lower bound on $M_0(k,\ell)$ is proved.

Let us now show that the set $A_1(k,\ell)$ defined above satisfies all but possibly condition (3) of a (k,ℓ)-good set. Showing that the same holds for the sets $A_2(k,\ell)$ and $A_3(k,\ell)$ is analogous.

Thus, assume that $A^0(k-1,\ell-1)$ is a $(k-1,\ell-1)$-good set with a good sequence of rectangles $P_0 \subset P_1 \subset \ldots \subset P_r = [k-1]\times[\ell-1]$ associated with it. First, clearly $|A_1(k,\ell)| = |A^0(k-1,\ell-1)|+1 = (k+\ell-2)/2+1 = (k+\ell)/2$. Now consider the sequence $P_0 \subset P_1 \subset \ldots \subset P_r = [k-1]\times[\ell-1] \subset P_{r+1} = [k]\times[\ell]$ which describes the infection of $[k]\times[\ell]$ with $A_1(k,\ell)$ as the set of initially infected sites. This sequence clearly satisfies properties (1) and (2) of (k,ℓ)-good sets since it is obtained from a $(k-1,\ell-1)$-good set. It satisfies property (4) for $i = r+1$ since, as we noticed, in the infection started from $A_1(k,\ell)$ at least one of the corner sites $(k,1),(1,\ell)$ becomes infected at the last time step. It satisfies property (5) for $i = r+1$ since (k,ℓ) is at distance 2 from $(k-1,\ell-1)$ (which is infected last) and at distance at least 3 from any other site in $P_r = [k-1]\times[\ell-1]$. Properties (4) and (5) for $i \leq r$ are satisfied for this sequence since it is obtained from one associated with a $(k-1,\ell-1)$-good set.

We shall show that at least one of the sets $A_1(k,\ell)$, $A_2(k,\ell)$ and $A_3(k,\ell)$ is (k,ℓ)-good by proving an upper bound on $M_0(k,\ell)$ analogous to inequality (1.4), that is,

$$M_0(k,\ell) \leq \max\begin{cases} M_0(k-1,\ell-1)+\max\{k,\ell\}-1, \\ M_0(k-2,\ell)+\ell+1, \\ M_0(k,\ell-2)+k+1. \end{cases} \tag{1.5}$$

This will mean that at least one of these sets satisfies the missing property (3) of a (k, ℓ)-good set. Note that, as we have already shown, when $k = 3$ then $M_0(k-2, \ell) + \ell + 1$ is not larger than $M_0(k-1, \ell-1) + \max\{k, \ell\} - 1$, and analogously for $\ell = 3$. Thus the maximal time is obtained by some set satisfying all properties of a (k, ℓ)-good set.

Consider any set A which internally spans the rectangle $R = [k] \times [\ell]$ in time $M_0(k, \ell)$ and is such that $|A| = (k + \ell)/2$. By Proposition 1.6, there exist disjoint subsets of A, say A' and A'', and two rectangles R' and R'' satisfying conditions (1)–(3) of Proposition 1.6. By Proposition 1.3 and condition (3) of Proposition 1.6, we have that

$$\Phi(R' \cup R'') \geq \Phi(\langle R' \cup R'' \rangle) = \Phi(R) = k + \ell.$$

By Fact 1.2, condition (2) of Proposition 1.6 and Corollary 1.4,

$$\Phi(R' \cup R'') \leq \Phi(R') + \Phi(R'') \leq 2|A'| + 2|A''| \leq 2|A| = k + \ell.$$

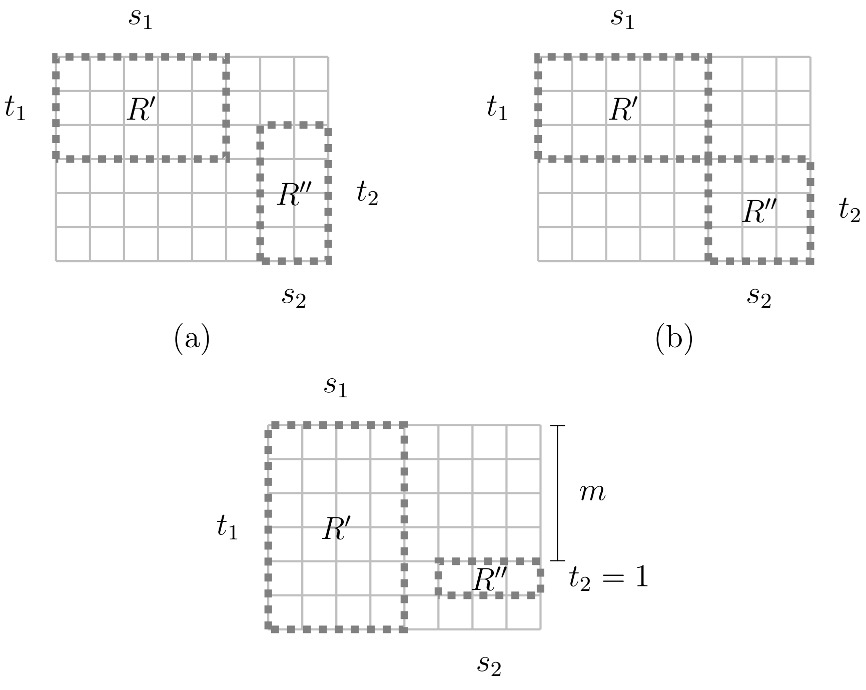
Therefore, each of the above inequalities must be an equality. In particular, we have $\Phi(R' \cup R'') = \Phi(R') + \Phi(R'')$. Fact 1.2 implies that $\operatorname{dist}(R', R'') \geq 2$, which together with condition (3) of Proposition 1.6 gives that R' and R'' must be at distance exactly 2. Also, we must have $\Phi(R') = 2|A'|$ and $\Phi(R'') = 2|A''|$, therefore, both $\Phi(R')$ and $\Phi(R'')$ are even.

Let $s_1, t_1, s_2, t_2 \geq 1$ be such that $R' \in \mathrm{Rec}(s_1, t_1)$ and $R'' \in \mathrm{Rec}(s_2, t_2)$. We have $\Phi(R') + \Phi(R'') = \Phi(R)$, so $s_1 + s_2 + t_1 + t_2 = k + \ell$. Since R' and R'' must be at distance exactly 2, the values of s_1, t_1, s_2, t_2 and the positions of R' and R'' inside R, must satisfy exactly one of the following conditions (to avoid redundancy we do not list cases analogous to Conditions (a), (b) and (c) when the alignment of R' and R'' in R is a rotation by 90 degrees of the one we consider here).

Condition (a): rectangles R' and R'' align as in Figure 1.5 (a) with $s_1 + s_2 = k - 1$ and $t_1 + t_2 = \ell + 1$.

Condition (b): rectangles R' and R'' align as in Figure 1.5 (b) with $s_1+s_2=k$, $t_1+t_2=\ell$.

Condition (c): there is an $0 \leq m \leq t_1-t_2$ so that the rectangles R' and R'' align as in Figure 1.5 (c) with $s_1+s_2=k-1$, $t_1=\ell$ and $t_2=1$.



(a) (b)

(c)

FIGURE 1.5. Three possible alignments of rectangles R' and R''.

Additionally, the rectangles R' and R'' are nonempty and internally spanned by $\frac{s_1+t_1}{2}$ and $\frac{s_2+t_2}{2}$ sites respectively.

Note now that no matter which of the Conditions (a), (b) or (c) holds, if at least one of s_1, t_1, s_2, t_2 equals 1 (which for Condition (c) is true by definition with $t_2=1$) then, just by possibly moving sites from A' to A'' or the other way, we can find a partition of A, say into sets $\tilde{A}'$ and $\tilde{A}''$, such that $\left\langle \tilde{A}' \right\rangle = \tilde{R}'$ is a rectangle, $\left\langle \tilde{A}'' \right\rangle = \tilde{R}''$ is a single site and $\left\langle \tilde{R}' \cup \tilde{R}'' \right\rangle = R$. This follows from the fact that, given $s \geq 1$ odd, any set of $(s+1)/2$ infected sites internally spanning an $s \times 1$ rectangle S must occupy every other site in S.

Now, returning to the intuitions we gave at the beginning of this section, we can bound from above the time that A takes to percolate $[k] \times [\ell]$ by the larger of the maximum times needed to internally span R' or R'', plus the time to grow from $R' \cup R''$ to R, that is, to infect all sites in $R \setminus (R' \cup R'')$ given that all sites in R' and R'' are infected. So if such $\tilde{R}''$ consisting of a single site can be found then the percolation time clearly cannot be greater than the lower bound given by inequality (1.4), in which case we are done. Assume therefore this is not the case which allows us to ignore Condition (c). Thus we only need to consider Conditions (a) and (b) with $s_1, t_1, s_2, t_2 \geq 2$. For these conditions we are also free to assume that $M_0(R') \geq M_0(R'')$.

Therefore, the time A takes to percolate is at most

$$\begin{cases} M_0(s_1, t_1) + \max\{s_1 + t_2, s_2 + t_1\}, & \text{if Condition (a) holds,} \\ M_0(s_1, t_1) + \max\{s_1 + t_2, s_2 + t_1\} - 1, & \text{if Condition (b) holds.} \end{cases} \tag{1.6}$$

From (1.4) and small case analysis when s or t equals 2, we have that the bound $M_0(s, t) \geq M_0(s-1, t-1) + \max\{s, t\} - 1$ holds for all $2 \leq s \leq k$, $2 \leq t \leq \ell$, $s+t$ even. By the same argument, inequalities $M_0(s+2, t) \geq M_0(s, t)$ and $M_0(s, t+2) \geq M_0(s, t)$ hold for all $1 \leq s \leq k$, $1 \leq t \leq \ell$, $s+t$ even.

If Condition (a) holds then since $s_1, t_1, s_2, t_2 \geq 2$ we also have $s_1, s_2 \leq k-3$ and $t_1, t_2 \leq \ell - 1$. Then

$$\begin{aligned} M_0(s_1, t_1) + \max\{s_1 + t_2, s_2 + t_1\} &\leq M_0(k-3, \ell-1) + k + \ell - 4 \\ &\leq M_0(k-2, \ell) + k + \ell - 4 \\ &\qquad - (\max\{k-2, \ell\} - 1) \\ &\leq M_0(k-2, \ell) + \min\{\ell - 1, k-3\} \\ &< M_0(k-2, \ell) + \ell + 1, \end{aligned}$$

where the second inequality follows from the fact that $M_0(s, t) \geq M_0(s-1, t-1) + \max\{s, t\} - 1$. In the case when the rectangles R' and R'' satisfy an analogous condition obtained by rotating Condition (a) by 90 degrees, we get an analogous bound $M_0(k, \ell - 2) + k + 1$ for the percolation time of A.

If Condition (b) holds then since $s_1, t_1, s_2, t_2 \geq 2$ we also have $s_1, s_2 \leq k-2$ and $t_1, t_2 \leq \ell - 2$. Then

$$\begin{aligned} M_0(s_1,t_1) + \max\{s_1+t_2, s_2+t_1\} - 1 &\leq M_0(k-2,\ell-2) + k + \ell - 5 \\ &\leq M_0(k-1,\ell-1) + k + \ell - 5 \\ &\qquad - (\max\{k,\ell\} - 2) \\ &\leq M_0(k-1,\ell-1) + \min\{\ell,k\} - 3 \\ &< M_0(k-1,\ell-1) + \max\{k,\ell\} - 1, \end{aligned}$$

where again the second inequality follows from the fact that $M_0(s,t) \geq M_0(s-1,t-1) + \max\{s,t\} - 1$.

Thus we conclude that the weakest upper bound on percolation time of A, equal to

$$\max\{M_0(k-1,\ell-1)+\max\{k,\ell\}-1,\ M_0(k-2,\ell)+\ell+1,\ M_0(k,\ell-2)+k+1\},$$

is obtained when one of R' or R'' is a single site. Since A was arbitrary with $|A| = (k+\ell)/2$ and $T(A) = M_0(k,\ell)$, this is an upper bound on $M_0(k,\ell)$ and so (1.5) is proved. Since this upper bound matches the percolation time of at least one of the sets $A_1(k,\ell)$, $A_2(k,\ell)$, $A_3(k,\ell)$ constructed in the proof of the lower bound on $M_0(k,\ell)$, we see that at least one of them percolates in time $M_0(k,\ell)$. Additionally, if $k=3$ or $\ell=3$ then we know that this maximum is obtained by $A_1(k,\ell)$. This was the last step needed to show that one of them is a (k,ℓ)-good set. This completes the proof of Theorem 1.11. $\square$

By Theorem 1.11 for every $n \geq 4$ there exists an (n,n)-good set which percolates $[n]^2$ in the maximum time $M_0(n)$. So, it is enough to determine s_0, t_0 and the sequence of Move 1s, 2s and 3s which takes the longest time to percolate. In the next lemma we treat a number of small cases to exclude some, a priori possible, values for the numbers s_0 and t_0. We shall ask for $\min\{s_0,t_0\} = 2$ so that, in the infection process started from our (k,ℓ)-good set, for each $i \geq 1$ the infection of the sites in $P_i \setminus P_{i-1}$ starts only after all sites in P_{i-1} are infected. Making sure that $(s_0, t_0) \neq (3,3)$ will also allow us to later simplify the description of good sets and, consequently, give an exact answer to the question about the value of $M_0(n,n)$.

LEMMA 1.12. *Let k and ℓ be such that $k \geq 4, \ell \geq 2$ and $k+\ell$ is even. Then there exists a (k,ℓ)-good set $A^0(k,\ell)$ with the sequence $P_0 \subset P_1 \subset \ldots \subset P_r = [k] \times [\ell]$ of rectangles associated with it, with $P_0 \in \mathrm{Rec}(s,2) \cup \mathrm{Rec}(2,s)$ for some even $s \geq 4$.*

PROOF. Given k, ℓ, with $k \geq 4, \ell \geq 2$ and $k+\ell$ even, consider any (k,ℓ)-good set, $A^0(k,\ell)$, and its associated good sequence of rectangles $P_0 \subset P_1 \subset \ldots \subset P_r = [k] \times [\ell]$. If $\ell = 2$ then we have $r = 0$ and the lemma is trivial. Thus assume that $\ell \geq 3$. Then since $k \geq 4$ we also have $r \geq 1$.

Suppose for a contradiction that $P_0 \in \mathrm{Rec}(s,1)$, for some odd s. By the definition of a (k,ℓ)-good set we have $P_1 \in \mathrm{Rec}(s_1,t_1)$ with $s_1, t_1 \geq 3$ and $\max\{s_1,t_1\} \geq 4$. The only move we can apply to P_0 to satisfy this is Move 3, so we must have $P_1 \in \mathrm{Rec}(s,3)$ with $s \geq 5$ (recall that $s_1 + t_1$ is even). This implies $s-1 \geq 4$ and so $M_0(s-1,2) \geq 4$. By inequality (1.4) we obtain $M_0(P_1) = M_0(s,3) \geq M_0(s-1,2) + s - 1 \geq s+3$. However, if we apply Move 3 to $P_0 \in \mathrm{Rec}(s,1)$ we will percolate $P_1 \in \mathrm{Rec}(s,3)$ in time at most $M_0(P_0) + s + 1 = s + 2$. This contradicts the fact that $A^0(k,\ell)$ is (k,ℓ)-good (more precisely, property (3) of Definition 1.7 will not hold for P_1). We deal with the case $P_0 \in \mathrm{Rec}(1,s)$ analogously.

Suppose now that $P_0 \in \mathrm{Rec}(3,3)$. We can assume that either $P_1 \in \mathrm{Rec}(4,4)$ (if we use Move 1 at moment 1) or $P_1 \in \mathrm{Rec}(5,3)$ (if we use Move 2), as the case $P_1 \in \mathrm{Rec}(3,5)$ (where we use Move 3) is analogous. In the first case, $M_0(P_0) = M_0(3) = 4$ and it takes 3 time steps to finish the infection of P_1 after P_0 has been fully infected. Thus P_1 becomes fully infected after at most $4 + 3 = 7$ time steps. However, by inequality (1.4) we know that $M_0(P_1) = M_0(4) \geq M_0(4,2) + 4 + 1 = 9$. So, as in the previous paragraph, we have a contradiction to $A^0(k,\ell)$ being (k,ℓ)-good. In the second case, where $P_1 \in \mathrm{Rec}(5,3)$, it takes 4 time steps to apply Move 2 to P_0 and finish the infection of P_1 after P_0 is fully infected. Thus P_1 is fully infected at time $M_0(P_0) + 4 = 8$. However, starting from $P_0' \in \mathrm{Rec}(4, 2)$ and using Move 1 at moment 1 we infect a rectangle $P_1 \in \mathrm{Rec}(5, 3)$ and again obtain infection time of P_1 equal to 8, as $M_0(4, 2) + 4 = 8$. This does not contradict the (k, ℓ)-goodness of $A^0(k, \ell)$ but shows that there exists a (k, ℓ)-good set $A'(k, \ell)$ with the sequence $P_0' \subset P_1 \subset \ldots \subset P_r = [k] \times [\ell]$ of rectangles associated with it, where $P_0' \in \mathrm{Rec}(4, 2)$. This completes the proof of Lemma 1.12. □

Let k and ℓ be such that $k \geq 4, \ell \geq 2$ and $k + \ell$ is even. By Lemma 1.12 we know that there exists a (k, ℓ)-good set $A^0(k, \ell)$ with the sequence $P_0 \subset P_1 \subset \ldots \subset P_r = [k] \times [\ell]$ of rectangles associated with it, with $P_0 \in \mathrm{Rec}(s, 2) \cup \mathrm{Rec}(2, s)$ for some even $s \geq 4$. Recall that, with such P_0, for each $i \geq 1$ the infection of the sites in $P_i \setminus P_{i-1}$ starts only after all sites in P_{i-1} are infected, which by the definition of (k, ℓ)-good sets happens at time $M_0(P_{i-1})$. The following two observations are crucial to determine the precise value of $M_0(n)$. In fact, with those observations and equation (1.3) we shall be able to find an (n, n)-good percolating set, i.e., a set which takes time exactly $M_0(n)$ to percolate.

OBSERVATION 1.13. *For any $i \geq 1$, no matter which of Move 1s, 2s or 3s is used at moment i to extend the rectangle P_{i-1} to P_i, at most two new sites become infected at each time step between $M_0(P_{i-1}) + 1$ and $M_0(P_i)$.*

By Observation 1.13, having fixed P_0 and remembering that in our problem the number of initially infected sites is fixed, a sequence of Move 1s, 2s and 3s that maximizes the time to infect a rectangle R must also maximize the number of time steps after $M_0(P_0)$ at which only one new site of $R \setminus A$ becomes infected. This observation also allows us to change the way we think about maximizing percolation time. Instead of thinking of the exact time it takes to apply a particular Move j at step i we shall think of a *score* of such move which is equal to the number of time steps at which exactly one new site becomes infected when we use Move j. Then our task becomes to maximize the cumulative score of our sequence of moves.

OBSERVATION 1.14. *For any $i \geq 1$ the following statements hold.*

(1) If Move 1 is used at moment i in order to extend the rectangle $P_{i-1} \in \mathrm{Rec}(s_{i-1}, t_{i-1})$ to $P_i \in \mathrm{Rec}(s_{i-1}+1, t_{i-1}+1)$ then only one new site becomes infected at exactly $|s_{i-1}-t_{i-1}|$ time steps between $M_0(P_{i-1})+1$ and $M_0(P_i)$, i.e., at $M_0(P_i)-|s_{i-1}-t_{i-1}|+1$, $M_0(P_i)-|s_{i-1}-t_{i-1}|+2$, ..., $M_0(P_i)-1$ and $M_0(P_i)$.

(2) If Move 2 or Move 3 is used at moment i to extend the rectangle P_{i-1} to P_i then only one new site becomes infected at exactly 3 time steps between $M_0(P_{i-1})+1$ and $M_0(P_i)$, i.e., at $M_0(P_{i-1})+1$, $M_0(P_{i-1})+2$ and $M_0(P_i)$.

Using these observations we get the next important claim. To talk about sequences of moves we shall use the following notation similar to that of regular expressions. We say that a finite (possibly empty) sequence is of the form $[a_1|a_2|\dots|a_r]^*$ if all its terms belong to $\{a_1, \dots, a_r\} \subset \{1,2,3\}$. We concatenate these expressions to create more general ones which describe the corresponding sets of concatenated sequences. For example, each of the sequences 22133232, 112333, 121233 is of the form $[1]^*[2]^*[1]^*[2|3]^*$, but 122331 is not.

CLAIM 1.15. *For $k \geq 4, \ell \geq 2$, there exists a (k,ℓ)-good set A internally spanning the rectangle $R \in \mathrm{Rec}(k,\ell)$, with a good sequence $P_0 \subset P_1 \subset \dots \subset P_r = R$ associated with it, with $P_0 \in \mathrm{Rec}(s,2) \cup \mathrm{Rec}(2,s)$ for some $s \geq 4$, such that the sequence of moves $(m_1, m_2, \dots, m_r)$ used to fully infect P_r from P_0 is of the form $[2]^*[1]^*[3]^*$ or of the form $[3]^*[1]^*[2]^*$.*

PROOF. Let us fix an even $s \geq 4$ and assume that $P_0 \in \mathrm{Rec}(s,2) \cup \mathrm{Rec}(2,s)$. Note that this uniquely defines $r = (k+\ell)/2 - s/2 - 1$, which is also the number of initially infected sites outside P_0. By Observation 1.14 we immediately see that in such a sequence we should apply Move 1s to rectangles $P_i \in \mathrm{Rec}(s_i, t_i)$ with as large as possible difference $|s_i - t_i|$ between the length of the longer side and the length of the shorter side of P_i. We also note that whenever Move 1 is applied, say to obtain $P_{i+1} \in \text{Rec}(s_{i+1}, t_{i+1})$ from $P_i \in \text{Rec}(s_i, t_i)$, then this difference does not change, i.e., $|s_{i+1} - t_{i+1}| = |s_i + 1 - (t_i + 1)| = |s_i - t_i|$.

If Move 1 does not occur in $(m_1, m_2, \ldots, m_r)$ then every move in the sequence has a constant score 3 depending neither on the step at which it is applied nor on the dimensions of the rectangle it is applied to. Thus every permutation of $(m_1, m_2, \ldots, m_r)$ has the same score and we can clearly rearrange the sequence of moves to make it be of the form $[2]^*[1]^*[3]^*$ (or in fact $[2]^*[3]^*$) without changing percolation time.

Assume that Move 1 occurs only once in $(m_1, m_2, \ldots, m_r)$, say that $m_k = 1$ and $m_j \in \{2, 3\}$ for $j \in [r] \setminus \{k\}$. Assume first that $P_{k-1} \in \text{Rec}(s_{k-1}, t_{k-1})$ with $s_{k-1} > t_{k-1}$, so that the score of Move 1 at step k equals $s_{k-1} - t_{k-1}$. For a contradiction, let $m_j = 3$ for some $1 \leq j < k \leq r$. Consider a new sequence of moves $(m'_1, m'_2, \ldots, m'_r)$, obtained from $(m_i)_{i=1}^r$ by moving m_j to position k and shifting $m_{j+1}, \ldots, m_k$ to positions $j, \ldots, k-1$ respectively: more formally let $m'_i = m_i$ if $i < j$ or $i > k$, $m'_i = m_{i+1}$ for $j \leq i \leq k-1$ and $m'_k = m_j = 3$.

Let $P'_0 \subset P'_1 \subset \ldots \subset P'_r = R$ be a sequence of rectangles obtained using the sequence of moves $(m'_i)_{i=1}^r$ (since for all $i \geq k$ the dimensions of rectangles P'_i equal the dimensions of rectangles P_i we indeed have $P'_r = R$). Then the only Move 1 in this new sequence is applied to the rectangle $P'_{k-2} \in \text{Rec}(s_{k-1}, t_{k-1} - 2)$ (this is because there is one less Move 3 among $(m'_1, m'_2, \ldots, m'_{k-2})$ as compared to $(m_1, m_2, \ldots, m_{k-1})$) and so this Move 1 has score $s_{k-1} - t_{k-1} + 2$. Note that the scores of other moves do not change, as they are still equal to 3. Thus the cumulative score of the sequence $(m'_i)_{i=1}^r$ is greater than the one of the sequence $(m_i)_{i=1}^r$ and consequently percolation time of A is not maximum, contradicting the fact that A is (k, ℓ)-good. Thus for all $1 \leq i \leq k-1$ we must have $m_i = 2$. In an analogous way we prove that $m_i = 3$ for all $k+1 \leq i \leq r$. So in this case $(m_i)_{i=1}^r$ must be of the form $[2]^*[1]^*[3]^*$.

If Move 1 occurs only once in $(m_1, m_2, \ldots, m_r)$, say that again $m_k = 1$ and $m_j \in \{2, 3\}$ for $j \in [r] \setminus \{k\}$, and additionally we have $P_{k-1} \in \mathrm{Rec}(s_{k-1}, t_{k-1})$ with $s_{k-1} < t_{k-1}$, then in an analogous way we show that, this time, $(m_i)_{i=1}^r$ must be of the form $[3]^*[1]^*[2]^*$.

In the remaining case where P_{k-1} is a square, i.e., $s_{k-1} = t_{k-1}$, also in a completely analogous way, we can show that we must have $r = 1$ and $m_1 = 1$. If that was not the case, i.e., if we had $r \geq 2$ and there was some $m_j \in \{2, 3\}$ then moving m_j to the opposite side of the only occurrence of Move 1 in $(m_i)_{i=1}^r$ would increase the cumulative score (as Move 1 would no longer have score 0) contradicting the (k, ℓ)-goodness of A. Thus in this case $(m_i)_{i=1}^r = (1)$, which is at the same time of the form $[2]^*[1]^*[3]^*$ and of the form $[3]^*[1]^*[2]^*$.

Thus assume that Move 1 occurs more than once in $(m_1, m_2, \ldots, m_r)$. If all occurrences of it constitute a subsequence of consecutive m_i's then we deal with this case exactly as we did with the one where Move 1 occurred only once. This is straightforward because, as we already noticed, using Move 1 does not change the difference between the length of the longer side and the length of the shorter side of the rectangle it is applied to.

Thus assume that there is some $1 \leq j < t < k \leq r$ such that $m_j = m_k = 1$ and $m_t \in \{2, 3\}$. For $P_j \in \mathrm{Rec}(s_j, t_j)$ and $P_k \in \mathrm{Rec}(s_k, t_k)$ assume that $|s_j - t_j| \geq |s_k - t_k|$. Consider a new sequence of moves $(m'_1, m'_2, \ldots, m'_r)$ obtained from $(m_i)_{i=1}^r$ by moving m_k to position $j + 1$, and shifting $m_{j+1}, \ldots, m_{k-1}$ to positions $j + 2, \ldots, k$ respectively, that is, let $m'_i = m_i$ if $i \leq j$ or $i > k$, $m'_{j+1} = m_k = 1$ and for $j + 2 \leq i \leq k$ let $m'_i = m_{i-1}$.

Let $P'_0 \subset P'_1 \subset \ldots \subset P'_r = R$ be a sequence of rectangles obtained using the sequence $(m'_i)_{i=1}^r$ (note that as previously $P'_r = P_r = R$). Then using Move $m'_{j+1} = 1$ at step $j + 1$ we finish the infection of $P'_{j+1} \in \mathrm{Rec}(s_j + 1, t_j + 1)$ and so this move has score $|s_j - t_j|$ which is at least as big as the score of the move m_k at time k. Note that if $i \leq j$ or $i > k$ then the score of the move m'_i at time i equals the score of the move m_i at time i. Finally if $j + 2 \leq i \leq k$ then the score of the move m'_i at time i equals the score of the move m_{i-1} at time $i-1$. Thus the cumulative score of the sequence $(m'_i)_{i=1}^r$ is at least as big as that of the sequence $(m_i)_{i=1}^r$. Thus applying this modification (which does not decrease the score) of the sequence $(m_i)_{i=1}^r$ repetitively we could obtain a sequence describing another (k,ℓ)-good set in which all Move 1s occur in consecutive positions of the sequence. However, we already know that such sequence must be of the form $[2]^*[1]^*[3]^*$ or of the form $[3]^*[1]^*[2]^*$. When $|s_j - t_j| < |s_k - t_k|$ we proceed analogously, moving $m_j = 1$ to position $k-1$. This completes the proof of the claim. $\square$

By Lemma 1.12 there exists (k,ℓ)-good set A for which $P_0 \in \mathrm{Rec}(s,2) \cup \mathrm{Rec}(2,s)$, with $s \geq 4$. The construction we give in Lemma 1.10 shows that in this case P_0 can be obtained from some $P' \in \mathrm{Rec}(2,2)$ either by, if $P_0 \in \mathrm{Rec}(s,2)$, applying $(s-2)/2$ times Move 2, or by applying Move 3 if $P_0 \in \mathrm{Rec}(2,s)$. Note that indeed for all these occurrences of move 2 or 3 we infect one new site at exactly three time steps.

OBSERVATION 1.16. *The proof of Claim 1.15 actually tells us that, for a brief moment slightly abusing the notation (relaxing condition (1) in Definition 1.7) and for $i \geq 1$ allowing $P'_i \in \mathrm{Rec}(s'_i,2) \cup \mathrm{Rec}(2,s'_i)$ for $s'_i \geq 4$ and even, there exists a (k,ℓ)-good set A and a good sequence of rectangles $P'_0 \subset P'_1 \subset \ldots \subset P'_r \in \mathrm{Rec}(k,\ell)$ associated with it, with $P'_0 \in \mathrm{Rec}(2,2)$, such that the sequence of moves $(m'_1, m'_2, \ldots, m'_r)$ used to fully infect P'_r from P'_0 is of the form $[2]^*[1]^*[3]^*$ or of the form $[3]^*[1]^*[2]^*$. Since in Claim 1.15 we have $P_0 \in \mathrm{Rec}(s,2) \cup \mathrm{Rec}(2,s)$, with $s \geq 4$, we see that if $(m'_i)_{i=1}^r$ is of the form $[2]^*[1]^*[3]^*$ then the subsequence of Move 2s is nonempty. Analogously, if $(m'_i)_{i=1}^r$ is of the form $[3]^*[1]^*[2]^*$ then the subsequence of Move 3s is nonempty. Applying a nonempty sequence of Move 2s to $P'_0 \in \mathrm{Rec}(2,2)$ fully infects a rectangle $P''_0 \in \mathrm{Rec}(s'',2)$, with $s'' \geq 4$ and even. Analogously, applying a nonempty sequence of Move 3s to $P'_0 \in \mathrm{Rec}(2,2)$ fully infects a rectangle $P''_0 \in \mathrm{Rec}(2,s'')$, with $s'' \geq 4$ and even.*

Thus by Observation 1.16 we obtain the following lemma which, for any k and ℓ such that $k \geq 4, \ell \geq 2$ and $k+\ell$ is even, fully characterizes a good sequence of rectangles associated with at least one (k,ℓ)-good set of initially infected sites.

LEMMA 1.17. *Let k and ℓ be such that $k \geq 4, \ell \geq 2$ and $k+\ell$ is even. Then there exists a (k,ℓ)-good set A and a good sequence of rectangles $P_0 \subset P_1 \subset \ldots \subset P_r \in \mathrm{Rec}(k,\ell)$ associated with it, with $P_0 \in \mathrm{Rec}(s,2) \cup \mathrm{Rec}(2,s)$ for some $s \geq 4$, such that the sequence of moves $(m_1, m_2, \ldots, m_r)$ used to fully infect P_r from P_0 is either of the form $[1]^*[3]^*$ if $P_0 \in \mathrm{Rec}(s,2)$, or of the form $[1]^*[2]^*$ if $P_0 \in \mathrm{Rec}(2,s)$.*

□

COROLLARY 1.18. *For $n \geq 4$, there is a (n,n)-good set A, whose good sequence of rectangles $P_0 \subset P_1 \subset \ldots \subset P_r \in \mathrm{Rec}(n,n)$ is such that $P_0 \in \mathrm{Rec}(s,2)$ and that the sequence of moves used to build it is of the form $[1]^*[3]^*$. Furthermore, if the number of times we use Move 1 equals m then $m = n-s$ and we must use Move 3 exactly $\frac{n-2-m}{2}$ times.*

PROOF. Apply Lemma 1.17 with $k = \ell = n$. By symmetry, we can assume that $P_0 \in \mathrm{Rec}(s,2)$ and the sequence of moves obtained is of type $[1]^*[3]^*$. It is trivial to check that, in order to obtain $P_r \in \mathrm{Rec}(n,n)$, we must have $m = n-s$ and we must use Move 3 exactly $\frac{n-2-m}{2}$ times. □

We are now ready to prove the exact formula for $M_0(n)$ for $n \geq 4$.

Proof of Theorem 1.1. Given $m \geq 0$, let A_m^n be (if it exists) the (n,n)-good set described in Corollary 1.18 for which during the infection process Move 1 is used exactly m times (note that when n and m have different parities then A_m^n definitely does not exist). For example, Figure 1.6 shows the set A_4^{12}.

Now, we notice that for every $n \geq 4$ and $0 \leq m \leq n-4$ (with n and m having the same parity) the percolation time of A_m^n (if it exists) can be given explicitly as follows:

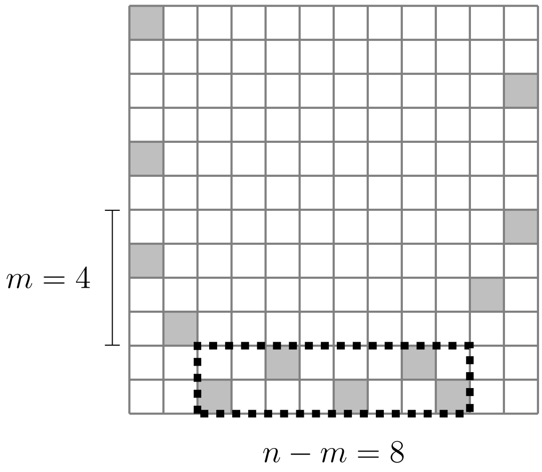


FIGURE 1.6. Set A_4^{12}.

(1) Infection of the rectangle $P_0 \in \mathrm{Rec}(n-m, 2)$ takes time

$$M_0(n-m,2) = \frac{3(n-m)-4}{2} = \frac{3(n-m)}{2} - 2;$$

(2) Applying m times Move 1 takes time

$$\sum_{i=0}^{m-1}(n-m+i) = mn - m^2 + \frac{m(m-1)}{2} = mn - \frac{m(m+1)}{2};$$

(3) Finishing the infection with $\frac{n-m-2}{2}$ applications of Move 3 takes time

$$\frac{n-m-2}{2}(n+1) = \frac{n^2-n-mn-m-2}{2}.$$

Letting $f(n,m)$ denote the percolation time of A_m^n, by the above calculations we have

$$f(n,m) = \frac{n^2 + n(m+2) - (m^2+5m+6)}{2}.$$

For a given n, the function $f_n(m) = f(n,m)$ is a quadratic function of m with maximum value at $m = \frac{n-5}{2}$. As our (n,n)-good set maximizes $f_n(m)$ subject to $m \in \mathbb{N}$ and m having the same parity as n, maximum percolation time is obtained for

$$m = m_0 = \left\lfloor \frac{n}{2} - \frac{5}{2} \right\rfloor + \mathbb{1}_{\{4|n-1\}} + \mathbb{1}_{\{4|n\}},$$

where in the above statement we use $\mathbb{1}_{\{\phi\}}$ to denote the indicator function,

$$\mathbb{1}_{\{\phi\}} = \begin{cases} 1, & \text{if the sentence } \phi \text{ is true,} \\ 0, & \text{otherwise.} \end{cases}$$

Now, by considering the possible values of $n \pmod 4$ we see that for all $n \geq 4$ we have $f(n, m_0) = \lfloor \frac{5n^2-2n}{8} \rceil$. This completes our proof. □

Using Lemma 1.17, given $\alpha \in (0,1)$ and n large, assuming $(1+\alpha)n$ is an even natural number we can determine the asymptotic value of $M_0(n, \alpha n)$. All we need to do is, for both $P_0 \in \mathrm{Rec}(s,2)$ and $P_0 \in \mathrm{Rec}(2,s)$, to optimize s to maximize the cumulative score of our sequence of moves knowing that the number of times we use Move 1 is fully determined by s and the horizontal or vertical alignment of P_0 in $[n] \times [\alpha n]$, and that the score of all occurrences of Move 1 equals $s-2$.

Corollary 1.19. *We have:*

1. *If $\frac{1}{2} \leq \alpha < 1$ then*

   $$M_0(n, \alpha n) = \left(\frac{\alpha}{2} + \frac{1}{8}\right) n^2 + O(n).$$

   To maximize percolation time we should first infect a roughly $\frac{n}{2} \times 2$ rectangle in time $O(n)$, then using Move 1 $\left(\frac{n}{2} + O(1)\right)$ times extend it to a roughly $n \times \frac{n}{2}$ one in time $\frac{3n^2}{8} + O(n)$, and then finish the infection in additional $\left(\frac{\alpha}{2} - \frac{1}{4}\right) n^2 + O(n)$ time steps using Move 3 $\left(\left(\frac{\alpha}{2} - \frac{1}{4}\right) n + O(1)\right)$ times.
2. *If $0 < \alpha < \frac{1}{2}$ then*

   $$M_0(n, \alpha n) = \left(\alpha - \frac{\alpha^2}{2}\right) n^2 + O(n).$$

   To maximize percolation time we should first infect a roughly $(1-\alpha)n \times 2$ rectangle in time $O(n)$, and then finish the infection in additional $\left(\alpha - \frac{\alpha^2}{2}\right) n^2 + O(n)$ time steps using Move 1 $(\alpha n + O(1))$ times.

□

CHAPTER 2

Maximum percolation time in two-dimensional bootstrap percolation

2.1. Introduction

In this chapter we consider a problem strongly related to the one we studied in Chapter 1. Answering another extremal problem posed by Bollobás we give the asymptotic value of the maximum time that any percolating subset of the set of vertices of $G = [n]^2$ can take to percolate under 2-neighbour bootstrap percolation. The notation and preliminary observations we use here are similar or even identical to the ones we defined in Section 1.2. We shall not repeat these redundant definitions here, referring to the concepts in Chapter 1 instead.

Recall that $T(A)$ denotes the time that A takes to percolate in $[n]^2$. Moreover, let

$$M(n) = \max\{T(A) : \langle A \rangle = [n]^2\}.$$

In this chapter we determine an asymptotic formula for $M(n)$ up to an $O(n)$ additive error. We believe that a constant additive error or even an exact formula could be found with similar techniques but with a much longer and more tedious proof. With our methods we prove the following theorem.

Theorem 2.1. *We have*

$$M(n) = \frac{13}{18}n^2 + O(n).$$

Theorem 2.1, together with Theorem 1.1 which in particular says that percolating sets of size n internally span the $n \times n$ grid in time at most $\frac{5}{8}n^2 + O(n)$, implies that, somewhat surprisingly, the slowest percolating sets do not have the minimum possible number of sites.

This chapter is joint work with Fabricio S. Benevides, with the exception of Section 2.5 which is solo work, and is based on our forthcoming paper, [**16**].

2.2. Notation

To solve the problem we consider in this chapter we shall mostly use the notation and preliminary observations presented in Section 1.2. Having defined

$M(n)$ in the previous section, we only need two extra definition before we start our investigations.

In this chapter we show that to infect $[n]^2$ in the maximum possible time one should first infect some smaller rectangular grid, not necessarily a square one, in maximum time. This motivates a definition of the maximum percolation time in rectangles, i.e., for any $k, \ell \in \mathbb{N}$ let

$$M(k, \ell) = \max\{T : \text{there exists a set } A \text{ percolating in time } T \text{ in } [k] \times [\ell]\}.$$

Note that clearly $M(k, \ell) = M(\ell, k)$. For a rectangle $R \in \mathrm{Rec}(k, \ell)$, to simplify our notation, we shall often write $M(R)$ instead of $M(k, \ell)$.

We shall be interested in infection time of particular sites. Thus, let $I_A(v)$ be the minimum T such that $v \in A_T$ starting from $A_0 = A$. If starting from A the site v never becomes infected, i.e., $v \notin \langle A \rangle$, then we set $I_A(v) = \infty$.

2.3. Slowly percolating sets

In this section we prove a recursive formula for $M(k, \ell)$ in order to later prove an asymptotic formula for $M(n)$. Let us start by giving a trivial upper bound and a natural lower bound on $M(n)$. Since every percolating set in $[n]^2$ contains at least n sites and for the infection to continue we need to infect at least one new site at every step we have $M(n) \leq n^2 - n$. On the other hand, the example shown in Figure 2.1 for the $[7]^2$ grid, generalizing in a self–explanatory way to $[n]^2$, shows that there exist initially infected sets of size linear in n for which at approximately half of the number of steps only one site becomes infected while the other steps, with the exception of the first one, yield infection of only two new sites. This clearly implies that $M(n) \geq \frac{2n^2}{3} + O(n)$. We will prove that for every n there is a set which percolates $[n]^2$ in time $M(n)$, for which at every time step at most two new sites become infected, but the number of steps for which a single site becomes infected is significantly larger than in the example in Figure 2.1.

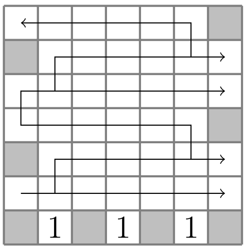


FIGURE 2.1. An initial set giving a lower bound $M(n) \geq \frac{2n^2}{3} + O(n)$.

The outline of our proof is as follows. First we define a notion of a (k, ℓ)-perfect set of initially infected sites; next, we prove that the function $M(k, \ell)$ satisfies a certain recursive relation and simultaneously show that (k, ℓ)-perfect sets exist and that their percolation time satisfies the same relation as $M(k, \ell)$. Although we do not find an exact solution for the recursion, we are able to find good lower and upper bounds on $M(n)$. For the lower bound we construct an explicit set of initially infected sites which is “almost” (n, n)-perfect. Finally, for the upper bound, we define a relaxed version of the infection process and for any (n, n)-perfect set A we build an appropriate instance of this new process; from this new instance we get an upper bound for the time that A takes to percolate. Let us now make our arguments formal.

DEFINITION 2.2. *Given $k, \ell \in \mathbb{N}$ we say that a set A is (k, ℓ)-perfect if the infection process starting from A can be described in the following way. There exists a nested sequence of rectangles $P_0 \subset P_1 \subset \ldots \subset P_r \in \mathrm{Rec}(k, \ell)$, such that $P_i \in \mathrm{Rec}(s_i, t_i)$, with the following properties:*

(a) either $s_0 \leq 2$ or $t_0 \leq 2$ or $s_0 = t_0 = 3$; and $s_1, t_1 \geq 3$ with $(s_1, t_1) \neq (3, 3)$,

(b) for each $1 \leq i \leq r$,

$$\begin{aligned} P_i \in\, &\mathrm{Rec}(s_{i-1}+1, t_{i-1}+1) \cup \mathrm{Rec}(s_{i-1}+2, t_{i-1}) \cup \mathrm{Rec}(s_{i-1}, t_{i-1}+2) \cup \\ &\mathrm{Rec}(s_{i-1}+2, t_{i-1}+1) \cup \mathrm{Rec}(s_{i-1}+1, t_{i-1}+2) \cup \mathrm{Rec}(s_{i-1}, t_{i-1}+3) \cup \\ &\mathrm{Rec}(s_{i-1}+3, t_{i-1}), \end{aligned}$$

(c) for every $0 \leq i \leq r$*, the rectangle* P_i *is internally spanned by* $A \cap P_i$ *in the maximum possible time, that is, in time* $M(P_i)$*,*

(d) for every $0 \leq i \leq r$*, if* P_i *has no side of length* 1 *then among the sites becoming infected last in* P_i *there is at least one of its corner sites,*

(e) for every $1 \leq i \leq r$*, if*

$$P_i \in \mathrm{Rec}(s_{i-1}+1, t_{i-1}+1) \cup \mathrm{Rec}(s_{i-1}, t_{i-1}+2) \cup \mathrm{Rec}(s_{i-1}+2, t_{i-1})$$

then there exists a site $v_{i-1} \in A$ *such that* $P_{i-1} \cup \{v_{i-1}\}$ *internally spans* P_i *and* v_{i-1} *is at distance exactly 2 from one of the corner sites in* P_{i-1} *(one which becomes infected last in* P_{i-1}*, if there is such) and at distance at least 3 from any other site in* P_{i-1} *(see Figure 1.3 in the previous chapter),*

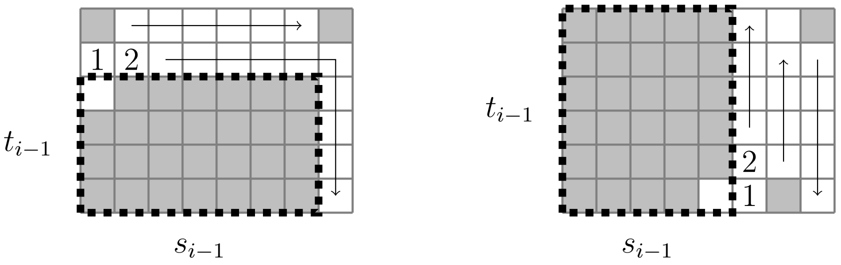
(f) for every $1 \leq i \leq r$*, if*

$$P_i \in \mathrm{Rec}(s_{i-1}+2, t_{i-1}+1) \cup \mathrm{Rec}(s_{i-1}+1, t_{i-1}+2) \cup \mathrm{Rec}(s_{i-1}, t_{i-1}+3) \cup \mathrm{Rec}(s_{i-1}+3, t_{i-1})$$

then there exists a pair of sites $v_{i-1}, w_{i-1} \in A$ *such that* $P_{i-1} \cup \{v_{i-1}, w_{i-1}\}$ *internally spans* P_i *and* v_{i-1} *is at distance exactly 2 from one of the corner sites in* P_{i-1} *(one which becomes infected last in* P_{i-1}*, if there is such) and at distance at least 3 from any other site in* P_{i-1}*, while* w_{i-1} *is at distance exactly 1 from one of the last corner sites to become infected in* $\langle P_{i-1} \cup \{v_{i-1}\} \rangle$ *and at distance at least 2 from any other site in* $\langle P_{i-1} \cup \{v_{i-1}\} \rangle$ *(see Figure 2.2).*

From condition (b) it follows that for every $1 \leq i \leq r$ we have $\Phi(P_{i-1})+2 \leq \Phi(P_i) \leq \Phi(P_{i-1})+3$. From condition (c), taking $i = r$, it follows that any (k,ℓ)-perfect set infects a rectangle in $\mathrm{Rec}(k,\ell)$ in time $M(k,\ell)$. In particular, any (n,n)-perfect set maximizes percolation time in $[n]^2$.

Given a (k,ℓ)-perfect set and a sequence $P_0 \subset P_1 \subset \ldots \subset P_r \in \mathrm{Rec}(k,\ell)$ associated with it, for $1 \leq i \leq r$ and $1 \leq m \leq 7$, we say that we use *Move m*



Move 5 at moment i Move 7 at moment i

FIGURE 2.2. Move 5 and 7 (Move 4 and 6 are obtained by rotating the above figures by 90 degrees).

at moment i (to construct P_i from P_{i-1}) if P_i belongs to the m-th term of the following list:

(1) $\mathrm{Rec}(s_{i-1}+1, t_{i-1}+1)$,
(2) $\mathrm{Rec}(s_{i-1}+2, t_{i-1})$,
(3) $\mathrm{Rec}(s_{i-1}, t_{i-1}+2)$,
(4) $\mathrm{Rec}(s_{i-1}+2, t_{i-1}+1)$,
(5) $\mathrm{Rec}(s_{i-1}+1, t_{i-1}+2)$,
(6) $\mathrm{Rec}(s_{i-1}, t_{i-1}+3)$,
(7) $\mathrm{Rec}(s_{i-1}+3, t_{i-1})$.

Let us recall and extend the notation we used for sequences of moves in Chapter 1, which we shall also use here. We say a finite (possibly empty) sequence of moves is of the form $[a_1|a_2|\dots|a_r]^*$ if all its terms belong to $\{a_1, a_2, \dots, a_r\} \subseteq [7]$; we say that it is of the form $[a_1|a_2|\dots|a_r]^{\leq j}$ if, in addition, it has at most j terms. We shall concatenate these expressions to create more general ones which describe the corresponding sets of concatenated sequences of moves. For example, all of the sequences 1444336366, 43333, 16633 are of the form $[1]^{\leq 1}[4]^*[3|6]^*$, but 144334 is not.

In the next lemma we determine the value of $M(k,2)$ and give an example of a $(k,2)$-perfect set for each natural k.

LEMMA 2.3. *For any natural number k we have $M(k,2) = \left\lfloor \frac{3(k-1)}{2} \right\rfloor$. Furthermore, there is a $(k,2)$-perfect set, $A^0(k,2)$, which percolates $[k] \times [2]$ in time $M(k,2)$.*

Proof. First let us consider the case when k is even. Let A be any set that percolates $[k] \times [2]$. Since percolation time is at most the number of initially healthy sites, if $|A| \geq k/2 + 2$ then it percolates in time at most $2k - (k/2 + 2) = (3k - 4)/2$. On the other hand, by Corollary 1.4, we must have $|A| \geq k/2 + 1$. Therefore we may assume that the cardinality of A is exactly $k/2 + 1$. Then the lemma for k even follows from Lemma 1.10

For k odd, the set in Figure 2.3 has the minimum cardinality necessary for a set to percolate $[k] \times [2]$ and at each time step causes infection of only one site. Therefore it percolates in the maximum time which is indeed $\left\lfloor \frac{3(k-1)}{2} \right\rfloor$. Thus it is an immediate observation that it satisfies all conditions of a $(k, 2)$-perfect set. □

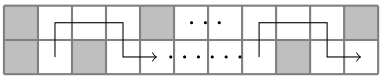


Figure 2.3. A $(k, 2)$-perfect set achieving maximum percolation time on $[k] \times [2]$ for k odd.

In the next theorem we state a recursive formula for $M(k, \ell)$. We should keep in mind the description of (k, ℓ)-perfect initial sets because the proof of the theorem is built on the proof of existence and a construction of such sets. Since $M(k, \ell) = M(\ell, k)$, we shall omit some cases where $k < \ell$.

Theorem 2.4. *We have* $M(1, 1) = M(2, 1) = 0$; $M(k, 1) = 1$ *for all* $k \geq 3$; $M(k, 2) = \left\lfloor \frac{3(k-1)}{2} \right\rfloor$; *and* $M(3, 3) = 4$. *For* $k, \ell \geq 3$ *such that* $(k, \ell) \neq (3, 3)$, *we* *have*

$$M(k,\ell) = \max \begin{cases} M(k-1,\ell-1) + \max\{k,\ell\} - 1, \\ M(k-2,\ell) + \ell + 1, \\ M(k,\ell-2) + k + 1, \\ M(k-2,\ell-1) + k + \ell - 2, \\ M(k-1,\ell-2) + k + \ell - 2, \\ M(k,\ell-3) + 2k - 1, \\ M(k-3,\ell) + 2\ell - 1, \end{cases} \tag{2.1}$$

where we assume $M(k,0) = M(0,\ell) = -\infty$. *Furthermore, for any* $k, \ell > 0$ *there exists a* (k,ℓ)*-perfect set.*

Proof. We prove Theorem 2.4 by induction on $k+\ell$. A small case analysis immediately gives the result for $\ell = 1$ and for $(k,\ell) = (3,3)$. For $\ell = 2$ we use Lemma 2.3. Note that in all these cases there exist (k,ℓ)-perfect initial sets for which, in the definition of (k,ℓ)-perfect sets, we have $r = 0$.

Now, assume that we are given $k, \ell \geq 3$ such that $(k,\ell) \neq (3,3)$. Our induction hypothesis is that for any $k', \ell' \geq 1$ such that $k' + \ell' < k + \ell$, there exists a (k',ℓ')-perfect set $A^M(k',\ell')$ which percolates in time $M(k',\ell')$, as in the statement of Theorem 2.4.

We shall first prove that the following inequality holds.

$$M(k,\ell) \geq \max \begin{cases} M(k-1,\ell-1) + \max\{k,\ell\} - 1, \\ M(k-2,\ell) + \ell + 1, \\ M(k,\ell-2) + k + 1, \\ M(k-2,\ell-1) + k + \ell - 2, \\ M(k-1,\ell-2) + k + \ell - 2, \\ M(k,\ell-3) + 2k - 1, \\ M(k-3,\ell) + 2\ell - 1. \end{cases} \tag{2.2}$$

Assume without loss of generality that $k \geq 4$. Recall that, for $k', \ell' \geq 2$, from the definition of (k', ℓ')-perfect sets we may assume that one of the corners of the rectangle spanned by $A^M(k', \ell')$ becomes infected at time $M(k', \ell')$. Now, consider the following seven ways of infecting $[k] \times [\ell]$ (see again Figure 1.3 in the previous chapter and Figure 2.2).

(1) Let $\langle A^M(k-1, \ell-1) \rangle = [k-1] \times [\ell-1]$. Since $k-1, \ell-1 \geq 2$, we may assume that $(k-1, \ell-1)$ becomes infected at time $M(k-1, \ell-1)$. Let $A^{(1)} = A^M(k-1, \ell-1) \cup \{(k, \ell)\}$. Then $A^{(1)}$ takes time $M(k-1, \ell-1) + \max\{k, \ell\} - 1$ to percolate.

(2) Let $\langle A^M(k-2, \ell) \rangle = [k-2] \times [\ell]$. Since $k-2, \ell \geq 2$, we may assume that $(k-2, \ell)$ becomes infected at time $M(k-2, \ell)$. Let $A^{(2)} = A^M(k-2, \ell) \cup \{(k, \ell)\}$. Then $A^{(2)}$ takes time $M(k-2, \ell) + \ell + 1$ to percolate.

(3) When $\ell \geq 4$, we have $k, \ell-2 \geq 2$. Let $\langle A^M(k, \ell-2) \rangle = [k] \times [\ell-2]$. We may assume that $(k, \ell-2)$ becomes infected at time $M(k, \ell-2)$. Let $A^{(3)} = A^M(k, \ell-2) \cup \{(k, \ell)\}$. Then $A^{(2)}$ percolates in time $M(k, \ell-2) + k + 1$.

(4) Let $\langle A^M(k-2, \ell-1) \rangle = [k-2] \times [\ell-1]$. Since $k-2, \ell-1 \geq 2$, we assume that $(k-2, 1)$ becomes infected at time $M(k-2, \ell-1)$. Let $A^{(4)} = A^M(k-2, \ell-1) \cup \{(k, 1), (k, \ell)\}$. Then $A^{(4)}$ takes time $M(k-2, \ell-1) + k + \ell - 2$ to percolate.

(5) When $\ell \geq 4$, we have $k-1, \ell-2 \geq 2$. Let $\langle A^M(k-1, \ell-2) \rangle = [k-1] \times [\ell-2]$. We may assume that $(1, \ell-2)$ becomes infected at time $M(k-1, \ell-2)$. Let $A^{(5)} = A^M(k-1, \ell-2) \cup \{(1, \ell), (k, \ell)\}$. Then $A^{(4)}$ takes time $M(k-1, \ell-2) + k + \ell - 2$ to percolate.

(6) When $\ell \geq 5$, we have $k, \ell-3 \geq 2$. Let $\langle A^M(k, \ell-3) \rangle = [k] \times [\ell-3]$ and assume that $(k, \ell-3)$ becomes infected at time $M(k, \ell-3)$. Let $A^{(6)} = A^M(k, \ell-3) \cup \{(k, \ell-1), (1, \ell)\}$. Then $A^{(6)}$ percolates in time $M(k, \ell-3) + 2k - 1$.

(7) When $k \geq 5$, an analogous construction to case (6), with a $(k-3,\ell)$-perfect set $A^M(k-3,\ell)$ spanning $[k-3]\times[\ell]$ in time $M(k-3,\ell)$. Taking $A^{(7)} = A^M(k-3,\ell)\cup\{(k-1,\ell),(k,1)\}$ we obtain a set spanning $[k]\times[\ell]$ in time $M(k-3,\ell)+2\ell-1$.

The above constructions show that inequality (2.2) holds when $k,\ell \geq 5$. We now check that inequality (2.2) also holds for the small values of k and ℓ for which some of these constructions do not apply. Constructions (3) and (5) do not apply when $\ell = 3$ since then we cannot ask for one of the corners of smaller rectangles to become infected respectively at times $M(k,\ell-2)=1$ and $M(k-1,\ell-2)=1$. However, since $k \geq 4$, in these cases we have $M(k,\ell-2)+k+1 = k+2$ and $M(k-1,\ell-2)+k+\ell-2 = k+2$ which is at most $M(k-1,\ell-1)+k-1 = \left\lfloor \frac{3(k-2)}{2} \right\rfloor + k - 1 \geq k+2$.

Construction (6) does not apply for $\ell = 4$ since then again we cannot ask for one of the corners of $[k]\times[\ell-3]$ to become infected at time $M(k,\ell-3)=1$. However, for $\ell = 4$ we have $M(k,\ell-3)+2k-1 = 2k$ which is less than $M(k,\ell-2)+k+1 = \left\lfloor \frac{3(k-1)}{2} \right\rfloor + k + 1 \geq \left\lfloor \frac{2k+1}{2} \right\rfloor + k + 1 = 2k+1$. Analogously we deal with the fact that construction (7) does not apply for $k = 4$. Thus the lower bound on $M(k,\ell)$ is proved.

For each of the sets $A^{(j)}$ constructed above, among the sites of $\langle A^{(j)} \rangle$ that become infected last there is a corner of $[k]\times[\ell]$. Thus it is clear that all sets $A^{(j)}$ satisfy the conditions (a)-(f) to be (k,ℓ)-perfect sets except for, possibly, condition (c). To finish the proof of Theorem 2.4, we only need to prove the upper bound on $M(k,\ell)$ analogous to inequality (2.2), since this will imply that at least one of the sets $A^{(j)}$ percolates in time $M(k,\ell)$ and therefore is (k,ℓ)-perfect. So, it remains to show that

$$M(k,\ell) \le \max \begin{cases} M(k-1,\ell-1) + \max\{k,\ell\} - 1, \\ M(k-2,\ell) + \ell + 1, \\ M(k,\ell-2) + k + 1, \\ M(k-2,\ell-1) + k + \ell - 2, \\ M(k-1,\ell-2) + k + \ell - 2, \\ M(k,\ell-3) + 2k - 1, \\ M(k-3,\ell) + 2\ell - 1. \end{cases} \tag{2.3}$$

Let A be any set which internally spans the rectangle $R = [k] \times [\ell]$ in time $M(k,\ell)$. Consider disjoint sets A', A'' and rectangles R', R'' satisfying conditions (1), (2) and (3) of Proposition 1.6. Define, $T(R',R'')$ as the time to grow from $R' \cup R''$ to $R = \langle R' \cup R'' \rangle$, that is, the time needed to infect all sites in $R \setminus (R' \cup R'')$ given that all sites in R' and R'' are infected and no site in $R \setminus (R' \cup R'')$ is. Let

$$S(R',R'') = \max\{M(R'), M(R'')\} + T(R',R'').$$

It is clearly seen that, for any choice of $A', A'' \subset A$ satisfying Proposition 1.6, $S(R',R'')$ is an upper bound on the time that A takes to percolate. As we shall see, for most choices of A a simple upper bound on $S(R',R'')$ will be enough to show that the time that A takes to percolate is at most the right hand side of inequality (2.3). However, in one particular case we will have to look carefully for a better bound.

Our technique of bounding $S(R',R'')$ will require the following claim which says that, under our induction hypothesis, maximum percolation time is strictly increasing.

Claim 2.5. *Let s, t be such that $s + t < k + \ell$. If $s \ge 1$ and $t \ge 2$ then $M(s+1,t) \ge M(s,t) + 1$. Similarly, if $s \ge 2$ and $t \ge 1$ then $M(s,t+1) \ge M(s,t) + 1$.*

Proof of Claim. Let $s \geq 1$ and $t \geq 2$. For $s = 1$, the result is trivial (as $M(2,2) \geq 1$ and $M(1,2) = 0$ and, for $t \geq 3$, $M(2,t) \geq 3$ and $M(1,t) = 1$). For $s, t \geq 2$, by the induction hypothesis, we may assume that there exists a set $A^M(s,t)$ which internally spans the rectangle $[s] \times [t]$ in time $M(s,t)$ and such that

$$I_{A^M(s,t)}(s,t) = M(s,t) \geq 1.$$

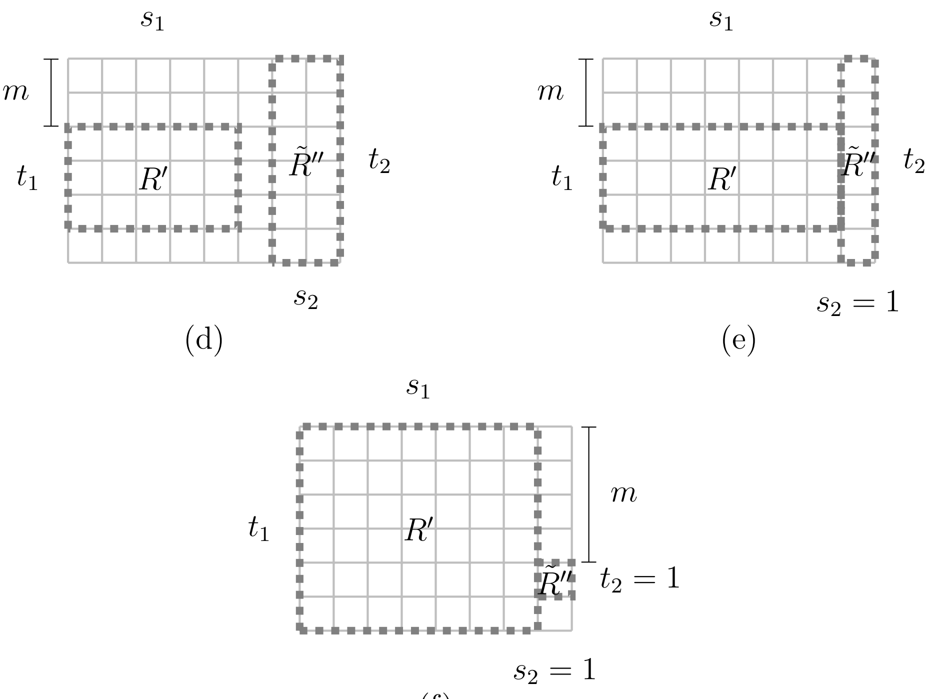
Note that we must have some $1 \leq i \leq t-1$ such that $(s,i) \in A^M(s,t)$. Let i^* be the smallest such i. Let $\tilde{A} = A^M(s,t) \cup \{(s+1, i^*)\}$. Clearly $\left\langle \tilde{A} \right\rangle = [s+1] \times [t]$ and for any $j \in [t] \setminus \{i^*\}$ we have $I_{\tilde{A}}(s+1,j) \geq I_{A^M(s,t)}(s,j) + 1$. Thus $M(s+1,t) \geq I_{\tilde{A}}(s+1,t) \geq M(s,t) + 1$. □

Assume without loss of generality that $M(R') \geq M(R'')$. Note that, in order to internally span R, the rectangles R' and R'' must be at distance 0, 1 or 2. Consider some minimal non-empty rectangle $\tilde{R}'' \subset R''$ such that $R' \cup \tilde{R}''$ spans R. Whenever R' and R'' intersect, that is $\text{dist}(R', R'') = 0$, we can choose $\tilde{R}''$ so that it is disjoint from R'. Furthermore, whenever $\text{dist}(R', R'') = 1$ then unless R'' has a side of length 1 we can always choose $\tilde{R}''$ such that $\text{dist}(R', \tilde{R}'') = 2$. Since $T(R', R'') \leq T(R', \tilde{R}'')$ and $M(R') \geq M(R'') \geq M(\tilde{R}'')$, we have $S(R', R'') \leq S(R', \tilde{R}'')$. Denote $R' \in \text{Rec}(s_1, t_1)$ and $\tilde{R}'' \in \text{Rec}(s_2, t_2)$. With case analysis we find that, since $\tilde{R}''$ is chosen to be minimal, R' and $\tilde{R}''$ must either satisfy one of the Conditions (a), (b) or (c) considered in the previous chapter for R' and R'' (see Figure 1.5), or one of the following conditions (or their analogues obtained by swapping k with ℓ).

Condition (d): there is an $0 \leq m \leq \ell - t_1$ such that the rectangles R' and $\tilde{R}''$ align as in Figure 2.4 (d) with $s_1 + s_2 = k - 1$, $t_1 < \ell$, $t_2 = \ell$.

Condition (e): there is an $0 \leq m \leq \ell - t_1$ such that the rectangles R' and $\tilde{R}''$ align as in Figure 2.4 (e) with $s_1 = k - 1$, $s_2 = 1$, $t_1 < \ell$, $t_2 = \ell$.

Condition (f): there is an $0 \leq m \leq \ell - 1$ such that the rectangles R' and $\tilde{R}''$ align as in Figure 2.4 (f) with $s_1 = k - 1$, $s_2 = 1$, $t_1 = \ell$, $t_2 = 1$.



(d) (e)

(f)

FIGURE 2.4. Additional alignments of rectangles R' and $\tilde{R}''$ that need to be considered.

Assume first that Condition (b) holds. Note that, in this case,

$$S(R', \tilde{R}'') = M(R') + \max\{s_1 + t_2 - 1, s_2 + t_1 - 1\}.$$

It is easy to check that $S(R', \tilde{R}'')$ cannot decrease if we "extend" the rectangle R' and "shrink" $\tilde{R}''$. In fact, when $\max\{s_1, t_1\} \geq 2$ then we can use Claim 2.5 and so, for any $i < s_2$ and $j < t_2$, we have $M(s_1+i, t_1+j) \geq M(s_1, t_1)+i+j$. Together with

$$\max\{(s_1 + i) + (t_2 - j) - 1, (s_2 - i) + (t_1 + j) - 1\} \geq \\ \max\{s_1 + t_2 - 1, s_2 + t_1 - 1\} - \max\{i, j\},$$

we conclude that the largest value of $S(R', \tilde{R}'')$ is given when $\tilde{R}''$ is a single site. Therefore, $S(R', \tilde{R}'') \leq M(k-1, \ell-1) + \max\{k, \ell\} - 1$. When $\max\{s_1, t_1\} = 1$ then R' is a single site. Since we assume $M(R') \geq M(\tilde{R}'')$ we would require

$\tilde{R}'' \in \mathrm{Rec}(1,1) \cup \mathrm{Rec}(1,2) \cup \mathrm{Rec}(2,1)$. This yields $\max\{k,\ell\} \leq 3$ which contradicts our assumption that $k,\ell \geq 3$ are such that $(k,\ell) \neq (3,3)$.

Now, assume that Condition (a) (or its analogue with k and ℓ swapped) holds. Observe that in this case

$$S(R',\tilde{R}'') = \begin{cases} M(R') + \max\{s_1+t_2, s_2+t_1\}, & \text{if } t_1,t_2 \geq 2, \\ M(R') + s_2 + t_1, & \text{if } t_2 = 1, \\ M(R') + s_1 + t_2, & \text{if } t_1 = 1. \end{cases}$$

If $t_1,t_2 \geq 2$ it is easy to reduce it to the previous case: by Claim 2.5 we have $M(s_1+1,t_1) \geq M(s_1,t_1)+1$, while

$$\max\{(s_1+1)+(t_2-1)-1, s_2+t_1-1\} = \max\{s_1+t_2, s_2+t_1\} - 1.$$

Putting these inequalities together we have $S(R',\tilde{R}'') \leq S(R^+,R^-)$ where $R^+ \in \mathrm{Rec}(s_1+1,t_1), R^- \in \mathrm{Rec}(s_2,t_2-1)$ and R^+,R^- satisfy Condition (b). If $t_2 = 1$, then $t_1 \geq 3$ (recall, $k,\ell \geq 3$). Thus, as for Condition (b), we can use Claim 2.5 and extend R' rightwards to bound $S(R',\tilde{R}'')$ from above using the case where $\tilde{R}''$ is a single site and obtain $S(R',\tilde{R}'') \leq M(k-2,\ell)+\ell+1$. Note that swapping k and ℓ gives the bound $S(R',\tilde{R}'') \leq M(k,\ell-2)+k+1$.

Finally, if $t_1 = 1$ then $t_2 \geq 3$ and, since $M(R') \geq M(\tilde{R}'')$, also $s_2 = 1$. Then, R becomes infected after at most $k+\ell-2$ steps which is not more than $M(k-1,\ell-1)+\max\{k,\ell\}-1$ for all $k,\ell \geq 3$.

Suppose now that Condition (c) holds. Note that, for a fixed R' and given m, we have $S(R',\tilde{R}'') = M(R')+\max\{m+s_2+1, t_1-m+s_2\}$ which is maximum when $m = 0$ or $m = t_1-1$ and this case is equivalent to Condition (a) with $t_2 = 1$. Thus we see that

$$\max\{M(k-1,\ell-1)+\max\{k,\ell\}-1, M(k-2,\ell)+\ell+1, M(k,\ell-2)+k+1\} \quad (2.4)$$

is the maximum percolation time in $[k]\times[\ell]$ if we limit ourselves to Conditions (a), (b) and (c) only.

Now we consider the case when Condition (d) applies to R', $\tilde{R}''$. Recall $M(R') \geq M(\tilde{R}'')$. Thus given m we have

$$S(R', \tilde{R}'') = M(R') + \max\{s_1 + m + 1, s_1 + t_2 - m - t_1 + 1\}.$$

which is maximum when $m = 0$ or $m = t_2 - t_1$. However, for these values of m we could further shrink $\tilde{R}''$ by setting $t_2 = \ell - t_1 + 1$. This is a contradiction by the minimality of $\tilde{R}''$ thus Condition (d) cannot yield a larger upper bound on $S(R', \tilde{R}'')$.

We deal with R' and R'' satisfying Condition (e) in an analogous way, bounding $S(R', \tilde{R}'')$ from above by taking $m = 0$ and then using the minimality of $\tilde{R}''$ to obtain a contradiction.

Finally let us consider the case where Condition (f), or its version with k and ℓ swapped, applies to R' and $\tilde{R}''$. In this case we need to be more careful: using similar arguments as before, we can only conclude that

$$S(R', \tilde{R}'') = \\ \begin{cases} M(R') + \max\{m, \ell - m - 1\} \leq M(R') + \ell - 1, & \text{if } R' \in \mathrm{Rec}(k-1, \ell), \\ M(R') + \max\{m, k - m - 1\} \leq M(R') + k - 1, & \text{if } R' \in \mathrm{Rec}(k, \ell - 1). \end{cases} \tag{2.5}$$

However, this bound is not good enough. To improve it, we need to analyze how the proximity of $\tilde{R}''$ affects the infection process inside R'.

Recall that we initially chose R' and R'' together with $A', A'' \subsetneq A$ spanning them according to Proposition 1.6. We later chose $\tilde{R}'' \subset R''$ and we assumed that Condition (f) applies to R' and $\tilde{R}''$. However, assuming that $R' = [k-1] \times [\ell]$, A'' must contain a site of the form (k, i) for some $1 \leq i \leq \ell$ as R' and R'' together span R. Thus we can assume that in fact R', internally spanned by A', and R'', which is a single site, satisfy Condition (f) (dropping some sites from A'' could not decrease percolation time).

We will find the following claim necessary.

CLAIM 2.6. *Let A be a set of sites percolating in $R = [k] \times [\ell]$, where $k, \ell \geq 2$. Then for any site $(i, j) \in R \setminus \{(1,1), (1,\ell), (k,1), (k,\ell)\}$ we have $I_A(i,j) < M(k,\ell)$.*

Proof of Claim. It is enough to prove the claim for all percolating sets minimal under containment (as for any $A \subset B$ we have $I_B(i,j) \leq I_A(i,j)$ for all i, j). Let A be such set. Applying Proposition 1.6 to R and A we obtain disjoint sets A' and A'' that partition A and internally span two rectangles $R', R'' \subsetneq R$ such that $\langle R' \cup R'' \rangle = R$. Note that, by minimality of A, $R \setminus (R' \cup R'')$ contains no initially infected sites.

If $k = \ell = 2$ then all sites in $[k] \times [\ell]$ are corners and the claim is trivial. If, without loss of generality, $k > 2$ then $M(k,\ell) > 1$. By Claim 2.5, we have $\max\{M(R'), M(R'')\} < M(k,\ell)$. So, for any $(i,j) \in R' \cup R''$ we have $I_A(i,j) \leq \max\{M(R'), M(R'')\} < M(k,\ell)$. Now, let

$$B = R \setminus \left(R' \cup R'' \cup \{(1,1), (1,\ell), (k,1), (k,\ell)\}\right).$$

If $\{(1,1), (1,\ell), (k,1), (k,\ell)\} \subset R' \cup R''$ and $B \neq \emptyset$ then $\Phi(R'), \Phi(R'') \leq k + \ell - 2$ (see Figure 2.5) so by Claim 2.5 we have $M(R'), M(R'') \leq M(R) - 2$ and therefore for any $(i,j) \in B$ we have $I_A(i,j) \leq M(k,\ell) - 1$. So, we may assume that $R \setminus (R' \cup R'')$ contains some corner site of R. Let (i,j) be any site of B. We consider the two following cases:

- If $\operatorname{dist}(R', R'') = 2$ then $M(R'), M(R'') \leq M(R) - 2$. Thus, if we have $\operatorname{dist}((i,j), R') = \operatorname{dist}((i,j), R'') = 1$ then

  $$I_A(i,j) \leq \max\{M(R'), M(R'')\} + 1 \leq M(k,\ell) - 1.$$

- If either $\operatorname{dist}(R', R'') = 2$ and $\operatorname{dist}((i,j), R') \neq 1$ or $\operatorname{dist}((i,j), R'') \neq 1$, or if $\operatorname{dist}(R', R'') \neq 2$, then no matter how the rectangles R' and R'' are aligned we can find a corner site $(k', \ell') \in R \setminus (R' \cup R'')$ such that to infect (k', ℓ') in the process we need to infect (i,j) first. This follows from the fact that the rectangular region in $R\setminus(R'\cup R'')$ which contains (k',ℓ') becomes infected starting from its own corner opposite (k',ℓ'). Thus $I_A(i,j) < I_A(k',\ell') \leq M(k,\ell)$.

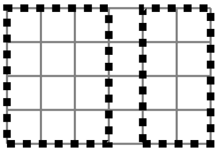


FIGURE 2.5. The alignment of R' and R'' containing all 4 corner sites

Thus the proof of the claim is complete. □

An important consequence of Claim 2.6 is that when rectangles R' and R'' in R satisfy Condition (f) then, no matter how we locate R'' in R, the infection of $R \setminus (R' \cup R'')$ starts at latest at time $M(R') - 1$. This improves the bound on the time that A takes to percolate given by equation (2.5) to

$$\max\begin{cases} M(R') + \ell - 2, & \text{if } R' \in \mathrm{Rec}(k-1,\ell) \\ M(R') + k - 2 & \text{if } R' \in \mathrm{Rec}(k,\ell-1) \end{cases} \tag{2.6}$$

To finish the proof, we apply Proposition 1.6 to R' (we can do this as $k,\ell \geq 3$ and R'' is a single site). So let A' be partitioned into disjoint sets A'_1 and A'_2 spanning rectangles R'_1 and R'_2 respectively, satisfying Proposition 1.6. Assume that $M(R'_1) \geq M(R'_2)$.

If R'_1 and R'_2 satisfy Condition (f) inside R', with R'_2 being a single site, then we can bound the time that A takes to percolate in a much better way than using equation (2.6). In fact, considering the possible cases it can be bounded from above by

$$\max\begin{cases} M(k-1,\ell-1) + \max\{k,\ell\} - 1, \\ M(k-2,\ell) + \ell + 1, \\ M(k,\ell-2) + k + 1, \end{cases}$$

because $\mathrm{dist}(R'_1, R'') \leq 2$ and so, with R'_1 fully infected, the processes of infecting $R' \setminus (R'_1 \cup R'_2)$ and $\langle R'_1 \cup R'' \rangle \setminus (R'_1 \cup R'')$ run simultaneously.

In the remainder, we assume that R_1' and R_2' satisfy one of the conditions (a)-(e) in R' and improve the bound (2.6) by replacing $M(R')$ with a better bound on the time that A' takes to percolate in R'.

If R_1' and R_2' satisfy Condition (a) or (c) in R' then, by what we already know about the bounds for these conditions (upper bound on $M(R')$ is the weakest when R_2' is a single site, see (2.4)), the bound in (2.6) is at most

$$\max \begin{cases} M(k-2,\ell-1)+k+\ell-2, \\ M(k-1,\ell-2)+k+\ell-2, \\ M(k,\ell-3)+2k-1, \\ M(k-3,\ell)+2\ell-1. \end{cases}$$

If $R_1' \in \mathrm{Rec}(s_1,t_1)$ and $R_2' \in \mathrm{Rec}(s_2,t_2)$ inside R' satisfy Condition (b) then R'', R_1' and R_2' are, up to some rotations, for some $m \le t_1+t_2-1$ mutually aligned as in Figure 2.6 (where R'' is depicted with a shaded square).

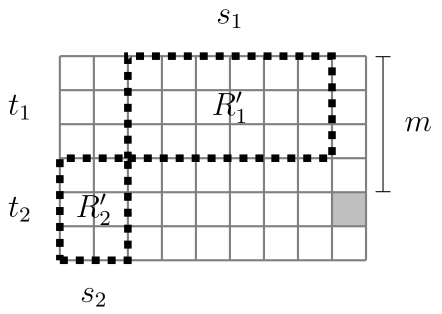


FIGURE 2.6. Condition (b) followed by Condition (f)

Let us analyze the possible cases conditioned on the value of t_2. If $t_2 = 1$ then we have $\mathrm{dist}(R_1', R'') \le 2$ so the infection of $\langle R_1' \cup R'' \rangle \setminus (R_1' \cup R'')$ starts at latest at time $M(R_1')$. Thus, by Claim 2.5, the bound on percolation time is maximized for $s_2 = 1$ and $m = 0$ which as an upper bound on $M(k,\ell)$ gives

$$\max \begin{cases} M(k-1,\ell-2)+\max\{k,\ell\}-1 \\ M(k-2,\ell-1)+\max\{k,\ell\}-1 \end{cases} < M(k-1,\ell-1)+\max\{k,\ell\}-1.$$

If $t_2 > 1$ then, by Claim 2.5 and Claim 2.6, the bound on percolation time is maximized either for $t_2 = 2$, $s_2 = 1$ and $m = t_1 + t_2 - 1$ which as the upper bound on $M(k, \ell)$ gives

$$M(k-2, \ell-2) + k + \ell - 3 < M(k-2, \ell-1) + k + \ell - 2,$$

or for $s_1 = 2$, $t_1 = 1$ and $m = t_1 + t_2 - 1$ which as the upper bound gives

$$\max\begin{cases} M(k-1, \ell-3) + 2k - 2 \\ M(k-3, \ell-1) + 2\ell - 2 \end{cases} < \max\begin{cases} M(k, \ell-3) + 2k - 1 \\ M(k-3, \ell) + 2\ell - 1 \end{cases},$$

or for $s_1 = 1$, $t_1 = 1$ and $m = t_1 + t_2 - 1$ which as the upper bound gives

$$\begin{aligned} &\max\begin{cases} M(k-1, \ell-2) + \max\{k+1, \ell-2\} \\ M(k-2, \ell-1) + \max\{k-2, \ell+1\} \end{cases} \\ &\leq \max\begin{cases} M(k-1, \ell-2) + k + \ell - 2 \\ M(k-2, \ell-1) + k + \ell - 2 \end{cases}. \end{aligned}$$

Thus the upper bound on the percolation time of A obtained when Condition (b) holds for R'_1, R'_2 inside R' is at most the maximum in inequality (2.3).

Finally, if R'_1 and R'_2 inside R' satisfy Condition (d) or (e) with $M(R'_1) \geq M(R'_2)$ then, as already noted, by setting $m = 0$ and shrinking R'_2 we can bound from above the percolation time of A' by the bounds obtained under conditions (a) and (b). That completes the proof of the upper bound on $M(k, \ell)$ and of Theorem 2.4. □

REMARK. *Relation* (2.1) *does not allow us to immediately give an exact formula for* $M(n)$. *However, with the use of a computer, it is possible to write a program evaluating* $M(n)$ *and at the same time finding an* (n, n)*-perfect set. Our simulations suggest that these sets have size approximately* $\frac{23n}{18} + O(1)$ *(for example, for* $n = 1000$ *it is* 1277*). In the next section we find the asymptotic* *formula for* $M(n)$*. For the lower bound we shall use sets similar to those suggested by our simulations.*

2.4. Computing the asymptotic value of $M(n)$

In this section we use the existence of (n, n)-perfect sets to compute the asymptotic value of $M(n)$. We say that a (k, ℓ)-perfect set A together with the sequence of rectangles $P_0 \subset P_1 \subset \ldots \subset P_r \in \mathrm{Rec}(k, \ell)$ associated with it are *described by a triple* $(s_0, t_0, m_1 m_2 \ldots m_r)$ if $P_0 \in \mathrm{Rec}(s_0, t_0)$ and, for $1 \leq i \leq r$, Move m_i is used to obtain P_i from P_{i-1}. We write $T_0 = M(P_0)$ and, for $i \geq 1$, we denote by T_i the additional time it takes to infect the sites of P_i after all sites of P_{i-1} are infected. We say that $T_0, T_1, \ldots, T_r$ is the *time sequence* of A. Finally, we say that a triple $(s_0, t_0, m_1 m_2 \ldots m_r)$ is a *scheme* that solves $M(k, \ell)$ if it describes a (k, ℓ)-perfect set.

Note that a triple $(s_0, t_0, m_1 m_2 \ldots m_r)$ may describe multiple (n, n)-perfect sets since it only determines the dimensions of the rectangles P_i but not their precise coordinates. Nevertheless, all (n, n)-perfect sets described by $(s_0, t_0, m_1 m_2 \ldots m_r)$ have the same time-sequence. Note that if $T_0, T_1, \ldots, T_r$ is the time sequence of an (n, n)-perfect set then $M(n) = \sum_{i=0}^{r} T_i$.

OBSERVATION 2.7. *Let* $(s_0, t_0, m_1 m_2 \ldots m_r)$ *be a scheme and* $P_0 \subset P_1 \subset \ldots \subset P_r$ *be the sequence of rectangles generated by it. Then for any* $1 \leq j \leq r$*, the triple* $(s_0, t_0, m_1 m_2 \ldots m_j)$ *is a scheme. In particular, it describes a set that percolates* P_j *in maximum time.*

REMARK. *In Appendix 2.7 we consider a number of small cases and show that for any* $k, \ell \geq 3$*,* $(k, \ell) \neq (3, 3)$*, there exists a scheme* $(s_0, t_0, m_1 m_2 \ldots m_r)$ *that solves* $M(k, \ell)$ *and is such that either* $s_0 \geq 3$ *and* $t_0 = 2$ *or* $s_0 = 2$ *and* $t_0 \geq 3$.

Let a, b be natural numbers and let $x_1 \ldots x_a$ and $y_1 \ldots y_b$ be sequences of moves. We say that these sequences are compatible if applying moves $x_1 \ldots x_a$ to a certain rectangle R yields a rectangle with the same dimensions as when applying moves $y_1 \dots y_b$ to R. For example, for any $1 \leq i, j \leq 7$, the sequence ij is compatible with ji, the sequence 61 is compatible with 35, the sequence 111 is compatible with 45, but 12 is not compatible with 13 (because the order of dimensions matters).

Fix $1 \leq i \leq r$ and denote $P_i \in \mathrm{Rec}(k, \ell)$. Clearly the value of T_i depends only on k, ℓ and m_i. We list its possible values in Table 1 (see also equation (2.1)). For $2 \leq i \leq r$, applying this argument twice, we can compute the value of $T_i + T_{i-1}$, as a function of only k, ℓ, m_i and m_{i-1}. In Table 2 we list the values of $T_i + T_{i-1}$ for $m_i, m_{i-1} \in \{2, 3, 4, 5, 6, 7\}$ and in Table 3 we list the values of $T_i + T_{i-1}$ when either $m_i = 1$ or $m_{i-1} = 1$.

m_i	P_{i-1}	T_i
1	$(k-1, \ell-1)$	$\max\{k, \ell\} - 1$
2	$(k-2, \ell)$	$\ell + 1$
3	$(k, \ell-2)$	$k + 1$
4	$(k-2, \ell-1)$	$k + \ell - 2$
5	$(k-1, \ell-2)$	$k + \ell - 2$
6	$(k, \ell-3)$	$2k - 1$
7	$(k-3, \ell)$	$2\ell - 1$

TABLE 1. Dimensions of P_{i-1} and value of T_i given m_i, assuming that $P_i \in \mathrm{Rec}(k, \ell)$.

Initially, the object of our interest in Table 2 and Table 3 is, for each pair (a, b) with $1 \leq a, b \leq 7$, whether for $P_i \in \mathrm{Rec}(k, \ell)$ the value of $(T_i + T_{i-1})$ is larger when $(m_{i-1}, m_i) = (a, b)$ or when $(m_{i-1}, m_i) = (b, a)$. We summarize the answer to that question in Figure 2.7 which tells us which pairs of consecutive moves are prohibited in a scheme (for one could swap them and obtain a slower percolating process). A solid directed edge from a to b means that, no matter what the values of k and ℓ are, it takes strictly longer to apply Move b right before Move a than it takes to apply them in the opposite order. Thus in this case the consecutive pair of moves ab inside a scheme is prohibited. A dashed directed edge from a to b means that no matter what the values of k and ℓ are, it always takes at least as much time to apply Move b followed by Move a as it takes to do the opposite. A dashed undirected edge means that the order of

	$m_i = 2$	$m_i = 3$	$m_i = 4$	$m_i = 5$	$m_i = 6$	$m_i = 7$
$m_{i-1} = 2$	$2\ell + 2$	$k + \ell$	$k + 2\ell - 2$	$k + 2\ell - 3$	$2k + \ell - 3$	3ℓ
$m_{i-1} = 3$	$k + \ell$	$2k + 2$	$2k + \ell - 3$	$2k + \ell - 2$	$3k$	$k + 2\ell - 3$
$m_{i-1} = 4$	$k + 2\ell - 3$	$2k + \ell - 3$	$2k + 2\ell - 7$	$2k + 2\ell - 7$	$3k + \ell - 6$	$k + 3\ell - 6$
$m_{i-1} = 5$	$k + 2\ell - 3$	$2k + \ell - 3$	$2k + 2\ell - 7$	$2k + 2\ell - 7$	$3k + \ell - 6$	$k + 3\ell - 6$
$m_{i-1} = 6$	$2k + \ell - 4$	$3k$	$3k + \ell - 7$	$3k + \ell - 5$	$4k - 2$	$2k + 2\ell - 8$
$m_{i-1} = 7$	3ℓ	$k + 2\ell - 4$	$k + 3\ell - 5$	$k + 3\ell - 7$	$2k + 2\ell - 8$	$4\ell - 2$

TABLE 2. Values of $(T_i + T_{i-1})$ for $m_i, m_{i-1} \in \{2, 3, 4, 5, 6, 7\}$, assuming that $P_i \in \text{Rec}(k, \ell)$.

	$(m_{i-1}, m_i) = (j, 1)$	$(m_{i-1}, m_i) = (1, j)$
$j = 1$	$2\max\{k, \ell\} - 3$	$2\max\{k, \ell\} - 3$
$j = 2$	$\max\{k, \ell\} + \ell - 1$	$\ell + \max\{k, \ell - 2\}$
$j = 3$	$\max\{k, \ell\} + k - 1$	$k + \max\{k - 2, \ell\}$
$j = 4$	$\max\{k, \ell\} + k + \ell - 5$	$k + \ell + \max\{k - 2, \ell - 1\} - 3$
$j = 5$	$\max\{k, \ell\} + k + \ell - 5$	$k + \ell + \max\{k - 1, \ell - 2\} - 3$
$j = 6$	$\max\{k, \ell\} + 2k - 4$	$2k + \max\{k, \ell - 3\} - 2$
$j = 7$	$\max\{k, \ell\} + 2\ell - 4$	$2\ell + \max\{k - 3, \ell\} - 2$

TABLE 3. Values of $(T_i + T_{i-1})$ for $m_i = 1$ or $m_{i-1} = 1$, assuming that $P_i \in \text{Rec}(k, \ell)$.

moves a and b maximizing the value of $(T_i + T_{i-1})$ depends on the values of k and ℓ. No edge between a and b means that the order we use does not affect the value of $(T_i + T_{i-1})$.

Next, we prove a series of propositions about schemes for $M(k, \ell)$.

PROPOSITION 2.8. *For any* $k, \ell \geq 3$, $(k, \ell) \neq (3, 3)$, *there exists a scheme solving* $M(k, \ell)$ *of the form* $(s_0, t_0, [1|2|3]^*[4|5|6|7]^*)$ *with* $s_0 \geq 3, t_0 = 2$ *or* $s_0 = 2, t_0 \geq 3$.

PROOF. Given k, ℓ, consider a scheme $Q = (s_0, t_0, m_1 m_2 \dots m_r)$ with $s_0 \geq 3, t_0 = 2$ or $s_0 = 2, t_0 \geq 3$ that solves $M(k, \ell)$ (which exists by Remark 2.4)

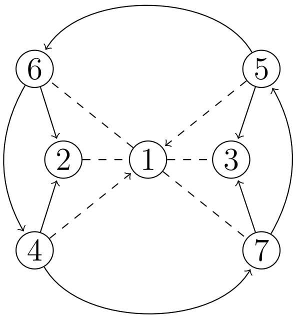


FIGURE 2.7. Relation between pairs of consecutive moves (m_{i-1}, m_i) and the value of $(T_i + T_{i-1})$.

which minimizes the sum $S = \sum_{m_i \in \{1,2,3\}} i$. Proposition 2.8 follows immediately from the following claim: in such a scheme, for any i with $2 \le i \le s$, if m_i is equal to 1, 2 or 3 then m_{i-1} is equal to 1, 2, or 3. Let us check that this claim holds.

Fix $2 \le i \le r$. Assume first that $m_i = 2$. From Figure 2.7 we see that $m_{i-1} \notin \{4, 6\}$ and if $m_{i-1} \in \{5, 7\}$ then we could swap the order of (m_{i-1}, m_i) without changing percolation time and decreasing the value of S, contradicting the choice of Q. Therefore, m_{i-1} must be either 1, 2 or 3. The case where $m_i = 3$ is analogous.

Assume now that $m_i = 1$. If $m_{i-1} \in \{4, 5\}$ then we could swap the order of (m_{i-1}, m_i) without decreasing percolation time and decreasing the value of S, contradicting the choice of Q. Now, suppose that $m_{i-1} = 6$. If $k \ge \ell$ then, by Table 3,

$$T_{i-1} + T_i = \max\{k, \ell\} + 2k - 4 < 2k + \max\{k, \ell - 3\} - 2$$

in which case we could set $(m_{i-1}, m_i) = (1, 6)$ and increase percolation time. If $k < \ell$ then again by Table 3 we have

$$T_{i-1} + T_i = \max\{k, \ell\} + 2k - 4 < 2k + \ell - 2$$

in which case we can set $(m_{i-1}, m_i) = (3, 5)$ and increase percolation time. In either case, we contradict the fact that Q is a scheme. Therefore $m_{i-1} \neq 6$. We show that $m_{i-1} \neq 7$ in an analogous way: one could either swap $(7, 1)$ or replace it by $(2,4)$ in order to increase percolation time (doing one or the other depending on the values of k and ℓ). Therefore we must have m_{i-1} equal to 1, 2 or 3. $\square$

Before we continue our investigations of the form of the schemes that solve $M(k,\ell)$ let us make the following observation analogous to Observation 1.13 in the previous chapter, about the infection process started from a (k,ℓ)-perfect set.

Observation 2.9. *For any $i \geq 1$, no matter which move $(1-7)$ is used at moment i, between time step $M(P_{i-1})+1$ and time step $M(P_i)$ (when the infection of the rectangle P_i is complete), at each step at most two new sites become infected.*

From Observation 2.9 and Observation 1.14 in the previous chapter the following claim follows. It is fully analogous to Claim 1.15 in the previous chapter therefore we leave it without proof.

Claim 2.10. *Suppose that there exists a (k,ℓ)-perfect set A internally spanning a rectangle $R \in \mathrm{Rec}(k,\ell)$ with a sequence of rectangles $P_0 \subset P_1 \subset \ldots \subset P_r \in \mathrm{Rec}(k,\ell)$ associated with it, described by a triple of the form $(s_0, t_0, [1|2|3]^*)$ with $s_0 \geq 3, t_0 = 2$ or $s_0 = 2, t_0 \geq 3$. Then there exists a (k,ℓ)-perfect set A' internally spanning the rectangle $R \in \mathrm{Rec}(k,\ell)$ described by a triple of the form $(s_0, t_0, [2]^*[1]^*[3]^*)$, or of the form $(s_0, t_0, [3]^*[1]^*[2]^*)$.*

$\square$

Proposition 2.11. *For any $n \geq 4$ there exists a scheme solving $M(n)$ of the form $(s_0, 2, [1]^*[3]^*[4|5|6|7]^*)$ or $(s_0, 2, [3]^*[1]^*[2]^*[4|5|6|7]^*)$ with $s_0 \geq 3$.*

Proof. Consider a scheme $Q = (s_0, 2, m_1 m_2 \ldots m_r)$ with $s_0 \geq 3$ and sequence $m_1 m_2 \ldots m_r$ of the form $[1|2|3]^*[4|5|6|7]^*$ which exists by Proposition 2.8 (by symmetry, when $k = \ell = n$ we might assume $t_0 = 2$).

Let $j = \max\{i : m_i \in \{1,2,3\}\}$. By Observation 2.7, the sequence of moves $m_1 \ldots m_j$ is such that the time taken to infect P_j is maximum. Therefore, by

Claim 2.10, we see that we may take $m_1 \dots m_j$ of the form $[2]^*[1]^*[3]^*$ or of the form $[3]^*[1]^*[2]^*$. We observe that in the first case we obtain a scheme Q' of the form $(s_0', 2, [1]^*[3]^*[4|5|6|7]^*)$, as the triple $(s_0, 2, [2]^*[1]^*[3]^*[4|5|6|7]^*)$ gets simplified to $(s_0', 2, [1]^*[3]^*[4|5|6|7]^*)$ (and $s_0' = s_0 + 2a$ where a is the number of times that Move 2 occurs in $m_1 \dots m_j$). In the second case we have a scheme of the form $(s_0', 2, [3]^*[1]^*[2]^*[4|5|6|7]^*)$. $\square$

PROPOSITION 2.12. *For any* $n \geq 4$ *there exists a scheme solving* $M(n)$ *of the form* $(s_0, 2, [1]^{\leq 1}[3]^{\leq 2}[4|5|6|7]^*)$ *or of the form* $(s_0, 2, [3]^{\leq 2}[1]^{\leq 1}[2]^*[4|5|6|7]^*)$.

PROOF. By Proposition 2.11 there exists a scheme $Q = (s_0, t_0, m_1 m_2 \dots m_r)$ of the form $(s_0, 2, [1]^*[3]^*[4|5|6|7]^*)$ or of the form $(s_0, 2, [3]^*[1]^*[2]^*[4|5|6|7]^*)$. Let us consider these cases separately.

Assume first that there exists Q of the form $(s_0, 2, [1]^*[3]^*[4|5|6|7]^*)$, and choose one for which the number of times it uses Move 1 is minimal. Let $j = \max\{i : m_i = 1\}$. Let $P_j \in \mathrm{Rec}(s_j, t_j)$. Assume that Move 3 was used at least three times. For $s_j \geq 5$, we could replace the last occurrence of the sequence 333 by the compatible sequence 66 without decreasing percolation time. For $3 \leq s_j \leq 4$, we consider all possible options for $Q' = (s_0, t_0, m_1 \dots m_j)$, and note that either:

(1) $Q' = (3, 2, 333)$, which takes strictly less time (15 steps) to span $R \in \mathrm{Rec}(3, 8)$ than $Q'' = (2, 7, 1)$ does (16 steps), or
(2) $Q' = (3, 2, 1333)$, which takes strictly less time (21 steps) to span $R \in \mathrm{Rec}(4, 9)$ than $Q'' = (2, 9, 2)$ does (22 steps), or
(3) $Q' = (4, 2, 333)$, which takes strictly less time (19 steps) to span $R \in \mathrm{Rec}(4, 8)$ than $Q'' = (2, 5, 15)$ does (21 steps).

By Observation 2.7, none of the above Q' can be an initial segment of Q. Thus there must exist Q of the form $(s_0, 2, [1]^*[3]^{\leq 2}[4|5|6|7]^*)$. Now, assume that Move 1 is used at least twice, say, Q is of the form $(s_0, 2, 11 m_3 m_4 \dots m_r)$. If $s_0 \geq 4$, then Q can be replaced by $(s_0 - 1, 2, 14 m_3 m_4 \dots m_r)$ for which we still have $P_2 \in \mathrm{Rec}(s_0 + 2, 4)$ and whose percolation time is at least as big as for Q because

$$T_0 + T_1 + T_2 = M(s_0, 2) + s_0 + (s_0 + 1) = \left\lfloor \frac{7s_0 - 1}{2} \right\rfloor$$

and the time sequence for the modified sequence of moves gives

$$T_0' + T_1' + T_2' = M(s_0 - 1, 2) + (s_0 - 1) + ((s_0 + 2) + 4 - 2) = \left\lfloor \frac{7s_0}{2} \right\rfloor .$$

In fact, as there is a dashed directed edge from 4 to 1 and no edge between 4 and 3 in Figure 2.7 we can move the new Move 4 further in the sequence and obtain $\tilde{Q}$ of the form $(s_0, 2, [1]^*[3]^{\leq 2}[4|5|6|7]^*)$ with a strictly smaller number of Move 1s used than in Q. This contradicts the minimality of the number of Move 1s used in Q. If $s_0 = 3$, it is enough to notice that $(3, 2, 11)$ takes strictly less time (10 steps) to percolate in $R \in \text{Rec}(5, 4)$ than $(5, 2, 3)$ does (12 steps). Therefore Move 1 must be used at most once. Thus Q is of the form $(s_0, 2, [1]^{\leq 1}[3]^{\leq 2}[4|5|6|7]^*)$ as stated.

In the second case, assume that there exists a scheme Q of the form $(s_0, 2, [3]^*[1]^*[2]^*[4|5|6|7]^*)$. By the same argument as in the first case, we can conclude the Move 3 is used at most two times. In fact, the only difference is that here we do not need to consider the subcase $Q' = (3, 2, 1333)$ in our analysis. Therefore, there must exist a scheme of the form $(s_0, 2, [3]^{\leq 2}[1]^*[2]^*[4|5|6|7]^*)$.

Assume that Move 1 is used at least twice. If Move 3 is not used then Q is of the form $(s_0, 2, 11m_3m_4 \dots m_r)$ and we can get a contradiction as in the first case. So, Move 3 must be used once or twice. It follows from Observation 1.14 that, when we limit ourselves to sequences of the form $(s_0, 2, [1|3]^*)$, the slowest sequences are obtained when Move 1s are applied to rectangles in which the difference between the length of their longer and their shorter side is maximum. This means that Move 3s could be used before Move 1 only if after using them the difference in lengths of the sides of the rectangle we obtained was at least as large as $s_0 - t_0 = s_0 - 2$. However, since Move 3 is used at most twice then, unless s_0 is small, by putting Move 1s before 3s we obtain a sequence slower than if we did it the other way. More precisely, the only cases in which putting

Move 3s before 1s could possibly increase the percolation time are those where $s_0 - 2 < 3$ and the initial sequences of steps in Q are:

(1) $Q' = (3, 2, 311)$ which takes strictly less time (16 steps) to span $R \in \mathrm{Rec}(5, 6)$ than $Q'' = (2, 5, 12)$ does (18 steps), or
(2) $Q' = (3, 2, 3311)$ which takes strictly less time (24 steps) to span $R \in \mathrm{Rec}(5, 8)$ than $Q'' = (2, 3, 155)$ does (25 steps), or
(3) $Q' = (4, 2, 3311)$ which takes strictly less time (27 steps) to span $R \in \mathrm{Rec}(6, 8)$ than $Q'' = (2, 7, 17)$ does (31 steps).

As in the first case, sets described by triples Q'' span the same rectangles as those spanned by sets described by corresponding triples Q'. Thus we see that the triples Q' are not initial segments of schemes. This implies that Move 1 is used at most once, that is, in the second case Q is of the form $(s_0, 2, [3]^{\leq 2}[1]^{\leq 1}[2]^*[4|5|6|7]^*)$ as stated. □

We are now ready to prove our main result.

Proof of Theorem 2.1. We begin proving that $M(n) \geq \frac{13}{18}n^2 + O(n)$ by constructing a particular family of percolating sets described by triples of the form $(s_0, 2, 1[4]^*[6]^*)$. These sets, however, are not necessarily (n, n)-perfect. We consider the following way of spanning $[n]^2$ for $n \geq 6$:

(1) choose a natural number $s \in (\frac{n}{3} - 3, \frac{n}{3} + 3]$ such that $6 | n + s - 5$ (note that, in particular, this implies $2 | n - s - 1$),
(2) in Phase 1 span a rectangle $P_0 \in \mathrm{Rec}(s, 2)$ in the maximum possible time,
(3) in Phase 2 obtain $P_1 \in \mathrm{Rec}(s + 1, 3)$ by applying Move 1 to P_0,
(4) in Phase 3 obtain $P_{\frac{n-s+1}{2}} \in \mathrm{Rec}(n, \frac{n-s+5}{2})$ by applying Move 4 $\frac{n-s-1}{2}$ times,
(5) in Phase 4 obtain $P_{\frac{2n-s-1}{3}} = [n]^2$ by applying Move 6 $\frac{n+s-5}{6}$ times.

Let us compute the time it takes to span $[n]^2$ this way:

(1) Phase 1 takes time $\left\lfloor \frac{3(s-1)}{2} \right\rfloor > \frac{n}{2} - 6$,
(2) Phase 2 takes time $s > \frac{n}{3} - 3$,

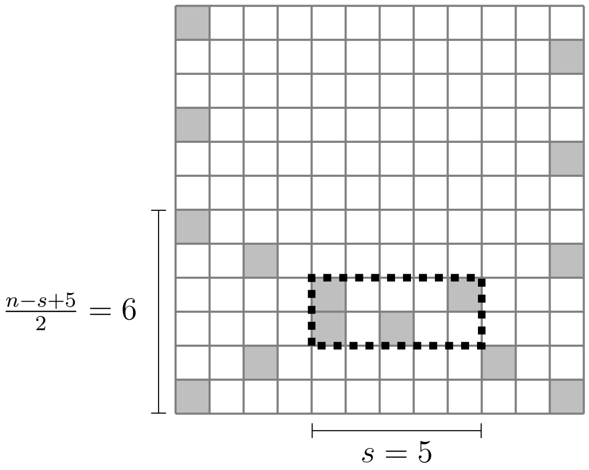


FIGURE 2.8. Example of a set giving a lower bound for $n = 12$

(3) Phase 3 takes time

$$\sum_{i=0}^{\frac{n-s-3}{2}} (s+5+3i) = \frac{3n^2 - 2sn - s^2 + 8n - 12s - 11}{8} > \frac{5n^2}{18} + \frac{n}{2} + 7,$$

(4) Phase 4 takes time

$$\frac{n+s-5}{6}(2n-1) = \frac{2n^2 - 11n + 2ns - s + 5}{6} > \frac{8n^2}{18} - \frac{26n}{9} + \frac{4}{3}.$$

Therefore, this way of infecting $[n]^2$ takes time at least $\frac{13n^2}{18} - \frac{14n}{9} - \frac{2}{3}$ to complete and the lower bound on $M(n)$ is proved.

To find an upper bound on $M(n)$, we would like to improve Proposition 2.12 and show that there is a scheme of the form $(s_0, 2, 1[4]^*[6]^*)$. The main issue is that, due to the cycle $4 \to 7 \to 5 \to 6 \to 4$ in Figure 2.7, there is no obvious way to order Move 4s, 5s, 6s and 7s in our schemes. So first we shall get rid of one type of move completely, so that the remaining ones will be easy to order. Another problem we would have to face is the fact that divisibility constraints restrict the number of times we can apply particular moves to eventually construct the $n \times n$ square.

To deal with our main issue we shall introduce a more general and rather abstract process in which fractional Moves 4, 5, 6 and 7 can be applied. In this process, our aim is also to infect the square $[n]^2$. It will be obvious that the maximum spanning time in this new process is at least as big as in the 2-neighbour bootstrap percolation. To be more precise, we will allow the following fractional moves. For $x \in (0, \infty)$

(1) Move $(4, x)$ applied to a rectangle $P \in \mathrm{Rec}(s, t)$ spans $P' \in \mathrm{Rec}(s + 2x, t + x)$ in time $x(s + t + 1) + 3(x^2 - x)/2$.
(2) Move $(5, x)$ applied to a rectangle $P \in \mathrm{Rec}(s, t)$ spans $P' \in \mathrm{Rec}(s + x, t + 2x)$ in time $x(s + t + 1) + 3(x^2 - x)/2$.
(3) Move $(6, x)$ applied to a rectangle $P \in \mathrm{Rec}(s, t)$ spans $P' \in \mathrm{Rec}(s, t + 3x)$ in time $x(2s - 1)$.
(4) Move $(7, x)$ applied to a rectangle $P \in \mathrm{Rec}(s, t)$ spans $P' \in \mathrm{Rec}(s + 3x, t)$ in time $x(2t - 1)$.

We note that when x is a natural number and $i \in \{4, 5, 6, 7\}$, then applying Move (i, x) is equivalent to applying the original Move i exactly x times.

Let $Q = (s_0, 2, m_1 m_2 \dots m_r)$ be a scheme solving $M(n)$ of the form

$$(s_0, 2, [1]^{\leq 1}[3]^{\leq 2}[4|5|6|7]^*) \text{ or } (s_0, 2, [3]^{\leq 2}[1]^{\leq 1}[2]^*[4|5|6|7]^*),$$

which exists by Proposition 2.12. Let A be an (n, n)-perfect set determined by Q and let $P_0 \subset P_1 \subset \dots \subset P_r \in \mathrm{Rec}(n, n)$ be the sequence of rectangles associated with it with $P_i \in \mathrm{Rec}(s_i, t_i)$. Let j_0 be such that P_{j_0} is the rectangle obtained after the last occurrence of any of the Move 1s, 2s or 3s. If there are no such moves, we set $j_0 = 0$. Since Move 1 is applied at most once and Move 3 at most twice we have $t_{j_0} \leq 7$. So there is an optimal scheme in which we first infect a rectangle $R \in \mathrm{Rec}(s_{j_0}, t_{j_0})$ where $t_{j_0} \leq 7$, and then apply only Move 4s, 5s, 6s or 7s. Without loss of generality assume that $s_{j_0} \geq t_{j_0}$.

We shall first construct a particular triple

$$Q' = (s_0, 2, m_1 \dots m_{j_0}(m'_{j_0+1}, x_{j_0+1})(m'_{j_0+2}, x_{j_0+2}) \dots (m'_{r'}, x_{r'}))$$

using (fractional) moves that infects $[n]^2$ in our generalized process in time at least as big as Q does in bootstrap percolation, and then bound from above the time it takes to perform Q'. Recall that by using Move m_i in Q we finish infection of a rectangle $P_i \in \text{Rec}(s_i, t_i)$. Set $k = j_0 + 1$ and, for $i = j_0 + 1, j_0 + 2, \dots, r$, build Q' using the following procedure, in which our aim is to ensure that at each step $j > j_0$ the rectangles $P'_j \in \text{Rec}(s'_j, t'_j)$ which we obtain in the generalized process satisfy $s'_j \geq t'_j$, which allows us to eliminate all occurrences of Move 5 (for an example of this procedure see Figure 2.9):

(1) If $m_i = 4$ or $m_i = 7$ put $m'_k = m_i$, $x_k = 1$ and increase k by 1.

(2) If $m_i = 6$ and $s_i \geq t_i$ put $m'_k = 6$, $x_k = 1$ and increase k by 1.

(3) If $m_i = 5$ and $s_i \geq t_i$ put $m'_k = 4$, $m'_{k+1} = 6$, $x_k = x_{k+1} = 1/2$ and increase k by 2; note that in the generalized process this pair of fractional moves takes $(s_{i-1} + t_{i-1} + 1)/2 - 3/8 + (2(s_{i-1} + 1) - 1)/2 = 3s_{i-1}/2 + t_{i-1}/2 + 5/8$ steps, while the original Move 5 takes $s_{i-1} + t_{i-1} + 1$ steps which is less than the former value as we must have $t_{i-1} \leq s_{i-1} - 1$.

(4) If $m_i = 5$ or $m_i = 6$, and $s_{i-1} = t_{i-1}$ then
   - redefine Q by, for $i \leq \ell \leq r$, changing each $m_\ell = 4$ to 5, $m_\ell = 5$ to 4, $m_\ell = 6$ to 7 and $m_\ell = 7$ to 6,
   - note that after this "mirror reflection" the spanning time of Q does not change,
   - as now $m_i = 4$ or $m_i = 7$ put $m'_k = m_i$, $x_k = 1$ and increase k by 1.

(5) If $m_i = 6$, $s_{i-1} = t_{i-1} + 2$ (and so $s_i = t_i - 1$) then
   - redefine Q by setting $m_i = 5$ so that $s_i = t_i + 1$ and, for $i + 1 \leq \ell \leq r$, by changing each $m_\ell = 4$ to 5, $m_\ell = 5$ to 4, $m_\ell = 6$ to 7 and $m_\ell = 7$ to 6,
   - note that both new and old Move m_i takes $2s_{i-1} - 1$ time steps and that after this modification Q still spans $[n]^2$ in maximum time,
   - put $m'_k = 4$, $m'_{k+1} = 6$, $x_k = x_{k+1} = 1/2$ and increase k by 2; note that in the generalized process this pair of fractional moves takes strictly more steps than the original Move 5.

(6) Finally we show that the only missing case $m_i = 6$, $s_{i-1} = t_{i-1}+1$ and $s_i = t_i - 2$ cannot occur: if it did then we could increase the spanning time of Q by 1 step, contradicting its maximality, by applying the following modifications:
  - redefine Q by setting $m_i = 4$ and, for $i+1 \le \ell \le r$, by changing each $m_\ell = 4$ to 5, $m_\ell = 5$ to 4, $m_\ell = 6$ to 7 and $m_\ell = 7$ to 6,
  - note that now $s_i = t_i + 2$ and that after this "mirror reflection" Q still spans $[n]^2$,
  - new Move m_i takes $s_{i-1}+t_{i-1}+1 = 2s_{i-1}$ time steps while the old Move m_i took $2s_{i-1} - 1$ time steps; further steps take the same time as before thus Q could not be a scheme.

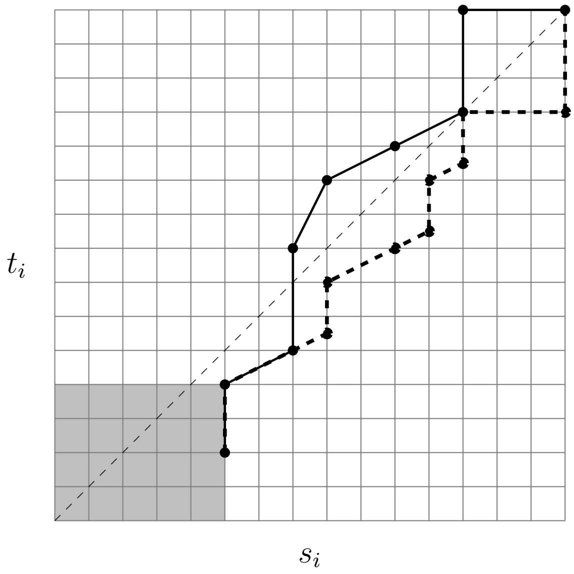


FIGURE 2.9. Example of the generalized infection process for $n = 15$. Circular marks depict dimensions of rectangles $P_i \in \mathrm{Rec}(s_i, t_i)$ and $P'_i \in \mathrm{Rec}(s'_i, t'_i)$ obtained after consecutive moves. In this example we have a triple (which is not a scheme for $M(15)$ but we use it for demonstration purpose) $Q = (5, 2, 34654467)$ (solid line) and its modification $Q' = (2, 5, 3(4,1)(4,1/2)(6,1/2)(4,1)(4,1/2)(6,1/2)(4,1/2)(6,1/2)(7,1)(6,1))$ (dashed line); note that here $j_0 = 1$, $s_{j_0} = 5$ and $t_{j_0} = 4$ (shaded rectangle represents the rectangle P_{j_0}).

We do not have any occurrences of Move 5 in Q' and Move 4s, 6s and 7s occur in multiples of 1/2, i.e., all x_i's are either 1/2 or 1. In Table 4 we show that wanting to maximize infection time we should keep the order of half–moves as suggested in Figure 2.7. That is, we should have Move 7s followed by 4s and finally by 6s.

	$m'_i = 4$	$m'_i = 6$	$m'_i = 7$
$m'_{i-1} = 4$	$k + \ell - 2$	$(3k + \ell)/2 - 15/8$	$(k + 3\ell)/2 - 15/8$
$m'_{i-1} = 6$	$(3k + \ell)/2 - 17/8$	$2k - 1$	$k + \ell - 5/2$
$m'_{i-1} = 7$	$(k + 3\ell)/2 - 13/8$	$k + \ell - 5/2$	$2\ell - 1$

TABLE 4. Time taken by consecutive half–Moves $(m'_{i-1}, 1/2)(m'_i, 1/2)$, assuming that $P'_i \in \mathrm{Rec}(k, \ell)$.

Thus we obtain $Q'' = (s_0, 2, m_1 \dots m_{j_0}(7, x)(4, y)(6, z))$, for some $x, y, z \in [0, \infty)$, which takes at least as long to infect $[n]^2$ in our generalized infection process as a scheme Q solving $M(n)$ does in bootstrap percolation. Denote the rectangle that we obtain when we apply Move $(7, x)$ to P_{j_0} by $P_{j_0+x} \in \mathrm{Rec}(s, t)$ and note that we must have $y = (n - s)/2$ and $z = (n - t - (n - s)/2)/3$. Recall that $P_{j_0} \in \mathrm{Rec}(s_{j_0}, t_{j_0})$, with $t_{j_0} \leq 7$, and therefore $s = s_{j_0} + 3x$ and $t = t_{j_0} \leq 7$. To bound the spanning time of Q'' from above, we may start by being generous and saying that $M(P_{j_0+x}) \leq st \leq 7s$; then we compute the time needed to apply Move $(4, y)$ and Move $(6, z)$. We conclude that the percolation time of Q'' can be bounded from above by

$$st + \frac{(n-s)}{2}(t+s+1) + \frac{3}{2}\frac{(n-s)}{2}\frac{(n-s-2)}{2} + \frac{(n-t-\frac{n-s}{2})}{3}(2n-1) \leq$$

$$\leq 7s + \frac{(n-s)(s+8)}{2} + \frac{3(n-s)(n-s-2)}{8} + \frac{(n+s)(2n-1)}{6} = f_n(s).$$

Maximizing $f_n(s)$ over $0 \leq s \leq n$ we find that its maximum is $f(\frac{n+43}{3}) = \frac{13}{18}n^2 + \frac{77}{18}n + \frac{1849}{72}$. That gives an upper bound on $M(n)$ and therefore completes the proof of Theorem 2.1. $\square$

2.5. Maximum percolation time in all dimensions

In this section we show that, for all $d \geq 2$, maximum percolation time in 2-neighbour bootstrap percolation in $[n]^d$ grows like a quadratic function of n.

We do not make any attempts at optimizing our bounds. However, our result allows us to formulate Conjecture 2.20 which we hope will be a starting point for further research in this area.

2.5.1. Notation. Given a site $v \in [n]^d$ and a number $t \in \mathbb{N} \cup \{0\}$, let $\mathrm{B}_v(t)$ be the l_1 discrete ball of radius t in $[n]^d$ centred at v, i.e.,

$$\mathrm{B}_v(t) = \{u \in [n]^d : \mathrm{dist}(u, v) \leq t\}.$$

Let $e_i = (0, \ldots, 0, 1, 0, \ldots, 0) \in \mathbb{Z}^d$, where 1 appears only in the i-th coordinate. Given two d-dimensional vectors $a = (a_i)_{i=1}^d$ and $b = (b_i)_{i=1}^d$ let $a + b = (a_i + b_i)_{i=1}^d$. Given two sets A and B of d-dimensional vectors let $A + B = \{a + b : a \in A, b \in B\}$. Finally, given $a = (a_i)_{i=1}^d$ and $c \in \mathbb{R}$ let $c \cdot a = (ca_i)_{i=1}^d$.

Let $[n_1, n_2] = \{n_1, n_1+1, \ldots, n_2\}$ (for $n_1 > n_2$ we assume that $[n_1, n_2] = \emptyset$). A *cuboid* in $[n]^d$ is, for some choice of $1 \leq j_i \leq k_i \leq n$ for $1 \leq i \leq d$, a set of the form $\prod_{i=1}^d [j_i, k_i]$. Similarly to percolation on $[n]^2$, for 2-neighbour bootstrap percolation in d dimensions we again have a nice characterization of closed sets.

FACT 2.13. *Given any set A of infected sites in $[n]^d$, $\langle A \rangle$ is a union of cuboids such that any distinct two of them are at distance at least* 3.

PROOF. This fact for general d follows by the same argument as Fact 1.5 for $d = 2$. The set A can be viewed as a union of $1 \times 1 \times \ldots \times 1$ cuboids. Also, any two fully infected cuboids within distance at most 2 span the minimal cuboid containing them both. Thus, in this "cuboid process" in which we replace a union of two infected cuboids at distance at most 2 by the minimal cuboid containing them both, at each step we decrease the number of cuboids. Therefore, trying to write $\langle A \rangle$ as a union of cuboids with the minimal number of cuboids, in finitely many steps we obtain a union of cuboids such that any distinct two of them are at distance at least 3. $\square$

The next proposition (see Lemma 2.3 in [**12**]), which is a d-dimensional analogue of Proposition 1.6, will be our main tool in bounding the percolation time from above.

Proposition 2.14. *Let C be a d-dimensional cuboid with volume at least* 2*. Suppose that C is internally spanned by a set of sites A. Then there exist disjoint subsets of A, say A' and A'', and cuboids C' and C'' such that:*

1. *$C' \subsetneq C$ and $C'' \subsetneq C$,*
2. *C' is internally spanned by A' and C'' is internally spanned by A'',*
3. *$\langle C' \cup C'' \rangle = C$; in particular, $\mathrm{dist}(C', C'') \le 2$.*

Proof. This proposition for general d follows by the same argument as Proposition 1.6 for $d = 2$ so we leave it without proof. □

Let $T_n^d(A)$ denote the time that A takes to percolate in $[n]^d$ under 2-neighbour bootstrap percolation, so that $T(A) = T_n^2(A)$. Then the maximum percolation time in 2-neighbour bootstrap percolation in $[n]^d$ is

$$M^d(n) = \max\{T_n^d(A) : \langle A \rangle = [n]^d\}$$

so that $M(n) = M^2(n)$. The following theorem is the main result of Section 2.5.

Theorem 2.15.

$$\frac{d^2 - d}{3} n^2 + O(n) \le M^d(n) \le \frac{d^2}{2} n^2 + O(n).$$

2.5.2. Quadratic percolation time. As usual, we prove the lower bound on $M^d(n)$ by giving a specific family of percolating sets. To prove the upper bound on $M^d(n)$ we use the following lemma.

Lemma 2.16. *Let $C, C_1, C_2 \subset [n]^d$ be cuboids in $[n]^d$ such that $\langle C_1 \cup C_2 \rangle = C$. Let $A_0 = C_1 \cup C_2$. Then there exists $v \in C$ such that for all $t \ge 0$ we have $\mathrm{B}_v(t) \cap C \subset A_{t+1}$.*

PROOF. Let $C = \prod_{i=1}^{d}[x_i, y_i]$, $C_1 = \prod_{i=1}^{d}[a_i, b_i]$ and $C_2 = \prod_{i=1}^{d}[c_i, d_i]$. Since $\langle C_1 \cup C_2 \rangle = C$, for all $1 \le i \le d$ we must have $\min\{a_i, c_i\} = x_i$ and $\max\{b_i, d_i\} = y_i$. Also, unless $C_1 \cup C_2 = C$ (in which case the lemma is trivial) there must exist some $v = (v_i)_{i=1}^{d} \in C$ such that $\operatorname{dist}(v, C_1) = \operatorname{dist}(v, C_2) = 1$.

CLAIM 2.17. *For any $i \in [d]$ and any $k \in [x_i - v_i, y_i - v_i]$ we have $v + k \cdot e_i \in A_{k+1}$.*

Proof of Claim. The claim holds for any i and $k = 0$ since $\operatorname{dist}(v, C_1) = \operatorname{dist}(v, C_2) = 1$. Note that, since the site v is adjacent to both cuboids C_1 and C_2, in whichever direction we go from v, we are initially either "inside" C_1 or C_2, or we remain adjacent to one of the faces of at least one of these cuboids. For contradiction, fix i and assume that $1 \le k \le y_i - v_i$ is the smallest number such that $v + k \cdot e_i$ is neither inside nor adjacent to any of C_1 or C_2. Then, knowing that $C_1, C_2 \subset C$ are cuboids in $[n]^d$, we could conclude that $\max\{b_i, d_i\} < v_i + k \le y_i$. However, this would contradict the fact that $\langle C_1 \cup C_2 \rangle = C$. We deal with $x_i - v_i \le k \le -1$ analogously. Thus the claim holds by induction on k. □

From the claim it follows that all sites at distance 1 from v belong to A_2. To prove the lemma it is now enough to notice that any site z in C with $\operatorname{dist}(z, v) = t + 1 \ge 2$, not of the form $v \pm (t + 1) \cdot e_i$, has at least 2 neighbours in C at distance t from v which by induction belong to A_{t+1}, so $z \in A_{t+2}$. Thus the lemma follows. □

COROLLARY 2.18. *Let $C_1, C_2 \subset [n]^d$ be cuboids in $[n]^d$ such that $\langle C_1 \cup C_2 \rangle = C \subseteq [n]^d$ with $C = \prod_{i=1}^{d}[j_i, k_i]$. Let $A_0 = C_1 \cup C_2$. Then $A_t = C$ for some $t \le \sum_{i=1}^{d}(k_i - j_i) + 1$.*

PROOF. By Lemma 2.16, infection of C ends in time equal to at most the diameter of C plus 1 time step. □

Proof of Theorem 2.15. We start by proving the upper bound on $M^d(n)$. Let A be any set of sites such that $\langle A \rangle = [n]^d$. By Proposition 2.14 there exist two cuboids $C_1, C_2 \subsetneq [n]^d$ internally spanned by disjoint subsets of A (say, C_1 by A_1 and C_2 by A_2) such that $\langle C_1 \cup C_2 \rangle = [n]^d$. By Corollary 2.18, $C_1 \cup C_2$ span $[n]^d$ in time at most $d(n-1)+1$. Let us apply the same argument to C_1: there exist two cuboids $C_1', C_2' \subsetneq C_1$ internally spanned by disjoint subsets of A_1 such that $\langle C_1' \cup C_2' \rangle = C_1$; since C_1 is a proper subset of $[n]^d$, by Corollary 2.18, $C_1' \cup C_2'$ spans C_1 in time at most $d(n-1)$. Of course, an analogous claim holds for C_2. Reapplying this argument inductively we see that $[n]^d$ is spanned in time at most

$$\sum_{i=1}^{d(n-1)+1} i = \frac{d(n-1)+2}{2}(d(n-1)+1) = \frac{d^2}{2}n^2 + O(n)$$

thus the upper bound on $M^d(n)$ is proved.

We now prove the lower bound $M^d(n) \geq \frac{d^2-d}{3}n^2 + O(n)$ with the following construction. Given $n \in \mathbb{N}$ let $n_0 = 3\lfloor \frac{n-1}{3} \rfloor + 1$. Let

$$A_1(n) = \{1, 2, \dots, n_0\}$$

and for $d \geq 1$ let

$$\begin{aligned} A_{d+1}(n) = \{&(a_1, a_2, \dots, a_d, 1) : (a_1, a_2, \dots, a_d) \in A_d\} \\ &\cup \left\{ (n_0, n_0, \dots, n_0, 3j), (1, 1, \dots, 1, 3j+1) : j = 1, 2, \dots, \frac{n_0 - 1}{3} \right\}. \end{aligned}$$

Then clearly $\langle A_{d+1} \rangle = [n_0]^{d+1}$.

LEMMA 2.19. *For any $d \geq 2$ and $n \in \mathbb{N}$ we have*

$$T_{n_0}^d(A_d(n)) = T_{n_0}^{d-1}(A_{d-1}(n)) + \frac{n_0 - 1}{3}(2(d-1)(n_0 - 1) + 1)$$

with $\{n_0\}^d$ becoming infected at time $T_{n_0}^d(A_d(n))$.

PROOF. Note that for all $d \geq 2$ the copy of $A_{d-1}(n)$ contained in $A_d(n)$ by itself spans the subcube $[n_0]^{d-1} \times \{1\}$ of $[n]^d$. Also, all other sites in $A_d(n)$ are at distance at least 2 from $[n_0]^{d-1} \times \{1\}$ and so they cannot interfere with the process of infecting it. Moreover, since the site $\{n_0\}^{d-1} \times \{3\}$ is at distance 2 from $\{n_0\}^{d-1} \times \{1\}$ and all other sites in $A_d(n)$ outside $[n_0]^{d-1} \times \{1\}$ are actually at distance at least 3 from $[n_0]^{d-1} \times \{1\}$, no site outside $[n_0]^{d-1} \times \{1\}$ becomes infected before or at the same time as $\{n_0\}^{d-1} \times \{1\}$.

Thus if $\{n_0\}^{d-1} \times \{1\}$ becomes infected at time $T^{d-1}_{n_0}(A_{d-1}(n))$ (and this is true for $d = 2$ with $T^1_{n_0}(A_1(n)) = 0$) then the infection of $[n_0]^{d-1} \times [2, n_0]$ starts only after $T^{d-1}_{n_0}(A_{d-1}(n))$ time steps. To infect a "new" dth dimension $A_d(n)$ infects $\frac{n_0-1}{3}$ stripes of the form $[n_0]^{d-1} \times [3(i-1)+2, 3i+1]$. The infection of the first such stripe goes at follows: on the first step the site $\{n_0\}^{d-1} \times \{2\}$ becomes infected and then, on step $t \geq 2$, all sites in $[n_0]^{d-1} \times \{2, 3\}$ at distance $(t-1)$ from $\{n_0\}^{d-1} \times \{2\}$ become infected. After infecting all sites in $[n_0]^{d-1} \times \{2, 3\}$ except $\{1\}^{d-1} \times \{3\}$, which takes $(d-1)(n_0-1)+1$ steps, all neighbours of $\{1\}^{d-1} \times \{4\}$ in $[n_0]^{d-1} \times \{4\}$ gain their second infected neighbour and the infection of $[n_0]^{d-1} \times \{4\}$ follows. All sites at distance $t \geq 1$ from $\{1\}^{d-1} \times \{4\}$ in $[n_0]^{d-1} \times \{4\}$ become infected at step $(d-1)(n_0-1)+1+t$. Thus it takes $2(d-1)(n_0-1)+1$ to fully infect $[n_0]^d \times [2, 4]$ and there are $\frac{n_0-1}{3}$ such stripes to infect, thus the lemma follows since clearly $\{n_0\}^d$ is the last site to become infected in $[n_0]^d$. □

If $n \neq 3k+1$ for some $k \in \mathbb{N} \cup \{0\}$ then we have $n_0 < n$ (but we still have $n_0 \geq n-2$). In that case, let

$$\tilde{A}_d(n) = A_d(n) \cup \left([n_0+1, n]^2 \times [n_0, n]^{d-2}\right).$$

Then $\left\langle \tilde{A}_d \right\rangle = [n]^d$ and the additional initially infected sites in $\tilde{A}_d(n)$ to not accelerate the infection of the sites in $[n_0]^d$. Thus, by Lemma 2.19,

$$\begin{aligned} M^d(n) \geq T^d_n(\tilde{A}_d(n)) \geq T^d_{n_0}(A_d(n)) \\ \geq \frac{(d^2-d)(n-3)^2 + (d-1)(n-3)}{3} \\ = \frac{d^2-d}{3} n^2 + O(n). \end{aligned}$$

This completes the proof of Theorem 2.15. □

2.6. Further questions

In this chapter we give the asymptotic formula for the maximum percolation time in the grid $[n]^2$ under 2-neighbour bootstrap percolation. We also prove that in $[n]^d$ we have

$$\frac{d^2-d}{3}n^2+O(n)\leq M^d(n)\leq \frac{d^2}{2}n^2+O(n).$$

This motivates the following natural conjecture.

Conjecture 2.20. *We have $M^d(n) = c_d n^2 + O(n)$, where c_d is some constant depending on d only.*

In this chapter we proved that $c_2 = 13/18$. If Conjecture 2.20 is correct then it would be interesting to analyse the behaviour of the constants c_d as d grows.

Problem 2.21. *If Conjecture 2.20 is correct, determine the growth of the function $f(d) = c_d$.*

Another natural question which we leave for further work is the one about the maximum percolation time for higher infection thresholds in $[n]^d$.

Question 2.22. *What is the maximum percolation time in r-neighbour bootstrap percolation on $[n]^d$ for $r \geq 3$?*

2.7. Appendix: analysis of small cases

Assume that $(s_0, t_0, m_1m_2\dots m_r)$ is a scheme for $M(k,\ell)$ for $k,\ell \geq 3$, $(k,\ell)\neq(3,3)$. Let A be a (k,ℓ)-perfect set described by it and let $P_0 \subset P_1 \subset \dots \subset P_r \in \mathrm{Rec}(k,\ell)$ be the sequence of rectangles associated with A. We treat a number of small cases to exclude some, a priori possible, values for the numbers s_0 and t_0.

Suppose for a contradiction that $P_0 \in \mathrm{Rec}(s,1)$. Since $P_1 \in \mathrm{Rec}(s_1,t_1)$ where $s_1, t_1 \geq 3$ and $\max\{s_1,t_1\} \geq 4$, one of the following cases must occur:

(1) $P_1 \in \mathrm{Rec}(s,3)$ with $s \geq 4$: since we have $M(s-1,2) \geq 3$, by applying Move 1 to $[s-1] \times [2]$ we see that $M(s,3) \geq (s-1)+3 = s+2$. However, for $P_0 \in \mathrm{Rec}(s,1)$ and $P_1 \in \mathrm{Rec}(s,3)$, as in the infection process defined by A, it takes time at most $s+1$ to infect all sites in P_1 since both ending sites of the rectangle P_0 must be initially infected. This contradicts the fact that at every step i the time that A takes to percolate P_i is maximum;

(2) $P_1 \in \mathrm{Rec}(s+1,3)$ with $s \geq 3$: since we have $M(s,2) \geq 3$, by applying Move 1 to $[s] \times [2]$ we see that $M(s+1,3) \geq s+3$. However, for $P_0 \in \mathrm{Rec}(s,1)$ and $P_1 \in \mathrm{Rec}(s+1,3)$, as in the infection process defined by A, it takes time at most $s+2$ to infect all sites of P_1 (by the same argument as above). This again contradicts the fact that A is (n,n)-perfect;

(3) $P_1 \in \mathrm{Rec}(s,4)$ with $s \geq 3$: since we have $M(s,2) \geq s$, by applying Move 3 to $[s] \times [2]$ we see that $M(s,4) \geq s+s+1 = 2s+1$. However, for $P_0 \in \mathrm{Rec}(s,1)$ and $P_1 \in \mathrm{Rec}(s,4)$, as in the infection process defined by A, using again the same argument it takes time at most $2s-1$ to infect all sites of P_1. This contradicts the fact that A is (n,n)-perfect.

Thus, we may assume that $P_0 \notin \mathrm{Rec}(s,1)$. We deal with $P_0 \in (1,t)$ analogously. Suppose now that $P_0 \in \mathrm{Rec}(3,3)$. Considering $P_1 \in \mathrm{Rec}(s_1,t_1)$ up to symmetries one of the following cases must occur:

(1) $P_1 \in \mathrm{Rec}(6,3)$: by applying Move 7 it takes time 5 to infect P_1 after P_0 is fully infected. This procedure takes time at most $M(3)+5 = 9$ to infect P_1. However, by applying Move 1 to $[5] \times [2]$ we see that $M(6,3) \geq M(5,2)+5 = 6+5 = 11$; this contradicts the fact that A is (n,n)-perfect;

(2) $P_1 \in \mathrm{Rec}(5,4)$: by applying Move 4 it takes time 7 to infect P_1 after P_0 is fully infected. This procedure takes time at most $M(3)+7 = 11$ to infect P_1. However, by applying Move 3 to $[5] \times [2]$ we see that

$M(5,4) \geq M(5,2) + 6 = 6 + 6 = 12$; this contradicts the fact that A is (n,n)-perfect;

(3) $P_1 \in \mathrm{Rec}(4,4)$: by applying Move 1 it takes time 3 to infect P_1 after P_0 is fully infected. This procedure takes time at most $M(3) + 3 = 7$ to infect P_1. However, by applying Move 3 to $[4] \times [2]$ we see that $M(4) \geq M(4,2) + 5 = 9$; this contradicts the fact that A is (n,n)-perfect;

(4) $P_1 \in \mathrm{Rec}(5,3)$: by applying Move 2 it takes time 4 to infect P_1 after P_0 is fully infected. This procedure takes time at most $M(3)+4 = 8$ to infect P_1. By applying Move 1 to $[4] \times [2]$ we also take time $M(4,2) + 4 = 8$. Although this does not contradict the (n,n)-perfectness of A, we can replace it by an (n,n)-perfect set A' whose infection process starts with a $P_0' \in \mathrm{Rec}(4,2)$ and expands to P_1, so that A' takes the same time to percolate in $[n]^2$ as A.

Thus, we may assume that $P_0 \notin \mathrm{Rec}(3,3)$. Therefore we have $P_0 \in \mathrm{Rec}(s,2) \cup \mathrm{Rec}(2,s)$ for some $s \geq 3$.

CHAPTER 3

Maximum percolation time in hypercubes

3.1. Introduction

In this chapter we consider yet another extremal problem in bootstrap percolation, posed by Bollobás. Namely, we study 2-neighbour bootstrap percolation on the n-dimensional hypercube Q_n, which we define precisely in Section 3.2, and again we look at extremal properties of the infection process when a set of initially infected sites is chosen in a deterministic way in order to maximize percolation time. As the main result of this chapter, we prove the following theorem.

THEOREM 3.1. *If $A \subset Q_n$ percolates, i.e., if $\langle A \rangle = Q_n$, then it percolates in at most $\left\lfloor \frac{n^2}{3} \right\rfloor$ steps. Moreover, this bound is tight for all $n \in \mathbb{N}$*

In other words, if in the definition of bootstrap percolation given in (1.1) we set $r = 2$, $A_0 = A$ and $G = Q_n$, then $A_t = Q_n$ for some $t \leq \left\lfloor \frac{n^2}{3} \right\rfloor$ whenever $\langle A \rangle = Q_n$. For $n \in \{1, 2, 3, 4\}$ sets obtaining the maximum percolation time can by found by exhaustive search. For $n \geq 5$ a family of optimal sets can be described as follows: a set A infecting Q_n in the maximum possible time consists of a small set initializing the process by infecting Q_2 if $n = 2$ (mod 3), Q_3 if $n = 0$ (mod 3) or Q_4 if $n = 1$ (mod 3) in the maximum time, and of pairs of sites each of which prolongs the process by infecting three "additional" dimensions in the maximum possible time. Details of this construction can be found in the proof of Theorem 3.14.

This chapter is solo work, and is based on my paper, [**47**].

3.2. Notation and basic observations

Let $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$. The n-dimensional hypercube Q_n is the graph with vertex set $\{0,1\}^n$ and edge set $\{\{x, y\} : x, y \in \{0,1\}^n, |\{i : x_i \neq y_i\}| = 1\}$. We shall write Q_l for any of the $\binom{n}{l} 2^{n-l}$ subcubes of dimension l in Q_n. For $x = (x_i)_1^n \in \{0, 1, *\}^n$, let Q^x be the subcube $\{z = (z_i)_1^n \in \{0,1\}^n : z_i = x_i \text{ if } x_i \neq *\}$. Clearly, $x \mapsto Q^x$ gives a $1-1$ correspondence between $\{0, 1, *\}^n$ and the subcubes of Q_n. Let $d(0, 1) = 1$, $d(0, 0) = d(1, 1) = d(*, *) =$

$d(0,*) = d(1,*) = 0$ be the distance of two coordinates. The *distance* of two subcubes Q^x, Q^y in Q_n is $d(Q^x, Q^y) = \sum_{i=1}^n d(x_i, y_i)$, where vectors x, y represent subcubes Q^x and Q^y. In the hypercube graph the distance between sets Q^x, Q^y is also $d(Q^x, Q^y)$.

For $p, q \in \mathbb{N}$ and $y_0, y_1, \ldots, y_p \in \{0, 1, *\}$ we denote by $[y_0]^q$ the sequence $(y_0, y_0, \ldots, y_0)$ of length q, and by $\overline{(y_1 y_2 \ldots y_p)}$ the set of all permutations of the multiset $\{y_1, \ldots, y_p\}$. We use a self explanatory notation to concatenate and nest such sequences, e.g.,

$$[0]^2\overline{([*]^2[1]^2)}0 = \{00{*}{*}110, 00{*}1{*}10, 00{*}11{*}0, 001{*}{*}10, 001{*}1{*}0, 0011{*}{*}0\}.$$

From now on let us consider 2-neighbour bootstrap percolation only. Recall that a set A is said to be closed under percolation if $\langle A \rangle = A$. Let us recall some simple results from Balogh and Bollobás [**8**], where the authors gave bounds on $p_c(Q_n, 2)$, the critical probability in 2-neighbour bootstrap percolation on the hypercube.

Lemma 3.2. *The only subsets of a hypercube that are closed under percolation are those which are a union of disjoint subcubes that are at distance at least 3 from each other.*

Proof. The lemma is equivalent to Fact 2.13. □

For vectors $x, y \in \{0, 1, *\}^n$ set $x \vee y = z = (z_i)$ where $z_i = x_i$ if $x_i = y_i$ and $*$ otherwise. It follows from the definition of $\vee$ that $Q^x, Q^y \subset Q^z$.

Lemma 3.3. *For any two vectors $x, y \in \{0, 1, *\}^n$ with $d(x, y) \leq 2$ we have $\langle Q^x \cup Q^y \rangle = Q^{x \vee y}$.*

□

Analogously to bootstrap percolation on grids, given an infection process on Q_n with an initial set $A \subset Q^n$, a subcube $Q_l \subset Q_n$ is said to be *internally spanned* if the restriction of the process to Q_l fully infects Q_l, i.e., if $\langle A \cap Q_l \rangle = Q_l$.

Lemma 3.4. *Let* $A \subset Q_n$ *be such that* $\langle A\rangle = Q_n$. *Then there is a nested sequence* $Q_0 = Q_{i_1}^{x_{i_1}} \subset Q_{i_2}^{x_{i_2}} \subset \ldots \subset Q_{i_t}^{x_{i_t}} = Q_n$, *of internally spanned subcubes (with respect to* A*), where* $2i_j + 2 \geq i_{j+1}$ *for all* j, $0 \leq j \leq t-1$. *Furthermore, for* $j \geq 2$ *each subcube* $Q_{i_j}^{x_{i_j}}$ *is spanned by two internally spanned cubes, namely by* $Q_{i_{j-1}}^{x_{i_{j-1}}}$ *and a subcube* $Q_{m_{j-1}}$ *of dimension* $m_{j-1} \leq i_{j-1}$ *which is not a member of the sequence.*

□

We call a longest nested sequence of internally spanned cubes as in Lemma 3.4 a *building sequence* of the hypercube. For a vector $x \in \{0,1,*\}^n$ we define the *dimension* of x as $\dim(x) = |\{i : x_i = *\}|$. Obviously, $\dim(x)$ equals $\dim(Q^x)$, the dimension of the cube Q^x.

For the sake of consistency with the notation introduced in Section 2.5.1, let $T_{Q_n}(A) = T_2^n(A) = \min\{t : A_t = Q_n\}$, where the sets A_t are defined as in (1.1). Throughout this chapter we shall shall refer to $T_{Q_n}(A)$ as to the *spreading time* of A in Q_n. Finally we define the maximum percolation time in the n-dimensional hypercube Q_n as

$$M_H(n) = \max_{A:\langle A\rangle = Q_n} T_{Q_n}(A).$$

3.3. Slow percolation in hypercubes

In this section we shall prove that $M_H(n) = \lfloor \frac{n^2}{3} \rfloor$ for all $n \in \mathbb{N}$. We start with the following simple lemma.

Lemma 3.5. *For any* $n \in \mathbb{N}$, $M_H(n) \leq M_H(n+1)$.

Proof. Let A be such that $\langle A\rangle = Q_n$ and $T_{Q_n}(A) = M_H(n)$. Let

$$\tilde{A} = \{(a_1,\ldots,a_n,j) : (a_1,\ldots,a_n) \in A \text{ and } j \in \{0,1\}\}.$$

Then $\left\langle \tilde{A} \right\rangle = Q_{n+1}$ and $M_H(n) = T_{Q_n}(A) = T_{Q_{n+1}}(\tilde{A}) \leq M_H(n+1)$. □

We shall now define a specific norm which at first sight might not be intuitive and might seem odd. However, due to the symmetries of the hypercube we shall highly benefit from it and not lose any generality by considering this particular norm. In the following series of lemmas, which will help us understand how infection spreads in Q_n depending on the configuration of the set of initially infected sites, the reader should think of the particular norm of x as a quantity that reflects (but is not always equal to) the sum of distances between x and S and between x and T. These six lemmas will be summarized in Lemma 3.12.

Let $n \in \mathbb{N}$ and $s, n_1, \ldots, n_s, d \in \mathbb{N}_0$ with $n \geq n_1 + \ldots + n_s + d$. For each $x \in \{0,1\}^n$ set

$$\|x\|_{n_1,\ldots,n_s}^{a_1\ldots a_d} = \begin{cases} \sum_{i=1}^{n-d} x_i, & \text{if } \sum_{j=n_1+\ldots+n_{i-1}+1}^{n_1+\ldots+n_i} x_j > 0 \text{ for all } i \in [s] \text{ with } n_i > 0 \\ & \qquad\qquad \text{and } x_{n-d+i} = a_i \text{ for all } i \in [d], \\ 0, & \text{otherwise.} \end{cases}$$

Note that, setting $s = 0$,

$$\|x\|^{a_1\ldots a_d} = \left(\sum_{i=1}^{n-d} x_i\right)\left(\prod_{i=1}^{d} \mathbb{1}_{\{x_{n-d+i}=a_i\}}\right),$$

so that, setting $s = d = 0$, $\|x\| = \sum_{j=1}^{n} x_j$. Note crucially that $\|x\|_{n_1,\ldots,n_s}^{a_1\ldots a_d} > 0$ only if x has at least one 1 in each of the sequences $(x_{n_1+\ldots+n_{i-1}+1}, \ldots, x_{n_1+\ldots+n_i})$ for each $i = 1, \ldots, s$ with $n_i > 0$ and the last d terms of $(x_1, \ldots, x_n)$ are $(a_1, \ldots, a_d)$.

LEMMA 3.6. *Let $k, l \in \mathbb{N}_0$, $n = k + l$, and set $S = [*]^k[0]^l$ and $T = [0]^k[*]^l$ and $A_0 = S \cup T$. Then*

$$A_t \supset \{x \in \{0,1\}^n : \|x\| \leq t+1\} = \overline{([*]^{t+1}[0]^{k+l-t-1})}$$

for every $t \in \mathbb{N}$.

PROOF. By induction on t, noting that $\|x\| \leq 1$ implies $x \in A_0$, and that every $x \in \{0,1\}^n$ with $\|x\| = t+1 \geq 2$ has at least two neighbours y with $\|y\| = t$. $\square$

LEMMA 3.7. *Let* $k, l \in \mathbb{N}_0$, $n = k + l + 1$, *and set* $S = [*]^k[0]^{l+1}$ *and* $T = [0]^k[*]^l1$ *and* $A_0 = S \cup T$. *Then*

$$\begin{aligned} A_t &\supset \big([0]^{k+l}*\big) \cup \big\{x \in \{0,1\}^n : 1 \leq \|x\|^0 \leq t \text{ or } 1 \leq \|x\|^1 \leq t\big\} \\ &= \overline{([*]^t[0]^{k+l-t})}0 \cup \overline{([*]^t[0]^{k+l-t})}1 \end{aligned}$$

for every $t \in \mathbb{N}$.

PROOF. Clearly we have $[0]^{k+l}* \subset S \cup T = A_0$. We shall show that both $\|x\|^0 = 1$ and $\|x\|^1 = 1$ imply $x \in A_1$. If $\|x\|^1 = 1$ then either $x \in T \subset A_0$ or $x_j = 1$ for some $1 \leq j \leq k$. In the latter case x has two neighbours in A_0: one is $[0]^{k+l}1$ (obtained by changing x_j to 0) and one is in S (obtained by changing x_n to 0), thus $x \in A_1$. In the same way we prove that $\|x\|^0 = 1$ implies $x \in A_1$.

Now we proceed by induction noting that every $x \in \{0,1\}^n$ with $\|x\|^1 = t + 1 \geq 2$ has at least two neighbours y with $\|y\|^1 = t$ and analogously for $\|x\|^0 = t + 1 \geq 2$. ☐

LEMMA 3.8. *Let* $k, l \in \mathbb{N}_0$, $n = k + l + 2$, *and set* $S = [*]^k[0]^{l+2}$ *and* $T = [0]^k[*]^l11$ *and* $A_0 = S \cup T$. *Then*

$$A_1 \supset [0]^{k+l} * *$$

and

$$\begin{aligned} A_t \supset\; &\big\{x \in \{0,1\}^n : 1 \leq \|x\|^{01} \leq t-1 \text{ or } 1 \leq \|x\|^{10} \leq t-1\big\} \\ &\cup \big\{x \in \{0,1\}^n : 1 \leq \|x\|^{00} \leq t-2 \text{ or } 1 \leq \|x\|^{11} \leq t-2\big\} \\ = \; &\overline{([*]^{t-1}[0]^{k+l-t+1})}01 \cup \overline{([*]^{t-1}[0]^{k+l-t+1})}10 \cup \overline{([*]^{t-2}[0]^{k+l-t+2})}00 \\ &\cup \overline{([*]^{t-2}[0]^{k+l-t+2})}11 \end{aligned}$$

for every $t \geq 2$.

PROOF. An example of this case is shown in Figure 3.1. Clearly we have $\{[0]^{k+l+2}, [0]^{k+l}11\} \subset S \cup T = A_0$. If $x \in \{[0]^{k+l}01, [0]^{k+l}10\}$ then x has two neighbours in A_0 obtained by changing the value of one of the two last coefficients, thus $x \in A_1$. Hence $[0]^{k+l} * * \subset A_1$.

We shall show that both $\|x\|^{01} = 1$ and $\|x\|^{10} = 1$ imply $x \in A_2$. Indeed, let $\|x\|^{01} = 1$ and $x_j = 1$ for some $1 \leq j \leq k+l$. Then x has two neighbours in A_1: one is $[0]^{k+l}01$ (obtained by changing x_j to 0) and one is in $S \cup T$ (obtained by changing x_n to 0 or x_{n-1} to 1, depending on whether $j \leq k$ or not), thus $x \in A_2$. In the same way we prove that $\|x\|^{10} = 1$ implies $x \in A_2$.

Now we proceed by induction noting that every $x \in \{0,1\}^n$ with $\|x\|^{01} = t + 1 \geq 2$ has at least two neighbours y with $\|y\|^{01} = t$ and analogously for $\|x\|^{10} = t + 1 \geq 2$.

Finally we show that, for every $t \geq 3$, both $\|x\|^{00} = t-2$ and $\|x\|^{11} = t-2$ imply $x \in A_t$. This is immediate as every such x has two neighbours y and z with $\|y\|^{01} = t-2$ and $\|z\|^{10} = t-2$ which, by what we have just proved, belong to A_{t-1}. □

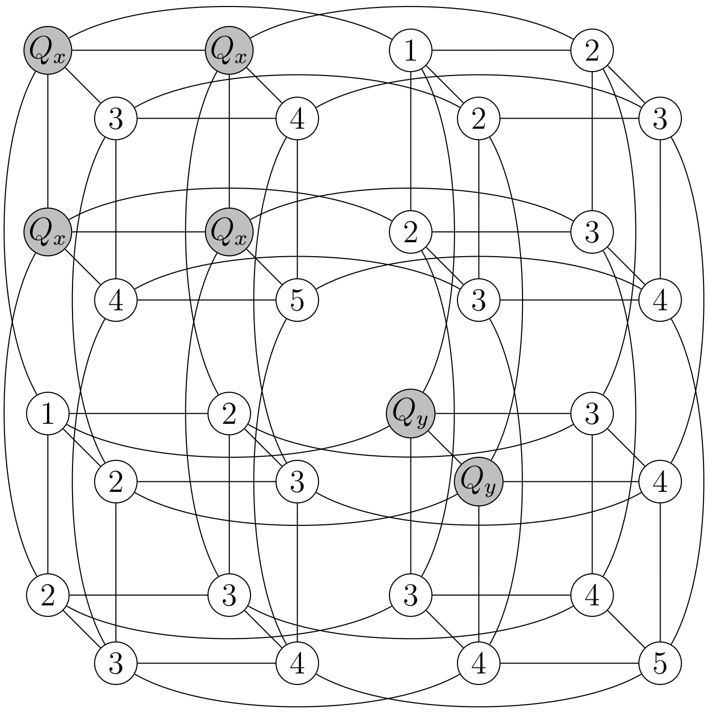


FIGURE 3.1. An example of spreading process on Q_5 for $x = **000$ and $y = 00*11$. Here $n = 5$, $k = 2$ and $l = 1$. Labels 1, 2, 3, 4 and 5 denote the time step at which vertices are infected. We see that here $T_{Q_n}(Q^x \cup Q^y) = 5$.

In the next lemma we assume $k, l > 0$ to avoid a trivial situation when $k = 0$ or $l = 0$ and $S \cup T = Q_n$.

LEMMA 3.9. *Let $k, l \in \mathbb{N}$, $n = k + l$, and set $S = [*]^k[0]^l$ and $T = [0]^k[*]^l$ and $A_0 = S \cup T$. Then*

$$A_t \cap \{x \in \{0,1\}^n : \|x\|_{k,l} \geq t + 2\} = \emptyset$$

for every $0 \leq t \leq k + l - 2$.

PROOF. By induction on t, noting that $\|x\|_{k,l} \geq 2$ implies $x \notin S \cup T = A_0$, and that for every $x \in \{0,1\}^n$ with $\|x\|_{k,l} = t + 1 \geq 3$, at most one of the neighbours y of x satisfies $\|y\|_{k,l} < t$ (there might be one neighbour z with $\|z\|_{k,l} = 0$ if $\sum_{j=1}^{k} x_j = 1$ or $\sum_{j=k+1}^{n} x_j = 1$). □

In the next lemma we avoid a trivial situation when $k = l = 0$ and $S \cup T = Q_1$ by assuming without loss of generality that $k > 0$.

LEMMA 3.10. *Let $k \in \mathbb{N}$, $l \in \mathbb{N}_0$, $n = k + l + 1$, and set $S = [*]^k[0]^{l+1}$ and $T = [0]^k[*]^l 1$ and $A_0 = S \cup T$. Then*

$$A_t \cap \left\{x \in \{0,1\}^n : \|x\|_k^1 \geq t + 1\right\} = \emptyset$$

for every $0 \leq t \leq k + l - 1$.

PROOF. By induction on t. Note first that $\|x\|_k^1 \geq 1$ implies $x \notin S \cup T = A_0$. Now, for $t \geq 1$ assume that every x with $\|x\|_k^1 \geq t$ does not belong to A_{t-1} and note that for every $x \in \{0,1\}^n$ with $\|x\|_k^1 \geq t + 1 \geq 2$, at most two of the neighbours y of x satisfy $\|y\|_k^1 < t$. These two might be w with $\|w\|_k^0 = t + 1$ obtained by changing x_n to 0 and, if $\sum_{i=1}^{k} x_i = 1$, z with $\|z\|_k^1 = 0$. We claim that z, if it exists, is not in A_{t-1}.

Indeed, for z to exist we must have $\sum_{i=1}^{k} x_i = 1$ and $\sum_{i=k+1}^{k+l} x_i = t \geq 1$, so in particular $l \geq 1$. Let z' denote the vector obtained by swapping the first k coordinates with the next l; that is,

$$z' = (z_{k+1}, \ldots, z_{k+l}, z_1, \ldots, z_k, z_{k+l+1}).$$

Then $\|z'\|_l^1 \geq t$, and so, by the case $t-1$ of the lemma (which we are assuming that we have already proved) applied to the sets $S' = [*]^l[0]^{k+1}$ and $T' = [0]^l[*]^k1$, it follows that z' is not infected after $t-1$ steps of the bootstrap process with initial set $S' \cup T'$. By symmetry (since we have only reordered the coordinates), it follows that $z \notin A_{t-1}$, as required.

Thus x can have at most one infected neighbour at time $t-1$ and therefore it does not belong to A_t. $\square$

In the next lemma we avoid a trivial situation when $k = l = 0$ and $A_1 = Q_2$ by assuming without loss of generality that $k > 0$.

LEMMA 3.11. *Let* $k \in \mathbb{N}$, $l \in \mathbb{N}_0$, $n = k+l+2$, *and set* $S = [*]^k[0]^{l+2}$ *and* $T = [0]^k[*]^l11$ *and* $A_0 = S \cup T$. *Then*

$$A_t \cap \left\{x \in \{0,1\}^n : \|x\|_k^{01} \geq t \text{ or } \|x\|_k^{10} \geq t\right\} = \emptyset$$

for every $1 \leq t \leq k+l$, *and*

$$A_t \cap \left\{x \in \{0,1\}^n : \|x\|_k^{11} \geq t-1\right\} = \emptyset$$

for every $2 \leq t \leq k+l+1$.

PROOF. Again, an example of this case is shown in Figure 3.1. Note first that $x \in [*]^{k+l}01$, $x \in [*]^{k+l}10$ and $\|x\|_k^{11} \geq 1$ each imply $x \notin S \cup T = A_0$. Also both $\|x\|_k^{01} \geq 1$ and $\|x\|_k^{10} \geq 1$ imply $x \notin A_1$ as such an x can have at most one neighbour y, obtained by changing respectively x_n and x_{n-1} to 0, in A_0. Similarly $\|x\|_k^{11} \geq 1$ implies $x \notin A_1$ as such an x can have at most one initially infected neighbour $y \in [*]^{k+l}11$ with $\|y\|_k^{11} = 0$, while all of its other neighbours y have either $\|y\|_k^{01} \geq 1$, $\|y\|_k^{10} \geq 1$ or $\|y\|_k^{11} \geq 1$. What is more, $\|x\|_k^{11} \geq 1$ implies $x \notin A_2$ as all these neighbours are not even in A_1.

Now, for $t \geq 1$ assume that every x with $\|x\|_k^{01} \geq t$ or $\|x\|_k^{10} \geq t$ does not belong to A_t and that every x with $\|x\|_k^{11} \geq t$ does not belong to A_{t+1}.

Note that for every $x \in \{0,1\}^n$ with $\|x\|_k^{01} \geq t+1$, at most three of its neighbours y satisfy $\|y\|_k^{01} < t$ which is a necessary condition to belong to A_t.

One of these three neighbours is v with $\|v\|_k^{11} = t+1 \geq 2$ obtained by changing x_{n-1} to 1, thus also $v \notin A_t$. The other two might be w with $\|w\|_k^{00} = t+1 \geq 2$ obtained by changing x_n to 0 and, if $\sum_{i=1}^k x_i = 1$, z with $\|z\|_k^{01} = 0$. We claim that z, if it exists, is not in A_t.

Indeed, for z to exist we must have $\sum_{i=1}^k x_i = 1$ and $\sum_{i=k+1}^{k+l} x_i = t \geq 1$, so in particular $l \geq 1$. We now follow steps similar to those in the proof of Lemma 3.10: let z' denote the vector obtained by swapping the first k coordinates with the next l; that is,

$$z' = (z_{k+1}, \ldots, z_{k+l}, z_1, \ldots, z_k, z_{k+l+1}, z_{k+l+2}).$$

Then $\|z'\|_l^{01} \geq t$, and so, by the case t of the lemma (which we are assuming that we have already proved) applied to the sets $S' = [*]^l[0]^{k+2}$ and $T' = [0]^l[*]^k 11$, it follows that z' is not infected after t steps of the bootstrap process with initial set $S' \cup T'$. By symmetry (since we have only reordered the coordinates), it follows that $z \notin A_t$, as required. Thus x can have at most one infected neighbour at time t and therefore it does not belong to A_{t+1}.

Finally, every $x \in \{0,1\}^n$ with $\|x\|_k^{11} = t+1 \geq 2$ has at most one neighbour y with $\|y\|_k^{11} = 0$ which might be in A_{t+1}. All other neighbours of x are either v with $\|v\|_k^{11} = t$, w with $\|w\|_k^{01} = t+1$ or y with $\|y\|_k^{10} = t+1$, none of which is in A_{t+1}. Thus $x \notin A_{t+2}$. $\square$

Let us now summarize what we know about the spreading time of $Q_k^x \cup Q_l^y$ in Q_n for particular choices of x and y.

LEMMA 3.12. *For vectors $x, y \in \{0,1,*\}^m$ such that dim$(x) = k$, dim$(y) = l$, dim$(x \vee y) = m$, where $k, l < m$, $d(x,y) = d \leq 2$, and such that $|\{i : x_i = y_i = *\}| = p$, the spreading time of $Q^x \cup Q^y$ in Q_m is given by*

$$T_{Q_n}(Q^x \cup Q^y) = \begin{cases} m-p, & \text{if } d = 2 \text{ and } (k,l) \neq (m-2, m-2), \\ m-p-1, & \text{otherwise.} \end{cases}$$

Proof. By the symmetry of the hypercube, without loss of generality assume that $l \leq k$ and that

$$x = [*]^k[0]^{m-k},\ y = [*]^p[0]^{k-p}[*]^{l-p}[1]^d.$$

Note that the first p coordinates, for which $x_i = y_i = *$, do not matter when we look at the spreading times since infection process will behave like 2^p parallel infection processes on identical $(m-p)$-dimensional subcubes which do not influence each other. Thus without loss of generality assume that $p = 0$. Then we have $m = k + l + d$ and $y = [0]^k[*]^l[1]^d$.

$d = 0$: by Lemma 3.6 we have $T_{Q_n}(Q^x \cup Q^y) \leq k + l - 1 = m - 1$ (note that in this case we must have $k, l > 0$ as $k, l < m$). Also, noting that the maximum value of the norm $\| \cdot \|_{k,l}$ in Lemma 3.9 is $k + l$, $T_{Q_n}(Q^x \cup Q^y) \geq k + l - 1 = m - 1$.

$d = 1$: by Lemma 3.7 we have $T_{Q_n}(Q^x \cup Q^y) \leq k + l = m - 1$. Also, noting that the maximum value of the norm $\| \cdot \|_k^1$ in Lemma 3.10 is $k + l$, $T_{Q_n}(Q^x \cup Q^y) \geq k + l = m - 1$. Note that if $k = l = 0$ then $m = 1$ and the formula on $T_{Q_n}(Q^x \cup Q^y)$ is also correct.

$d = 2$: if $(k, l) = (m - 2, m - 2) = (0, 0)$ then infection takes exactly one step and the formula for $T_{Q_n}(Q^x \cup Q^y)$ is correct. Otherwise, by Lemma 3.8, $T_{Q_n}(Q^x \cup Q^y) \leq k + l + 2 = m$. Also, noting that the maximum value of the norm $\| \cdot \|_k^{11}$ in Lemma 3.11 is $k + l$, $T_{Q_n}(Q^x \cup Q^y) \geq k + l + 2 = m$ (see Figure 3.1).

□

The next lemma will be used later to simplify a recurrence formula we shall obtain for $M_H(n)$.

Lemma 3.13. *Let* $a(1) = 0$, $a(2) = 1$, $a(3) = 3$ *and for* $n \geq 4$

$$a(n) = \max \begin{cases} a(n-2) + n, \\ a(n-3) + 2n - 3. \end{cases}$$

Then $a(n) = a(n-3) + 2n - 3$ *for all* $n \geq 4$.

PROOF. First, we immediately see that $a(4) = a(1) + 5 = a(2) + 4 = 5$. Similarly, it can be trivially checked that the lemma holds for $n \in \{5, 6\}$.

Now, we prove the lemma by induction. For $n \geq 4$ we assume that it holds for n, $n+1$ and $n+2$, and for $n+3$ we obtain

$$\begin{aligned} a(n+3) &= \max\{a(n) + 2(n+3) - 3, a(n+1) + n + 3\} \\ &= \max\{a(n-3) + 4n, a(n-2) + 3n + 2\} \\ &= a(n-3) + 4n \\ &= a(n) + 2(n+3) - 3, \end{aligned}$$

where the third equality follows from the fact that

$$\begin{aligned} a(n-3) + 4n &= a(n-3) + 2n - 3 + (2n+3) \\ &\geq a(n-2) + n + (2n+3) \\ &> a(n-2) + 3n + 2. \end{aligned}$$

□

Let us prove a recursion formula for the maximum percolation time which we shall later use to give a closed-form expression for $M_H(n)$.

THEOREM 3.14. *We have* $M_H(1) = 0$, $M_H(2) = 1$, $M_H(3) = 3$, $M_H(4) = 5$ *and for* $n \geq 5$

$$M_H(n) = \max \begin{cases} M_H(n-2) + n, \\ M_H(n-3) + 2n - 3. \end{cases}$$

PROOF. The values of $M_H(n)$ for $n \leq 4$ can be found by exhaustive search. The maximum percolation time can be obtained with the following sets of sites:

$$n = 1 : \{0, 1\},\ n = 2 : \{00, 11\},\ n = 3 : \{000, 110, 001\},$$

$$n = 4 : \{0000, 1100, 0111\}.$$

We shall first prove that for $n \geq 5$ the following holds.

$$M_H(n) \geq \max \begin{cases} M_H(n-2)+n, \\ M_H(n-3)+2n-3. \end{cases}$$

Consider the following two ways of infecting Q_n. Note that the second way corresponds to the optimal family briefly described at the end of Section 3.1.

(1) Let A^{n-2} be a set that internally spans the hypercube Q^x_{n-2} for $x = [*]^{n-2}00$ in time $M_H(n-2)$ and such that the site $[0]^n$ becomes infected at time $M_H(n-2)$. Let $\tilde{A}^{n-2} = A^{n-2} \cup [0]^{n-2}11$; then $\left\langle \tilde{A}^{n-2} \right\rangle = Q_n$ and, by Lemma 3.12 case $d = 2$, $T_{Q_n}(\tilde{A}^{n-2}) = M_H(n-2)+n$,

(2) Let A^{n-3} be a set that internally spans the hypercube Q^x_{n-3} for $x = [*]^{n-3}000$ in time $M_H(n-3)$ and such that the site $[0]^n$ becomes infected at time $M_H(n-3)$. Let $\tilde{A}^{n-3} = A^{n-3} \cup [0]^{n-3}110 \cup [1]^n$ (note that we require $n \geq 5$ here so that the distance between $[0]^{n-3}110$ and $[1]^n$ is ≥ 3). Then clearly $\left\langle \tilde{A}^{n-3} \right\rangle = Q_n$. The set of sites infected after $M_H(n-3)$ steps is $[*]^{n-3}000 \cup [0]^{n-3}110 \cup [1]^n$. By Lemmas 3.8 and 3.11, all neighbours y of $[1]^{n-1}0$ having norm $\|y\|^{110} = n-4$, $\|y\|^{010} = n-3$ or $\|y\|^{100} = n-3$ (i.e., all sites at distance two from $[1]^n$ in $[*]^{n-1}0$), become infected at time exactly $M_H(n-3)+n-2$, so at time $M_H(n-3)+n-2$ the only infected site in $[*]^{n-1}1$ is $[1]^n$. Thus by Lemma 3.12 it takes $n-1$ more steps to fully infect Q_n, and so $T_{Q_n}(\tilde{A}^{n-3}) = M_H(n-3)+2n-3$.

Now let us prove an upper bound on $M_H(n)$, i.e.,

$$M_H(n) \leq \max \begin{cases} M_H(n-2)+n, \\ M_H(n-3)+2n-3. \end{cases}$$

Let A be a set spanning the hypercube Q_n for $n \geq 5$. Let

$$Q_0 = Q^{x_{i_1}}_{i_1} \subset Q^{x_{i_2}}_{i_2} \subset \ldots \subset Q^{x_{i_{t-1}}}_{i_{t-1}} \subset Q^{x_{i_t}}_{i_t} = Q_n$$

be a building sequence of the hypercube. Let $Q_{m_1}^{z_{m_1}}, Q_{m_2}^{z_{m_2}}, \dots, Q_{m_{t-2}}^{z_{m_{t-2}}}, Q_{m_{t-1}}^{z_{m_{t-1}}}$ be the cubes that merge with cubes $Q_{i_j}^{x_{i_j}}$ as in the statement of Lemma 3.4. Recall that for each $1 \leq j \leq t-1$ we have $i_j \geq m_j$. As adding sites to a set that spans Q_n cannot increase its spreading time we may assume that A is a minimal under containment set spanning Q_n. Therefore $i_{t-1} < n$. Let us consider the possible scenarios of the infection process started from A.

(1) If $i_{t-1} \leq n-2$ then, by Lemma 3.5, after at most $M_H(i_{t-1}) \leq M_H(n-2)$ time steps both $Q_{i_{t-1}}^{x_{i_{t-1}}}$ and $Q_{m_{t-1}}^{z_{m_{t-1}}}$ are fully infected. Then, since $\left\langle Q_{i_{t-1}}^{x_{i_{t-1}}} \cup Q_{m_{t-1}}^{z_{m_{t-1}}} \right\rangle = Q_n$, by Lemma 3.12 after at most n more steps we have percolation. Thus in this case

$$T_{Q_n}(A) \leq M_H(n-2) + n.$$

(2) If $i_{t-1} = n-1$ and $i_{t-2} = n-2$ then (since $Q_{i_{t-1}}^{x_{i_{t-1}}}$ is internally spanned) we must have some site $v \in A \cap Q_{m_{t-2}}^{z_{m_{t-2}}}$ such that $d(x_{i_{t-2}}, v) = 1$ and $\left\langle Q_{i_{t-2}}^{x_{i_{t-2}}} \cup v \right\rangle = Q_{i_{t-1}}^{x_{i_{t-1}}}$. Also, there must exist some site $w \in A \cap Q_{m_{t-1}}^{z_{m_{t-1}}}$ such that $\left\langle Q_{i_{t-1}}^{x_{i_{t-1}}} \cup w \right\rangle = Q_n$. Note that, since $i_{t-2} = n-2$, either $d(x_{i_{t-2}}, w) = 1$ or $d(x_{i_{t-2}}, w) = 2$. Let us consider these situations separately.

If $d(x_{i_{t-2}}, w) = 2$ then $\left\langle Q_{i_{t-2}}^{x_{i_{t-2}}} \cup w \right\rangle = Q_n$ which contradicts the minimality of A, as $\langle A \setminus \{v\} \rangle = Q_n$.

If $d(x_{i_{t-2}}, w) = 1$ then, without loss of generality, we have

$$x_{i_{t-2}} = [*]^{n-2}00,\ x_{i_{t-2}} \vee v = [*]^{n-1}0,\ x_{i_{t-2}} \vee w = [*]^{n-2}0*.$$

Clearly, after at most $M_H(n-2)$ time steps the cube $Q_{i_{t-2}}^{x_{i_{t-2}}}$ is fully infected. Then, by Lemma 3.12 case $d=1$, after at most $(n-1)-1 = n-2$ more steps both $Q_{n-1}^{x_{i_{t-2}} \vee v}$ and $Q_{n-1}^{x_{i_{t-2}} \vee w}$ are fully infected. Clearly (or, by Lemma 3.12 case $d=0$), after one more step we have percolation. Thus in this case

$$T_{Q_n}(A) \leq M_H(n-2) + (n-2) + 1 = M_H(n-2) + n - 1.$$

(3) If $i_{t-1} = n-1$, $i_{t-2} \leq n-3$ and $d(x_{i_{t-2}}, z_{m_{t-2}}) \leq 1$ then after at most $M_H(n-3)$ time steps both $Q^{x_{i_{t-2}}}_{i_{t-2}}$ and $Q^{z_{m_{t-2}}}_{m_{t-2}}$ are fully infected. Then, by Lemma 3.12 case $d = 0$ or $d = 1$, after at most $i_{t-1} - 1 = n-2$ more time steps $Q^{x_{i_{t-1}}}_{i_{t-1}}$ is fully infected. Since $i_{t-1} = n-1$ we must have $d(x_{i_{t-1}}, z_{m_{t-1}}) \leq 1$ so, again by Lemma 3.12 case $d = 0$ or $d = 1$, after at most $n-1$ more time steps we have percolation. Thus in this case

$$T_{Q_n}(A) \leq M_H(n-3) + n - 2 + n - 1 = M_H(n-3) + 2n - 3.$$

(4) If $i_{t-1} = n-1$, $i_{t-2} \leq n-3$, $d(x_{i_{t-2}}, z_{m_{t-2}}) = 2$ and $m_{t-2} = n-3$ (note that since we assume that $m_{t-2} \leq i_{t-2}$ then this condition in fact implies $i_{t-2} = n-3$) then after at most $M_H(n-3)$ time steps both $Q^{x_{i_{t-2}}}_{i_{t-2}}$ and $Q^{z_{m_{t-2}}}_{m_{t-2}}$ are fully infected. Then, by Lemma 3.12 case $d = 2$, $(k,l) = (m-2, m-2)$, after at most $i_{t-1} - 1 = n-2$ more time steps $Q^{x_{i_{t-1}}}_{i_{t-1}}$ is fully infected. Again, since $i_{t-1} = n-1$ we must have $d(x_{i_{t-1}}, z_{m_{t-1}}) \leq 1$ so, again by Lemma 3.12 case $d = 0$ or $d = 1$, after at most $n-1$ more time steps we have percolation. Thus in this case again

$$T_{Q_n}(A) \leq M_H(n-3) + n - 2 + n - 1 = M_H(n-3) + 2n - 3.$$

(5) Finally we consider the case $i_{t-1} = n-1$, $i_{t-2} \leq n-3$, $d(x_{i_{t-2}}, z_{m_{t-2}}) = 2$ and $m_{t-2} < n-3$. Without loss of generality

$$x_{i_{t-1}} = [*]^{n-1}0,\ x_{i_{t-2}} = [*]^{i_{t-2}}[0]^{n-i_{t-2}},\ z_{m_{t-2}} = [*]^p[0]^{i_{t-2}-p}[*]^{m_{t-2}-p}110,$$

with $i_{t-2} - p > 0$, which follows from $m_{t-2} < n-3$. Again after at most $M_H(n-3)$ time steps both $Q_{i_{t-2}}^{x_{i_{t-2}}}$ and $Q_{m_{t-2}}^{z_{m_{t-2}}}$ are fully infected so let us assume this is the case and see how the process goes from this point.

Even if we limit our attention only to the initially infected sites in $Q_{i_{t-1}}^{x_{i_{t-1}}}$ then, by Lemma 3.8 (the p common $*$ coordinates in $x_{i_{t-2}}$ and $z_{m_{t-2}}$ do not play any role here), at most two sites in $Q_{i_{t-1}}^{x_{i_{t-1}}}$, $s = [1]^{n-1}0$ with $\|s\|^{110} = n-3$ and $t = [1]^{n-3}000$ with $\|t\|^{000} = n-3$, are not yet infected after $(n-1)-1 = n-2$ additional steps. Let $\tilde{y} \in A$ be such that $\tilde{y} \in [*]^{n-1}1$. Such a $\tilde{y}$ must exist as otherwise no site in $[*]^{n-1}1$ would ever become infected. If $d(\tilde{y}, s), d(\tilde{y}, t) \neq 2$ then all neighbours of $\tilde{y}$ in $[*]^{n-1}1$ have their neighbour in $[*]^{n-1}0$ already infected at time $M_H(n-3) + n - 2$ thus at latest at this moment the infection of the subcube $[*]^{n-1}1$ starts with $\tilde{y}$ as its "seed" and by Lemma 3.12 case $d = 1$ takes at most $n-1$ steps so again

$$T_{Q_n}(A) \leq M_H(n-3) + n - 2 + n - 1 \leq M_H(n-3) + 2n - 3.$$

If $d(\tilde{y}, s) = 2$ or $d(\tilde{y}, t) = 2$ (which strongly constrains our possible choices of $\tilde{y}$) then let $y^* \in [*]^{n-1}1$ be such that $d(y^*, \tilde{y}) = 1$, $d(y^*, s) = d(y^*, t) = 3$ (we do not require $y^* \in A$). Note that such a site can always be found as $d(s, t) = 2$. Note also that we must have $\|y^*\|^{011} = n-4$ or $\|y^*\|^{101} = n-4$. Let w^* be the neighbour of y^* in $[*]^{n-1}0$. Clearly $d(w^*, s) = d(w^*, t) = 2$ since w^* is obtained from y^* by changing y^*_n to 0. Also, $\|w^*\|^{010} = n-4$ or $\|w^*\|^{100} = n-4$.

Again by Lemma 3.8, in the process started from $Q_{i_{t-2}}^{x_{i_{t-2}}} \cup Q_{m_{t-2}}^{z_{m_{t-2}}}$ and constrained to $Q_{i_{t-1}}^{x_{i_{t-1}}}$, w^* becomes infected after at most $(n-1) - 2 = n-3$ steps. From this follows that y^* becomes infected after at most $n-2$ steps (recall that it is a neighbour of w^* and of an initially infected site $\tilde{y}$). If $n \geq 6$ then, also by Lemma 3.8, all sites v^* in $[*]^{n-1}0$ at distance 2 from y^* must have either $0 < \|v^*\|^{010} \leq n-3$,

$0 < \|v^*\|^{100} \leq n-3$, $\|v^*\|^{000} = n-4$ or $\|v^*\|^{110} = n-4$. Thus they are as well infected after at most $n-2$ steps. If $n=5$ then we could additionally have $v^* \in \{00010, 00100\}$. However, these two sites would become infected by $Q_{i_{t-2}}^{x_{i_{t-2}}} \cup Q_{m_{t-2}}^{z_{m_{t-2}}}$ on the first step. Therefore the infection of the subcube $[*]^{n-1}1$ starts in the worst case after $M_H(n-3)+n-2$ steps with y^* as its "seed" and it spreads undisturbed by the infection state of s and t. Thus by Lemma 3.12 case $d=1$ it can take at most $n-1$ additional time steps. Thus once again

$$T_{Q_n}(A) \leq M_H(n-3) + n - 2 + n - 1 \leq M_H(n-3) + 2n - 3.$$

This completes the proof.

□

From Lemma 3.13 and Theorem 3.14 we get the following corollary.

Corollary 3.15. *We have* $M_H(1) = 0$, $M_H(2) = 1$, $M_H(3) = 3$ *and for* $n \geq 4$, $M_H(n) = M_H(n-3) + 2n - 3$.

□

We are now ready to prove our main result.

Proof of Theorem 3.1. The theorem holds for $n \in \{1,2,3\}$. Assume that it holds for $n-3$. By Corollary 3.15 we obtain

$$\begin{aligned} M_H(n) &= M_H(n-3) + 2n - 3 \\ &= \left\lfloor \frac{(n-3)^2}{3} \right\rfloor + 2n - 3 \\ &= \left\lfloor \frac{n^2}{3} - 2n + 3 \right\rfloor + 2n - 3 = \\ &= \left\lfloor \frac{n^2}{3} \right\rfloor . \end{aligned}$$

□

3.4. Further questions

In this chapter we found the maximum percolation time in the n-dimensional hypercube under 2-neighbour bootstrap percolation. Another very interesting question asks how many small percolating subsets can be found in a hypercube. A simple result from Balogh and Bollobás [**8**] says that in 2-neighbour bootstrap percolation every percolating set in Q_n must contain at least $\lceil \frac{n}{2} \rceil + 1$ sites so the question can be formulated as follows.

PROBLEM 3.16. *For $\varepsilon > 0$ what is the number of percolating sets of size $(\frac{1}{2} + \varepsilon)n$ in Q_n?*

This problem can also be interpreted as determining the probability that a random $(\frac{1}{2} + \varepsilon)n$-set of vertices of Q_n percolates. Note that in our proof of the value of $M_H(n)$ we show that the maximum spreading time is obtained for a set of size roughly $\frac{2n}{3}$.

CHAPTER 4

Bootstrap percolation on infinite trees

4.1. Introduction

In this chapter we continue our investigations of the r-neighbour bootstrap percolation models, but we completely change the character of the questions we look at. From now on, they will have a probabilistic character and instead of grid-like graphs, we shall look at infinite trees.

For an infinite tree T, the critical probability for r-neighbour bootstrap percolation, denoted $p_c(T,r)$, is defined as

$$p_c(T,r) = \inf\{p : \mathbb{P}_p(T \text{ percolates in } r\text{-neighbour bootstrap percolation}) > 0\}.$$

Note that this definition of $p_c(T,r)$ is different from that given in (0.1) for general graphs. This modification is motivated by the fact that for a general infinite tree the exact probability of percolation could be highly affected by finite, yet difficult to infect from the outside, subtrees. The existence of such substructures does not matter when we care only about the probability of percolation being positive.

For every $d \geq 1$, let T_d denote the infinite $(d+1)$-regular tree. Balogh, Peres and Pete [**13**], expanding the work of Chalupa, Leath and Reich [**27**], gave a formula for $p_c(T_d,r)$ showing, in particular, that for any $d \geq 1$ and $r \geq 2$ we have $p_c(T_d,r) > 0$. They also showed that every infinite tree T with *branching number* $\mathrm{br}(T) < r$ has the property that $p_c(T,r) = 1$. (The branching number is defined in Section 4.2.) Given these results, the question was raised of finding the smallest critical probability among all trees with a fixed branching number. With a simple example of a Galton–Watson tree it was shown in [**13**] that for $b \geq r$ a $(b+1)$-regular tree does not, in general, minimize the critical probability for r-neighbour bootstrap percolation among all trees with branching number b. Defining a function f_r, for each $r \geq 2$, by

$$f_r(b) = \inf\{p_c(T,r) : \mathrm{br}(T) \leq b \text{ and } T \text{ has bounded degree}\},$$

Balogh, Peres and Pete [**13**] posed the following two problems:

(1) Is $f_r(b)$ strictly positive for all real $b \geq 1$?

(2) Is $f_r(b)$ continuous apart from at $b = r$?

In this chapter we answer both of these questions by showing that $f_r(b)$ is a step-function. More precisely, in Section 4.2, we prove the following theorem.

THEOREM 4.1. *For all $r \geq 2$ and $b \geq r$, $f_r(b) = 0$.*

Balogh, Peres and Pete [**13**] showed that $f_r(b) = 1$ for $b < r$. To briefly describe their proof, let us recall the following definition from [**13**], which we shall also find very useful in Chapter 5.

DEFINITION 4.2. *Let G be a graph and $k \in \mathbb{N}$. A finite or infinite set of vertices, $F \subset V(G)$, is called a k-*fort* if every vertex in F has at most k neighbours in $V(G) \setminus F$.*

If G contains an $(r-1)$-fort, F, with all vertices initially healthy, then G does not percolate in the r-neighbour bootstrap process. Moreover, the set of eternally healthy vertices is an $(r-1)$-fort, so a vertex remains healthy forever if and only if it belongs to a healthy $(r-1)$-fort.

In [**13**] the authors proved that if a tree T has $\mathrm{br}(T) = b < r$ then T contains infinitely many $(r-1)$-forts of bounded size. Then, infecting vertices initially with some $p < 1$, almost surely we obtain an initially healthy $(r-1)$-fort which, by the definition, remains healthy forever and prevents percolation. Combining Theorem 4.1 with the result of Balogh, Peres and Pete, we have

$$f_r(b) = \begin{cases} 1, & \text{if } b < r, \\ 0, & \text{otherwise.} \end{cases}$$

It is worth noticing that we shall prove Theorem 4.1 by producing trees with arbitrarily small, but positive, critical probabilities.

This chapter is joint work with Béla Bollobás, Karen Gunderson, Cecilia Holmgren, and Svante Janson. The chapter is based on Section 2 of our forthcoming paper, [**20**].

4.2. Trees with arbitrarily small critical probability

In this section, a construction is given for families of infinite trees with a fixed branching number and arbitrarily small critical probability.

The branching number is one of the most important invariants of infinite trees which we shall now define formally. (For further information, see, for example, Lyons [**41**].) Given a rooted tree T, for every edge e in the tree, let $|e|$ denote the number of edges (including e) in the path from e to the root. The branching number of a tree T, denoted $\mathrm{br}(T)$, is the supremum of real numbers $\lambda \geq 1$ such that there exists a positive flow in T from the root to infinity with capacities at every edge e bounded by $\lambda^{-|e|}$. For example, a binary tree in which every vertex has exactly 2 children has branching number 2. However, in Figure 4.1 we see a tree with 2^n vertices in the n-th level and branching number 1.

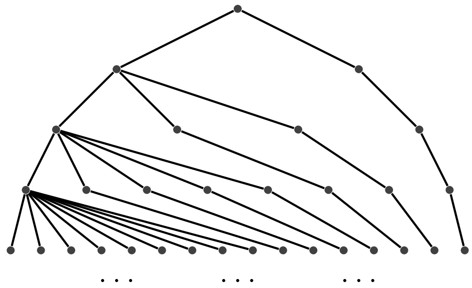


FIGURE 4.1. A tree with an exponentially growing size of levels and branching number 1.

It is easily seen that this value does not depend on the choice of the root. Though in this chapter, only infinite trees are considered, let us mention that for a finite tree T we define $\mathrm{br}(T) = 0$.

For $b \geq 2$, let T_b denote the infinite $(b+1)$-regular tree. As usual, for $n \geq 1$ and $p \in [0,1]$, write $\mathrm{Bin}(n,p)$ for a binomial random variable with parameters n and p. In [**27**], it was shown that, in r-neighbour bootstrap percolation, for each $b \geq r$, the critical probability $p_c(T_b, r)$ is equal to the supremum of all p for which the fixed-point equation

$$x = \mathbb{P}(\mathrm{Bin}(b, (1-x)(1-p)) \leq b - r) \tag{4.1}$$

has a solution $x \in [0,1)$. Note that $x = 1$ is always a solution to (4.1).

An interpretation of equation (4.1) is as follows. The complete occupation of T_b obeys the $0-1$ law and can be shown to be stochastically equivalent to complete occupation of a rooted b-ary tree, that is, a rooted infinite tree in which every vertex has exactly b descendants (so all vertices have degree $b+1$ except the root which has degree b). For $b \geq r$ the root of a b-ary tree, conditioned on being initially healthy, remains healthy forever iff at least $b-r+1$ of its children are initially healthy and remain healthy forever in the infection process limited to the subtrees rooted at them. Let x be the probability that, conditioned on being initially healthy, the root *does not* remain healthy forever. Then, one can show that x is the smallest solution to equation (4.1) in $[0,1]$. In particular, it was noted in [**27**] that $p_c(T_b,2) = 1 - \frac{(b-1)^{2b-3}}{b^{b-1}(b-2)^{b-2}}$ and later in [**13**] that $p_c(T_b,b) = 1 - \frac{1}{b}$. It can be shown that for every fixed r, as b tends to infinity, $p_c(T_b,r) = \left(1-\frac{1}{r}\right)\left(\frac{(r-1)!}{b^r}\right)^{1/(r-1)}(1+o(1))$. This calculation is given in Lemma 5.10 in the next chapter.

From equation (4.1) we see immediately that $p_c(T_b,r) > 0$ for any $b \geq r \geq 2$. In [**13**] the authors asked whether there exists $\varepsilon_{b,r} > 0$ such that for any tree T with branching number $\mathrm{br}(T) = b$ we have $p_c(T,r) \geq \varepsilon_{b,r}$, answering this question affirmatively for $r > b$ with $\varepsilon_{b,r} = 1$. Note that the question about the maximum of $p_c(T,r)$ among trees T with $\mathrm{br}(T) = b$ is trivial. For all values of $b \geq 1$ this maximum is equal to 1 as a tree T with $\mathrm{br}(T) = b \geq 1$ might have infinitely many leaves which would all need to be initially infected for percolation to occur.

With an explicit construction of a family of infinite trees with bounded degree we shall now show that $f_r(b) = 0$ for $b \geq r$. The condition that the tree T has bounded degree is included in the definition of the function $f_r(b)$ since one can easily construct infinite trees with unbounded degree and branching number b, and such that their critical probability is 0. We show an example of such construction at the end of this section.

Given $b \geq r \geq 2$ and $p \in (0,1)$, we shall show that there is an integer d and an infinite tree with branching number b where every vertex has either degree $d+1, d+2, b+1$ or $b+2$ and such that, infecting vertices with probability p, the tree almost surely percolates. The idea of the proof is that, when d is sufficiently large, vertices that are the roots of some number of levels of a copy of T_d are very likely to eventually become infected and these finite trees can be arranged within an infinite tree to cause the percolation of the entire tree.

First, it is shown that, for the infection threshold r and for d large enough, we can in fact obtain an arbitrarily small critical probability $p_c(T_d, r)$.

Lemma 4.3. *For each integer $r \geq 2$ and $d \geq r$, $p_c(T_d, r) \leq r/d$.*

Proof. Fix $r \geq 2$, $d \geq r$ and $p > r/d$. To prove this result, it suffices to show that for all $x \in [0,1)$ we have $\mathbb{P}(\mathrm{Bin}(d,(1-x)(1-p)) \leq d-r) > x$, or alternatively, $\mathbb{P}(\mathrm{Bin}(d,(1-x)(1-p)) \geq d-r+1) < 1-x$. Then there are no solutions of the fixed point equation (4.1) in $[0,1)$ and so $p_c(T_d, r) \leq p$.

Recall the following Chernoff-type inequality: if $X \sim \mathrm{Bin}(n,p)$ and $m \geq np$, then $\mathbb{P}(X \geq m) \leq e^{-np}(enp/m)^m$ (see, e.g., Appendix A in Alon and Spencer [**6**]). Since $dp > r$, we have $d(1-x)(1-p) \leq d-dp < d-r < d-r+1$, and thus

$$
\begin{aligned}
&\mathbb{P}(\mathrm{Bin}(d,(1-x)(1-p)) \geq d-r+1)\\
&\qquad \leq e^{d-r+1-d(1-x)(1-p)} \left(\frac{d(1-x)(1-p)}{d-r+1}\right)^{d-r+1}\\
&\qquad = e^{d-r+1-d(1-x)(1-p)} \left(\frac{d(1-p)}{d-r+1}\right)^{d-r+1} (1-x)^{d-r}(1-x)\\
&\qquad \leq e^{d-r+1-d(1-x)(1-p)} \left(1-\frac{dp-r+1}{d-r+1}\right)^{d-r+1} e^{-x(d-r)}(1-x)\\
&\qquad \leq \exp\left[d-r+1-d(1-x)(1-p)-(dp-r+1)-x(d-r)\right](1-x)\\
&\qquad = \exp(-x(dp-r))(1-x)\\
&\qquad < 1-x,
\end{aligned}
$$

for all $x \in [0, 1)$. Thus, there are no solutions of equation (4.1) in $[0, 1)$ and hence $p_c(T_d, r) \leq p$. $\square$

As a consequence of Lemma 4.3, for r fixed, $\lim_{d\to\infty} p_c(T_d, r) = 0$.

In the next lemma we show that, for any $\varepsilon \in (0, 1)$, there is a large number n_ε such that if we initially infect vertices in the first n_ε levels of T_d with probability $p \geq p_c(T_d, r)$, then the root of T_d will become infected in the r-neighbour bootstrap process with probability at least $1 - \varepsilon$. For any $d \geq 1$, $n \geq 0$, let T_d^n be the first $n + 1$ levels of a rooted, $(d + 1)$-regular tree. That is, the root has $d + 1$ children, there are $(d + 1)d^{n-1}$ leaves and every vertex except the root and the leaves has exactly d children.

LEMMA 4.4. *For $d \geq r \geq 2$, $p > p_c(T_d, r)$, and $n \geq 1$, let the vertices of T_d^n be infected independently with probability $p > 0$. For the r-neighbour bootstrap process,*

$$\mathbb{P}_p(\textit{the root of } T_d^n \textit{ is eventually infected}) \to 1$$

as $n \to \infty$.

PROOF. Note that if $p > p_c(T_d, r)$ then for r-neighbour bootstrap percolation on T_d, using a $0 - 1$ law argument, $\mathbb{P}_p(T_d \text{ percolates}) = 1$ and hence

$$\mathbb{P}_p(\text{root is eventually infected}) = \mathbb{P}_p(\cup_{t\geq 0}\{\text{root is infected by time } t\}) = 1.$$

Using induction, one can show that the root is infected by time t exactly when the eventual infection of the root depends on the infection status of vertices in the first t levels. Indeed, if the root is infected at time 0, this event depends only on the initial infection of the root itself. For $t \geq 1$, if the root becomes infected at time t, then at least r of its children are infected at time $t - 1$. By induction this event depends only on vertices at distance at most $t - 1$ from the children of the root and hence at distance at most t from the root itself.

Therefore, $\lim\limits_{t\to\infty} \mathbb{P}_p(\text{root infected based on first } t \text{ levels}) = 1$. $\square$

We are now ready to prove Theorem 4.1 with the construction given in the proof of Theorem 4.5 below. For simplicity we give a construction for integer values of b and later describe how to modify it for $b \in \mathbb{R}$.

THEOREM 4.5. *For every pair of integers $r \geq 2$ and $b \geq r$ and every $p \in (0,1)$, there is an infinite tree T with bounded degree and $\mathrm{br}(T) = b$ satisfying $p_c(T,r) < p$.*

PROOF. Fix $p \in (0,1)$ and integers r, b with $b \geq r$. Let $d > \max\{r/p, b\}$ so that, by Lemma 4.3, $p > r/d \geq p_c(T_d, r)$. Let $\{n_i\}_i$ and $\{m_i\}_i$ be sequences of integers, all to be defined precisely later in the proof. Our tree is constructed level-by-level, depending on these parameters; it will be shown that the sequences $\{n_i\}_i$ and $\{m_i\}_i$ can be chosen appropriately so that the resulting tree has the desired properties.

Begin with a copy of $T_d^{n_1}$. To each leaf of this tree attach a copy of $T_b^{m_1}$. Then to each leaf of the resulting tree attach a copy of $T_d^{n_2}$ and then to each new leaf attach a copy of $T_b^{m_2}$. Continue in this manner, alternating with $(d+1)$-regular trees and $(b+1)$-regular trees of depths given by the sequences $\{n_i\}_i$ and $\{m_i\}_i$ respectively and let T be the resulting infinite tree. We would like to show that there is a suitable choice for the sequences $\{n_i\}$ and $\{m_i\}$ so that $\mathrm{br}(T) = b$ and $p_c(T,r) < p$ (in other words, $\mathbb{P}_p(T \text{ percolates}) > 0$).

For each $\ell \geq 1$, let $N_\ell = \prod_{i=1}^{\ell-1}(d+1)d^{n_i-1}(b+1)b^{m_i-1}$ be the number of copies of $T_d^{n_\ell}$ added in the $(2\ell-1)$-th step of the construction and let $v_1^\ell, v_2^\ell, \ldots, v_{N_\ell}^\ell$ be the roots of those copies of $T_d^{n_\ell}$ and let $T_{d,i}^{n_\ell}$ denote the copy of $T_d^{n_\ell}$ rooted at v_i^ℓ. Define $t_\ell = \sum_{i=1}^{\ell-1}(n_i + m_i)$ to be the depth of these vertices in T. For each $\ell \geq 1$ and $i \in \{1, \ldots, N_\ell\}$, consider the event

$$A_{\ell,i} = \{v_i^\ell \text{ becomes infected based only on infection of vertices in } T_{d,i}^{n_\ell}\}.$$

Using Lemma 4.4, choose n_ℓ to be large enough so that $\mathbb{P}(A_{\ell,i}) \geq (1/2)^{1/N_\ell}$. Note that N_ℓ does not depend on n_ℓ, and that n_ℓ only depends on n_i and m_i for $i < \ell$. Set $A_\ell = \cap_i A_{\ell,i}$. If A_ℓ occurs, then all vertices in level t_ℓ are eventually infected and hence all vertices in levels at most t_ℓ are eventually infected. Further, if infinitely many events $\{A_\ell\}_\ell$ occur, then T percolates.

For ℓ fixed, since the events $\{A_{\ell,i}\}_i$ are independent, by the choice of n_ℓ we have

$$\mathbb{P}(A_\ell) = \mathbb{P}(\cap_i A_{\ell,i}) = \prod_{i=1}^{N_\ell} \mathbb{P}(A_{\ell,i}) \geq \prod_{i=1}^{N_\ell} \left(\frac{1}{2}\right)^{1/N_\ell} = \frac{1}{2}.$$

By the Borel-Cantelli lemma (see, for example, Lemma 2 in Chapter VIII of Feller [**29**]), since the events $\{A_\ell\}$ are independent and $\sum_\ell \mathbb{P}(A_\ell) \geq \sum_\ell \frac{1}{2} = \infty$, then $\mathbb{P}(T \text{ percolates}) = 1$.

Up to this point, no conditions have been imposed on the sequence $\{m_i\}_i$ and these can be chosen in such a way that $\mathrm{br}(T) = b$. Note that, since d was chosen with $d > b$, every vertex of T has at least b children and so $\mathrm{br}(T) \geq b$. By choosing the values of m_i recursively, depending on the sequence $\{n_i\}$, it is shown below that $\mathrm{br}(T) \leq b$.

For every n, let L_n be the n-th level of T, i.e., the vertices at distance n from the root of T. A standard upper bound on the branching number of an arbitrary tree gives $\mathrm{br}(T) \leq \liminf |L_n|^{1/n}$.

For $\ell \geq 1$, consider the level $t_{\ell+1} = \sum_{i=1}^{\ell}(n_i + m_i)$ with $\prod_{i=1}^{\ell}(d+1)d^{n_i-1}(b+1)b^{m_i-1}$ vertices. Clearly, if $m_\ell \geq \ell^2$ is large enough then

$$\left(\frac{d}{b}\right)^{\frac{\sum_{i=1}^{\ell} n_i}{t_{\ell+1}}} \leq 1 + \frac{1}{2^\ell}$$

and $\ell / t_{\ell+1} \to 0$ as $\ell \to \infty$ (note that m_ℓ only depends on n_i for $i \leq \ell$ and m_i for $i < \ell$). Then, the number of vertices in level $t_{\ell+1}$ satisfies

$$\begin{aligned} |L_{t_{\ell+1}}| &= \prod_{i=1}^{\ell}(d+1)d^{n_i-1}(b+1)b^{m_i-1} \\ &= b^{t_{\ell+1}} \left(\frac{d}{b}\right)^{\sum_{i=1}^{\ell} n_i} \left(1+\frac{1}{d}\right)^{\ell} \left(1+\frac{1}{b}\right)^{\ell} \\ &\leq b^{t_{\ell+1}} \left(1+\frac{1}{2^\ell}\right)^{t_{\ell+1}} \left(1+\frac{1}{d}\right)^{\ell} \left(1+\frac{1}{b}\right)^{\ell}. \end{aligned}$$

Thus, $\liminf |L_n|^{1/n} \leq b$ and so $\mathrm{br}(T) = b$. □

For simplicity, the proof of Theorem 4.5 assumes that b is an integer. For any real $b \geq r$, the construction can be easily modified to give an infinite tree with branching number b and arbitrarily small critical probability. Given $b \geq r$ let $b' = \lfloor b \rfloor \geq r$. Then we build our tree alternating $(d+1)$-regular and $(b'+1)$-regular trees with the heights m_i of the $(b'+1)$-regular trees chosen appropriately to obtain $\liminf |L_n|^{1/n} = b$.

By Theorem 4.5, for $b \geq r$, $f_r(b) = 0$, completing the proof of Theorem 4.1.

The construction in the proof of Theorem 4.5 can also be modified to produce examples of infinite trees with branching number b, unbounded degree and critical probability 0. Indeed, set $n_i \equiv 1$, and for each $\ell \geq 1$, at step $2\ell - 1$ of the construction replace d by d_ℓ, chosen to be large enough so that for the corresponding events $A_{\ell,i}$,

$$\mathbb{P}(A_{\ell,i}) = \mathbb{P}(\mathrm{Bin}(d_\ell + 1, 1/\ell) \geq r) \geq \left(\frac{1}{2}\right)^{1/N_\ell}.$$

The sequence $\{m_i\}_i$, giving the number of levels of the $(b+1)$-regular trees, can be chosen to ensure $\mathrm{br}(T) = b$. The resulting infinite tree T has branching number b, unbounded degree and $p_c(T, r) = 0$.

CHAPTER 5

Bootstrap percolation on Galton–Watson trees

5.1. Introduction

In this chapter we continue our studies of bootstrap percolation on infinite trees. Motivated by the non-homogeneous nature of trees with arbitrarily small critical probabilities constructed in the proof of Theorem 4.5 we also study a well-known family of well-behaved trees: *Galton-Watson trees.* For a non-negative integer-valued distribution ξ, let T_ξ be the Galton–Watson tree with offspring distribution ξ (a more formal definition is given in Section 5.2). We shall see in Section 5.3 that $p_c(T_\xi, r)$ is almost surely a constant (depending on the distribution ξ but not on the realization T_ξ); we let $p_c(T_\xi, r)$ denote also this constant, without risk of confusion. We define a new function $f_r^{GW}(b)$ by

$$f_r^{GW}(b) = \inf\{p_c(T_\xi, r) : \mathbb{E}(\xi) = b, \mathbb{P}(\xi = 0) = 0\}. \tag{5.1}$$

The condition that $\mathbb{P}(\xi = 0) = 0$ is included since any finite tree percolates with positive probability if the probability of initial infection, p, is positive. For this reason, we consider only offspring distributions for which the resulting tree is almost surely infinite. While the branching numbers of infinite trees can be difficult to determine, for Galton–Watson trees, Lyons [**41**] showed that, almost surely, $\mathrm{br}(T_\xi) = \mathbb{E}(\xi)$.

In Section 5.3, we shall investigate the function $f_r^{GW}(b)$ and we shall show it to be positive for all b and r. That is, the value of $\mathbb{E}(\xi)$ immediately leads to a non-trivial lower bound on $p_c(T_\xi, r)$. We shall also show that our bound is tight up to a factor of $O(b)$.

THEOREM 5.1. *For $b \geq 1$, let the function $f_r^{GW}(b)$ be defined as in* (5.1)*.*

1. *If $r > b \geq 1$ then $f_r^{GW}(b) = 1$.*
2. *For $r \geq 2$ there are constants c_r and C_r such that if $b \geq r$ then*

$$\frac{c_r}{b} e^{-\frac{b}{r-1}} \leq f_r^{GW}(b) \leq C_r e^{-\frac{b}{r-1}}.$$

Note that the b-ary tree is a Galton–Watson tree given by ξ with $\mathbb{P}(\xi = b) = 1$. The b-ary tree has the same critical probability as the $(b+1)$-regular tree T_b. By Theorem 5.1, for large b, the value of $f_r^{GW}(b)$ is extremely far from the value $p_c(T_b, 2) \sim \frac{1}{2b^2}$, obtained in [**13**]. Moreover, for the family of offspring distributions which we use to bound $f_r^{GW}(b)$ from above the variance grows exponentially in b. This discrepancy suggests that offspring distributions highly concentrated around their means might yield much higher values for the critical probability. This is in fact true as shown by the following theorem, proved in Section 5.3.2.1.

THEOREM 5.2. *For each $r \geq 2$ and $\alpha \in (0, r-1)$, there exists a constant $c_{r,\alpha} > 0$ such that for any offspring distribution ξ with $\mathbb{E}(\xi^{1+\alpha}) < \infty$ we have*

$$p_c(T_\xi, r) \geq c_{r,\alpha} \left(\mathbb{E}(\xi^{1+\alpha})\right)^{-1/\alpha}.$$

Also, for each $r \geq 2$ there exists a constant $A_r > 0$ such that

$$p_c(T_\xi, r) \leq c_r \mathbb{E}\left(\frac{1}{\xi^{r/(r-1)}}\right).$$

The lower bound in Theorem 5.2 is proved directly for $\alpha \notin \mathbb{N}$. Given r, as $\alpha \to n \in \{1, \ldots, r-2\}$ the constants $c_{r,\alpha}$ obtained in the theorem converge to $c_{r,n} > 0$ and hence by the monotone convergence theorem, the theorem holds for $\alpha = n$.

In fact, Theorem 5.2 holds also for $r = 2$ and $\alpha = 1$ as shown by the final result in this chapter, given in Section 5.3.2.2. Theorem 5.3, apart from a sharp lower bound on $p_c(T_\xi, 2)$ based on the second moment of ξ, also gives additional lower bounds on the critical probability in 2-neighbour bootstrap percolation, as well as a sharp upper bound on $p_c(T_\xi, 2)$ based on the second negative moment of ξ. Our bounds are sharp since the constants in them cannot be improved, as shown by the critical probability for regular trees.

THEOREM 5.3. *Let T_ξ be the Galton–Watson tree of an offspring distribution ξ. Then*

$$p_c(T_\xi, 2) \geq \max\left\{1 - \frac{1}{2\mathbb{P}(\xi = 2)}, \max_{k \geq 3}\left\{1 - \frac{(k-1)^{2k-3}}{k^{k-1}(k-2)^{k-2}\mathbb{P}(\xi = k)}\right\}\right\}, \tag{5.2}$$

and

$$p_c(T_\xi, 2) \leq \mathbb{E}\left(\frac{1}{(\xi-1)(2\xi-3)}\right) \leq \mathbb{E}\left(\frac{4}{\xi^2}\right). \tag{5.3}$$

Additionally, if ξ *has the property that* $\mathbb{E}(\xi^2) < \infty$*, then*

$$p_c(T_\xi, 2) \geq \frac{1}{2\mathbb{E}(\xi(\xi-1)) - 3} \geq \frac{1}{2\mathbb{E}\xi^2}. \tag{5.4}$$

Balogh, Peres and Pete **[13]** noted that as $b \to \infty$, the critical probability for the regular tree, T_b, is $p_c(T_b, 2) \sim \frac{1}{2b^2}$, which matches the bounds given in Theorem 5.3.

Finally, in Section 5.3.3 we shall present some examples of natural classes of Galton–Watson trees for which the critical probability for bootstrap percolation can be computed exactly and compare these to the bounds given by Theorem 5.3. To conclude, in Section 5.4, we state a few open questions and conjectures.

This chapter is again joint work with Béla Bollobás, Karen Gunderson, Cecilia Holmgren, and Svante Janson, with the exception of Section 5.3.2.1 which is my joint work with Karen Gunderson only. The chapter is based on Section 3 of our forthcoming paper, **[20]**.

5.2. Definitions, notation, and initial observations

In Chapter 4 we showed that the branching number $\mathrm{br}(T)$ of an infinite tree T does not lead to any nontrivial lower bound on the critical probability $p_c(T, r)$, except when $\mathrm{br}(T) < r$ and $p_c(T, r) = 1$, as shown in **[13]**. The trees constructed in the proof of Theorem 4.5 to show that if $b \geq r$, then $f_r(b) = 0$, are highly non-homogeneous and the irregularities in their construction seem crucial to their small critical probabilities. In this section we limit our attention to the well-studied family of Galton–Watson trees, for which these anomalies do not occur.

A Galton–Watson tree is the family tree of a Galton–Watson branching process. For a non-negative integer-valued distribution ξ, called the *offspring distribution*, we start with a single root vertex in level 0 and at each generation

$n = 1, 2, 3, \ldots$ each vertex in level $n - 1$ gives birth to a random number of children in level n, where the number of offspring of each vertex is distributed according to the distribution ξ and is independent of the number of children of any other vertex. This process can be formalized to define a probability measure on the space of finite and infinite rooted trees, and T_ξ is used to denote a randomly chosen Galton–Watson tree with offspring distribution ξ. As previously mentioned, if $\mathbb{P}(\xi = 0) > 0$ then T_ξ is finite with positive probability. Thus in this chapter we limit our attention to offspring distributions with $\mathbb{P}(\xi = 0) = 0$, for which T_ξ is almost surely infinite.

While the critical probability $p_c(T_\xi, r)$ is a random variable, which could take a range of values, depending on the tree T_ξ, it can be shown that in the space of Galton–Watson trees with offspring distribution ξ, conditioned on T_ξ being infinite, $p_c(T_\xi, r)$ is almost surely a constant. While this involves standard applications of results and techniques in the theory of branching processes, the details are given in this section for completeness.

For any rooted tree T, with root v_0, let $\{T_w : w \in N(v_0)\}$ be the collection of rooted sub-trees of T whose roots are the immediate descendants of v_0; that is, T_w is the connected component of $T - v_0$ containing w and rooted at w. A property $\mathcal{A}$ of rooted trees is called *inherited* if every finite tree T has this property and, furthermore, T has the property $\mathcal{A}$ only if for every w adjacent to the root, T_w has property $\mathcal{A}$. Now we note a general zero-one property of Galton–Watson branching processes. The next proposition is Proposition 5.6 in [**42**].

PROPOSITION 5.4. *Every inherited property of a Galton–Watson tree has conditional probability either* 0 *or* 1 *given nonextinction.*

PROOF. Let $\mathcal{T}$ be the set of trees possessing a given inherited property. Again, for any rooted tree T, with root v_0, let $\{T_w : w \in N(v_0)\}$ be the set of rooted sub-trees of T whose roots are the immediate descendants of v_0. For an offspring distribution ξ, let $f_\xi(x) = \sum_{k \geq 0} \mathbb{P}(\xi = k) x^k$ be the probability generating function of ξ. It is a well known fact in the branching processes theory that the extinction probability of the process is given by $q = \lim_{n\to\infty} f^{(n)}(0)$. Also, q and 1 are the only fixed points of f_ξ. We have

$$\begin{aligned}\mathbb{P}(T \in \mathcal{T}) &= \sum_{k\geq 0} \mathbb{P}(\xi = k)\mathbb{P}(T \in \mathcal{T} \mid |N(v_0)| = k)\\ &\leq \sum_{k\geq 0} \mathbb{P}(\xi = k)\mathbb{P}(T_w \in \mathcal{T} \text{ for all } w \in N(v_0) \mid |N(v_0)| = k)\end{aligned}$$

by definition of inherited. Since $\{T_w : w \in N(v_0)\}$ are i.i.d. given $|N(v_0)|$, the last quantity above is equal to

$$\sum_{k\geq 0} \mathbb{P}(\xi = k)(\mathbb{P}(T \in \mathcal{T}))^k = f_\xi(\mathbb{P}(T \in \mathcal{T})).$$

Thus $\mathbb{P}(T \in \mathcal{T}) \leq f_\xi(\mathbb{P}(T \in \mathcal{T}))$. On the other hand, $\mathbb{P}(T \in \mathcal{T}) \geq q$ since every finite tree is in $\mathcal{T}$. It follows from the observation about the fixed points of f_ξ that $\mathbb{P}(T \in \mathcal{T}) \in \{q, 1\}$, from which the desired conclusion follows. □

Given $p > 0$ and $r \geq 2$ consider the property

$$\mathcal{A}_p = \{\mathbb{P}_p(T \text{ percolates in the } r\text{-neighbour bootstrap process}) > 0\}.$$

If T is a Galton–Watson tree then the property $\mathcal{A}_p$ is inherited. This is because every finite tree is initially fully infected with positive probability, and an infinite Galton–Watson tree is fully infected with positive probability only if all the subtrees in $\{T_w : w \in N(v_0)\}$ are fully infected with positive probability, and these are also Galton–Watson trees with the same offspring distribution. Since we consider offspring distributions with $\mathbb{P}(\xi = 0) = 0$, the Galton–Watson process survives almost surely and we see that the probability that the Galton–Watson tree T_ξ has property $\mathcal{A}_p$ is either 0 or 1. By the definition of critical probability this implies that $p_c(T_\xi, r)$ is almost surely a constant.

Now we show that we may assume that $\mathbb{P}(\xi < r) = 0$, repeating the argument observed earlier in [**13**]. If there is a $k < r$ such that $\mathbb{P}(\xi = k) > 0$, then T_ξ almost surely contains infinitely many pairs of vertices u, v such that v is a child of u and $\deg(u) = \deg(v) = k + 1$. Then, if we initially infect vertices of T_ξ independently with some probability $p < 1$, almost surely we obtain such a pair with both u and v initially healthy, in which case $\{u, v\}$ is an initially healthy $(r-1)$-fort. Thus T_ξ almost surely does not percolate and so $p_c(T_\xi, r) = 1$.

Therefore from now on we assume that $\mathbb{P}(\xi < r) = 0$; in particular, $\mathbb{E}(\xi) = b \geq r$. In this case, almost surely, T_ξ contains no finite $(r-1)$-forts.

In [**13**], Balogh, Peres and Pete characterize the critical probability for a particular Galton–Watson tree in terms of the probability that the root of the tree remains healthy in the bootstrap process. The details are given here for arbitrary Galton–Watson trees.

For any tree T with root v_0, $r \geq 2$ and $p \geq 0$, initially infecting vertices with probability p, define

$$q(T, p) = \mathbb{P}_p(v_0 \text{ is in a healthy } (r-1)\text{-fort}),$$

the probability that v_0 is never infected. Since, in general, the random variable $q(T_\xi, p)$ depends on the tree T_ξ, consider its expected value, over the space of random Galton–Watson trees with offspring distribution ξ and set

$$q(p) = \mathbb{E}_{T_\xi}(q(T_\xi, p)).$$

In what follows, it is shown that $q(p) > 0$ iff $p < p_c(T_\xi, r)$.

Given a tree T with root v_0, denote the children of the root by $v_1, v_2, \ldots, v_k$ and the corresponding sub-trees by $T_1, T_2, \ldots, T_k$. The root v_0 is contained in an infinite healthy $(r-1)$-fort iff v_0 is initially healthy and at least $k - r + 1$ of its children are themselves contained in an infinite healthy $(r-1)$-fort in their sub-tree T_i. Since these k events are mutually independent,

$$q(T, p) = (1-p) \sum_{\substack{X \subseteq [1,k] \\ |X| \leq r-1}} \left(\prod_{i \in X} (1 - q(T_i, p)) \prod_{j \notin X} q(T_j, p) \right).$$

If T is a Galton–Watson tree with offspring distribution ξ then, given that the root has exactly k children, the sub-trees $T_1, T_2, \ldots, T_k$ are also such (independent) trees. Thus,

$$\begin{aligned} q(p) &= (1-p)\sum_{k\geq r}\mathbb{P}(\xi = k)\sum_{i\leq r-1}\binom{k}{i}(1-q(p))^i q(p)^{k-i} \\ &= (1-p)\sum_{k\geq r}\mathbb{P}(\xi = k)\mathbb{P}(\mathrm{Bin}(k, 1-q(p)) \leq r-1). \end{aligned} \tag{5.5}$$

Define a function $h_{r,p}(x)$, depending implicitly on the distribution ξ, by

$$h_{r,p}(x) = (1-p)\sum_{k\geq r}\mathbb{P}(\xi = k)\mathbb{P}(\mathrm{Bin}(k, 1-x) \leq r-1).$$

By equation (5.5), $q(p)$ is a fixed point of $h_{r,p}(x)$. Note that this is closely related to the fixed point equation (4.1) with x in place of $(1-p)(1-x)$.

The function $h_{r,p}(x)$ is continuous on $[0,1]$, $0 \leq h_{r,p}(x) \leq (1-p)$ and since

$$\frac{d}{dx}\mathbb{P}(\mathrm{Bin}(k, 1-x) \leq r-1) = k\mathbb{P}(\mathrm{Bin}(k-1, 1-x) = r-1) > 0 \tag{5.6}$$

for all $k \geq r$ and $0 < x < 1$, $h_{r,p}$ is strictly increasing in $[0,1]$ unless $p = 1$. Note that for any p, $h_{r,p}(0) = 0$ and so 0 is a fixed point of the function. Using standard techniques for branching processes, we show that the critical probability $p_c(T_\xi, r)$ is given as follows in terms of the function $h_{r,p}(x)$.

LEMMA 5.5. *The critical probability $p_c(T_\xi, r)$ is almost surely given by*

$$p_c(T_\xi, r) = \inf\{p : x = h_{r,p}(x) \textit{ has no solution for } x \in (0,1]\}.$$

The proof of Lemma 5.5 is given by Claim 5.6 and Lemma 5.7 below.

CLAIM 5.6. *For every p, $q(p)$ is the largest fixed point of $h_{r,p}(x)$ in $[0,1]$.*

PROOF. If $p = 1$ then $h_{r,p}(x) = 0$ for all $x \in [0,1]$ and so $x = 0$ is the only fixed point of $h_{r,p}(x)$ in $[0,1]$. Thus $q(p)$, itself being such a fixed point, must be equal to 0.

Therefore assume that $p < 1$. For any tree T, let T^n be the first n levels of T and define

$$q_n(T,p) = \mathbb{P}_p(v_0 \text{ is in a healthy } (r-1)\text{-fort of } T^n)$$

and $q_n(p) = \mathbb{E}_{T_\xi}(q_n(T_\xi, p))$.

Since the definition of a fort depends only on the neighbourhood of each vertex, a sub-tree $F \subseteq T$ is an $(r-1)$-fort iff for every $n \geq 0$, $F \cap T^n$ is an $(r-1)$-fort in T^n; furthermore, the latter event is decreasing in n. Therefore, $q_n(T,p) \searrow q(T,p)$ as $n \to \infty$ and so also $q_n(p) \searrow q(p)$.

Following the same recursive argument as before, we see that for every $n \geq 0$, $q_{n+1}(p) = h_{r,p}(q_n(p))$. Note also that for any tree T,

$$q_0(T,p) = \mathbb{P}_p(v_0 \text{ is initially healthy}) = 1 - p.$$

Suppose that x_0 is a fixed point of $h_{r,p}(x)$. Then, $x_0 = h_{r,p}(x_0) \leq 1 - p = q_0(p)$. Proceeding by induction, suppose that for some $n \geq 0$, $x_0 \leq q_n(p)$. Since $h_{r,p}(x)$ is increasing, $x_0 = h_{r,p}(x_0) \leq h_{r,p}(q_n(p)) = q_{n+1}(p)$. Therefore, $x_0 \leq \lim_{n\to\infty} q_n(p) = q(p)$, completing the proof. □

There is a small difference between the event that the root of a tree T is the root of a healthy $(r-1)$-fort and the event that some other vertex of T is the root of a healthy $(r-1)$-fort. Fix a vertex v in T that is not the root and consider the probability that v is the root of a healthy fort, in T. Since v already has a neighbour (its parent) not in the fort, then v is the root of a healthy $(r-1)$-fort iff v has at most $r-2$ children that are not, themselves, roots of healthy $(r-1)$-forts. Thus, for $T = T_\xi$, conditioning on v being a vertex of the tree,

$$\begin{aligned} &\mathbb{E}_{T_\xi}(\mathbb{P}_p(v \text{ is the root of a healthy } (r-1)\text{-fort}) \mid v \in V(T_\xi)) \\ &\qquad = (1-p)\sum_{k\geq r} \mathbb{P}(\xi = k)\mathbb{P}(\mathrm{Bin}(k, 1-q(p)) \leq r-2) \qquad (5.7) \\ &\qquad = h_{r-1,p}(q(p)). \end{aligned}$$

Since for all $s \geq 1$ and $p < 1$ we have $h_{s,p}(x) = 0$ iff $x = 0$ then in particular, $q(p) = 0$ iff $h_{r-1,p}(q(p)) = 0$.

LEMMA 5.7. *In the space of Galton–Watson trees for a fixed distribution* ξ, *if* $q(p) > 0$, *then* $\mathbb{P}_p(T_\xi$ *percolates*$) = 0$ *almost surely. If* $q(p) = 0$, *then* $\mathbb{P}_p(T_\xi$ *percolates*$) = 1$ *almost surely.*

PROOF. If $p = 1$ then $q(p) = 0$ and clearly $\mathbb{P}_p(T \text{ percolates}) = 1$. So assume that $p < 1$.

First, assume that $q(p) > 0$, with the aim of showing that

$$\mathbb{E}_{T_\xi}(\mathbb{P}_p(T_\xi \text{ percolates})) = 0.$$

By equation (5.7), there is a $\delta > 0$ be such that, for every vertex v,

$$\mathbb{E}_{T_\xi}(\mathbb{P}_p(v \text{ is in a healthy } (r-1)\text{-fort} | v \in V(T_\xi))) \geq \delta.$$

Since $\xi \geq r$ almost surely, at level t in the tree, there are at least r^t vertices. The events that these vertices are roots of healthy $(r-1)$-forts are independent; thus, for every t

$$\mathbb{E}_{T_\xi}(\mathbb{P}_p(\text{every vertex of } T_\xi \text{ at level } t \text{ is eventually infected})) \leq (1-\delta)^{r^t} \to 0$$

as $t \to \infty$. Thus, $\mathbb{E}_{T_\xi}(\mathbb{P}_p(T_\xi \text{ percolates})) = 0$ and hence the set

$$\{T : \mathbb{P}_p(T \text{ percolates}) > 0\}$$

has measure 0.

On the other hand, suppose that $\mathbb{E}_{T_\xi}(\mathbb{P}_p(T_\xi \text{ percolates})) < 1$ in hopes of showing that $q(p) > 0$. Then, the set of trees

$$\{T : \mathbb{P}_p(T \text{ percolates}) < 1\} = \{T : \mathbb{P}_p(T \text{ contains a healthy } (r-1)\text{-fort}) > 0\}$$

has positive measure.

Even though the number of infinite trees is uncountable, each tree has only a countable number of vertices and these can be thought of as a subset of a common countable set of vertices. Then, there is a vertex v for which, conditioning on v being a vertex of the tree,

$$\mathbb{E}_{T_\xi}(\mathbb{P}_p(v \text{ is the root of a healthy } (r-1)\text{-fort}) \mid v \in V(T_\xi)) > 0.$$

That is, either $q(p) > 0$ (if $v = v_0$) or $h_{r-1,p}(q(p)) > 0$. In either case, $q(p) > 0$, which completes the proof. $\square$

Thus, combining Claim 5.6 and Lemma 5.7, Lemma 5.5 holds and the critical probability is almost surely given by

$$p_c(T_\xi, r) = \inf\{p : x = h_{r,p}(x) \text{ has no solution } x \in (0,1]\}. \tag{5.8}$$

With equation (5.8) in mind, we define the following functions.

Definition 5.8. *For each $r \geq 2$ and $k \geq r$, define*

$$g_k^r(x) = \frac{\mathbb{P}(\mathrm{Bin}(k, 1-x) \leq r-1)}{x} = \sum_{i=0}^{r-1} \binom{k}{i} x^{k-i-1}(1-x)^i$$

and for any offspring distribution ξ, set

$$G_\xi^r(x) = \sum_{k \geq r} \mathbb{P}(\xi = k) g_k^r(x).$$

Using equation (5.8), the critical probability for T_ξ can be characterized in terms of the function $G_\xi^r(x)$. Note that for $p = 0$, the equation $h_{r,p}(x) = x$ has a solution at $x = 1$ and for $p = 1$, the only solution to $h_{r,p}(x) = x$ is $x = 0$. Since $h_{r,p}(x) = x(1-p)G_\xi^r(x)$, then for $p < 1$, $x = h_{r,p}(x)$ has a solution in $(0,1]$ iff $G_\xi^r(x) = \frac{1}{1-p}$ has a solution in $(0,1]$. Note that we have $G_\xi^r(1) = 1$, and so for $p > 0$, $(1-p)G_\xi^r(1) < 1$. Since $G_\xi^r(x)$ is continuous, by Lemma 5.5, if $p < p_c(T_\xi, r)$ then $\sup_{x \in (0,1]} G_\xi^r(x) \geq \frac{1}{1-p}$ and if $p_c(T_\xi, r) < p < 1$ then for every $x \in (0,1]$, $G_\xi^r(x) < \frac{1}{1-p}$. The following theorem summarizes the relation between $p_c(T_\xi, r)$ and $G_\xi^r(x)$.

THEOREM 5.9. *The critical probability for r-neighbour bootstrap percolation on the Galton–Watson tree T_ξ is, almost surely, given by*

$$p_c(T_\xi, r) = 1 - \frac{1}{\max_{x\in[0,1]} G_\xi^r(x)}. \tag{5.9}$$

Since $\max_{x\in[0,1]} G_\xi^r(x) \geq 1$, *this implies that*

$$p_c(T_\xi, r) \leq \max_{x\in[0,1]} G_\xi^r(x) - 1. \tag{5.10}$$

□

Before proceeding, we note a few facts about the functions $g_k^r(x)$. First, for all $r \geq 2$,

$$\begin{aligned} g_r^r(x) &= \frac{\mathbb{P}(\mathrm{Bin}(r, 1-x) \leq r-1)}{x} = \frac{1-(1-x)^r}{1-(1-x)} \\ &= 1 + (1-x) + (1-x)^2 + \ldots + (1-x)^{r-1} = \sum_{i=0}^{r-1} (1-x)^i. \end{aligned} \tag{5.11}$$

For any $k > r$, $\mathbb{P}(\mathrm{Bin}(k, 1-x) \leq r) = \mathbb{P}(\mathrm{Bin}(k, 1-x) \leq r-1) + \mathbb{P}(\mathrm{Bin}(k, 1-x) = r)$ and hence

$$g_k^{r+1}(x) = g_k^r(x) + \binom{k}{r} x^{k-r-1}(1-x)^r. \tag{5.12}$$

We claim that, for each fixed $r \geq 2$ and $k \geq r$,

$$g_{k+1}^r(x) - g_k^r(x) = -\binom{k}{r-1} x^{k-r}(1-x)^r. \tag{5.13}$$

Indeed, to prove equation (5.13), let $X \sim \mathrm{Bin}(k, 1-x)$ and $Y \sim \mathrm{Bin}(1, 1-x)$ be independent. Then, $X + Y \sim \mathrm{Bin}(k+1, 1-x)$ and so

$$\begin{aligned} x g_k^r(x) &= \mathbb{P}(X \leq r-1) \\ &= \mathbb{P}(X + Y \leq r-1) + \mathbb{P}(Y = 1 \text{ and } X = r-1) \\ &= x g_{k+1}^r(x) + (1-x) \cdot \binom{k}{r-1} (1-x)^{r-1} x^{k-r+1} \\ &= x \left(g_{k+1}^r(x) + \binom{k}{r-1} (1-x)^r x^{k-r} \right), \end{aligned}$$

which implies equation (5.13). Thus, by equation (5.13), for any $k \geq r$,

$$g^r_{k+1}(x) = g^r_r(x) - \sum_{i=r}^{k} \binom{i}{r-1} x^{i-r}(1-x)^r \leq g^r_r(x). \tag{5.14}$$

In particular, note that $G^r_\xi(x) \leq g^r_r(x)$.

One simple example of a Galton–Watson tree occurs when the offspring distribution is constant. When $\xi \equiv b$, T_ξ is the b-ary tree, which has the same critical probability as the $(b+1)$-regular tree, T_b. Note that, in this case, $G^r_\xi(x) = g^r_b(x)$. In the next lemma we give the asymptotic value of $p_c(T_b, r)$ as b tends to infinity for $r \geq 2$ fixed.

LEMMA 5.10. *For each* $r \geq 2$, $p_c(T_b, r) = (1 - 1/r)\left(\frac{(r-1)!}{b^r}\right)^{1/(r-1)}(1+o(1))$ *as* $b \to \infty$.

PROOF. Fix $r \geq 2$ and $b \geq r$. The critical probability for T_b in r-neighbour bootstrap percolation is given by

$$p_c(T_b, r) = 1 - \frac{1}{\max_{x\in[0,1]} g^r_b(x)} = \frac{\max_{x\in[0,1]} g^r_b(x) - 1}{\max_{x\in[0,1]} g^r_b(x)}. \tag{5.15}$$

For a lower bound on the critical probability, note that

$$\begin{aligned} g^r_b(1-y) &= \frac{\mathbb{P}(\mathrm{Bin}(b,y) \leq r-1)}{1-y} = \frac{1 - \mathbb{P}(\mathrm{Bin}(b,y) \geq r)}{1-y} \geq \frac{1 - \binom{b}{r} y^r}{1-y} \\ &\geq \frac{1 - \frac{(by)^r}{r!}}{1-y}. \end{aligned}$$

Set $y_0 = \left(\frac{(r-1)!}{b^r}\right)^{1/(r-1)}$ so that $b^r y_0^{r-1} = (r-1)!$ and consider

$$g^r_b(1-y_0) - 1 \geq \frac{y_0 - \frac{(by_0)^r}{r!}}{1-y_0} = \frac{y_0\left(1 - \frac{1}{r}\right)}{1-y_0}.$$

Then, a lower bound on the critical probability is given by

$$\begin{aligned} p_c(T_b, r) &\geq \frac{(1-1/r)\frac{y_0}{1-y_0}}{1 + (1-1/r)\frac{y_0}{1-y_0}} = \frac{(1-1/r)y_0}{1 - \frac{y_0}{r}} \geq \left(1 - \frac{1}{r}\right) y_0 \\ &= \left(1 - \frac{1}{r}\right)\left(\frac{(r-1)!}{b^r}\right)^{1/(r-1)}. \end{aligned}$$

For an upper bound on the function $g_b^r(1-y)$, consider separately different ranges for the value of y. Using Chebyshev's inequality, one can show that if $y \geq 2r/b$, then $g_b^r(1-y) < 1$. Indeed, we have

$$\begin{aligned} g_b^r(1-y) &= \frac{\mathbb{P}(\mathrm{Bin}(b,y) \leq r-1)}{1-y} \leq \frac{by(1-y)}{(by-r+1)^2(1-y)} \\ &< \frac{by}{(by-r)^2} \leq \frac{by}{(by/2)^2} = \frac{4}{by} \leq \frac{4}{2r} \leq 1. \end{aligned}$$

Consider the function

$$(1-y)(g_b^r(1-y)-1) = \mathbb{P}(\mathrm{Bin}(b,y) \leq r-1) - (1-y) = y - \mathbb{P}(\mathrm{Bin}(b,y) \geq r). \tag{5.16}$$

Suppose that $b > e^{4r}r$ and consider y such that $(r^r e^{4r} b^{-r})^{1/(r-1)} < y < 2r/b$. Then $2r/b < 1/2$ and, using the fact that $\binom{b}{r} \geq b^r/r^r$,

$$\begin{aligned} y - \mathbb{P}(\mathrm{Bin}(b,y) \geq r) &\leq y - \binom{b}{r} y^r (1-y)^{b-r} \\ &\leq y - \frac{b^r}{r^r} y^r e^{-2yb} \leq y - y\frac{b^r y^{r-1}}{r^r} e^{-4r} \\ &= y\left(1 - y^{r-1}\frac{b^r}{e^{4r}r^r}\right) < 0. \end{aligned}$$

Consider now $y \leq \left(\frac{r^r e^{4r}}{b^r}\right)^{1/(r-1)}$. Using equation (5.16) and (5.6) with y in place of $1-x$, the maximum value for $(1-y)(g_b^r(1-y)-1)$ occurs at y_1 with $\mathbb{P}(\mathrm{Bin}(b-1,y_1) = r-1) = \frac{1}{b}$ and hence $\binom{b}{r} y_1^{r-1}(1-y_1)^{b-r} = 1/r$. Thus,

$$y - \mathbb{P}(\mathrm{Bin}(b,y) \geq r) \leq y_1 - \mathbb{P}(\mathrm{Bin}(b,y_1) = r) = y_1\left(1 - \frac{1}{r}\right). \tag{5.17}$$

By the choice of y_1, noting that $y_1 b \leq \left(r^r e^{4r}\right)^{1/(r-1)} b^{-1/(r-1)} = o(1)$,

$$\begin{aligned} y_1^{r-1} &= \frac{1}{b\binom{b-1}{r-1}}(1-y_1)^{-(b-r)} \\ &\leq \frac{(r-1)!}{b^r}\frac{b^r}{b(b-1)\dots(b-r+1)}e^{2y_1 b} \\ &= \frac{(r-1)!}{b^r}(1+o(1)). \end{aligned} \tag{5.18}$$

Thus, by (5.16), (5.17) and (5.18),

$$\begin{aligned}\max_{y\in[0,1]}\left(g_b^r(1-y)-1\right) &\le \frac{1}{1-\left(\frac{r^r e^{4r}}{b^r}\right)^{1/(r-1)}}\left(1-\frac{1}{r}\right)y_1\\ &\le \left(1-\frac{1}{r}\right)\left(\frac{(r-1)!}{b^r}\right)^{1/(r-1)}(1+o(1)). \qquad (5.19)\end{aligned}$$

and the upper bound on $p_c(T_b,r)$ follows from (5.15). $\square$

5.3. Critical probabilities for Galton–Watson trees

5.3.1. Bounds for $f_r^{GW}(b)$. With the definitions from section 5.2, we are now ready to prove Theorem 5.1: For every $r\ge 2$ there are positive constants c_r and C_r so that for every $b\ge r$,

$$\frac{c_r}{b}e^{-\frac{b}{r-1}}\le f_r^{GW}(b)\le C_r e^{-\frac{b}{r-1}}.$$

The proof of Theorem 5.1 is given in two parts. The lower bound for $f_r^{GW}(b)$ is given in Lemma 5.11, to come, by examining properties of the function $G_\xi^r(x)$. The upper bound for $f_r^{GW}(b)$ is given in Lemma 5.13 by producing a family of Galton–Watson trees with fixed branching number and small critical probability for r-neighbour bootstrap percolation.

LEMMA 5.11. *For every $r\ge 2$ and for any offspring distribution ξ with $\mathbb{E}(\xi)=b\ge r$,*

$$p_c(T_\xi,r)\ge\frac{e^{-\frac{r-2}{r-1}}}{b}e^{-\frac{b}{r-1}}.$$

PROOF. In what follows, we shall need to consider integrals of functions related to $g_k^r(x)$ and so recall from the definition of the beta function that for all $a,b\in\mathbb{Z}^+$,

$$\int_0^1 x^a(1-x)^b\,dx=\frac{a!\;b!}{(a+b+1)!}.$$

By equation (5.14), for any $k \geq r$, using $H_\ell = \sum_{i=1}^{\ell} \frac{1}{i}$ to denote the ℓ-th harmonic number,

$$\begin{aligned} \int_0^1 \frac{g_r^r(x) - g_k^r(x)}{(1-x)^2}\,dx &= \sum_{i=r}^{k-1} \binom{i}{r-1} \int_0^1 x^{i-r}(1-x)^{r-2}\,dx \\ &= \sum_{i=r}^{k-1} \binom{i}{r-1} \frac{(i-r)!(r-2)!}{(i-1)!} \\ &= \sum_{i=r}^{k-1} \frac{1}{r-1}\frac{i}{i-r+1} \\ &= \frac{1}{r-1}\sum_{i=r}^{k-1}\left(1 + \frac{r-1}{i-r+1}\right) = \frac{k-r}{r-1} + H_{k-r}. \end{aligned} \tag{5.20}$$

Therefore, for any offspring distribution ξ, since $\xi \geq r$ almost surely,

$$\begin{aligned} \int_0^1 \frac{g_r^r(x) - G_\xi^r(x)}{(1-x)^2}\,dx &= \sum_{k \geq r} \mathbb{P}(\xi = k)\left(\frac{k-r}{r-1} + H_{k-r}\right) \\ &= \frac{\mathbb{E}\xi}{r-1} + \mathbb{E}(H_{\xi-r}) - \frac{r}{r-1}. \end{aligned} \tag{5.21}$$

On the other hand, let $M = \max_{x\in[0,1]} G_\xi^r(x)$. Then by equation (5.9), $p_c = p_c(T_\xi, r) = 1-\frac{1}{M}$. Note that, since by (5.11) $g_r^r(x)$ is decreasing and continuous, $g_r^r(0) = r$, $g_r^r(1) = 1$ and $G_\xi^r(x) \leq g_r^r(x)$, we have $M \in [1, r]$ and there is a unique $y \in [0,1]$ with $g_r^r(1-y) = M$. Then, by (5.11),

$$\begin{aligned} \int_0^{1-y} \frac{g_r^r(x) - M}{(1-x)^2}\,dx &= \left\{ -\frac{M-1}{1-x} - \log(1-x) - \sum_{i=2}^{r-1} \frac{(1-x)^{i-1}}{i-1} \right\}_{x=0}^{1-y} \\ &= (M-1)(1-1/y) - \log y + \sum_{i=1}^{r-2} \frac{1-y^i}{i}. \end{aligned}$$

Note that $(M-1)(1-1/y) = \frac{(y+y^2+\ldots+y^{r-1})(y-1)}{y} = y^{r-1} - 1$. Thus, the above expression can be simplified, as

$$\begin{aligned} \int_0^{1-y} \frac{g_r^r(x) - M}{(1-x)^2}\,dx &= y^{r-1} - 1 - \log y + \sum_{i=1}^{r-2} \frac{1-y^i}{i} \\ &\geq y^{r-1} - 1 - \log y. \end{aligned} \tag{5.22}$$

Now, using the definition of y,

$$p_c = 1 - \frac{1}{M} = \frac{M-1}{M} = \frac{y + y^2 + \ldots + y^{r-1}}{1 + y + y^2 + \ldots + y^{r-1}} = \frac{y(1-y^{r-1})}{1-y^r}. \tag{5.23}$$

Note that for any $y \in [0,1)$,

$$\log\left(\frac{1-y^r}{1-y^{r-1}}\right) \leq \log\left(\frac{1-y^{2r-2}}{1-y^{r-1}}\right) = \log(1+y^{r-1}) \leq y^{r-1}$$

and from this, using (5.23), we obtain

$$y^{r-1} - \log y \geq \log\left(\frac{1-y^r}{1-y^{r-1}}\right) - \log y = -\log\left(\frac{y(1-y^{r-1})}{1-y^r}\right) = -\log p_c.$$

Since $g_r^r(x) - G_\xi^r(x) \geq 0$ then, using (5.21) and (5.22),

$$\begin{aligned} -\log p_c - 1 &\leq \int_0^{1-y} \frac{g_r^r(x) - M}{(1-x)^2}\,dx \leq \int_0^1 \frac{g_r^r(x) - G_\xi^r(x)}{(1-x)^2}\,dx \\ &= \frac{\mathbb{E}\xi}{r-1} + \mathbb{E}(H_{\xi-r}) - \frac{r}{r-1} \end{aligned}$$

and hence

$$p_c(T_\xi, r) \geq \exp\left(-\frac{\mathbb{E}(\xi)-1}{r-1} - \mathbb{E}(H_{\xi-r})\right) \geq \exp\left(-\frac{b-1}{r-1} - \mathbb{E}(H_\xi)\right). \tag{5.24}$$

Using the inequality $H_n \leq \log n + 1$ for $n \geq 1$ and the concavity of the logarithm function we see that $\mathbb{E}(H_\xi) \leq \log b + 1$ and thus

$$p_c(T_\xi, r) \geq \exp\left(-\frac{r-2}{r-1}\right)\frac{e^{-\frac{b}{r-1}}}{b},$$

completing the proof of the lemma. □

By Lemma 5.11, the lower bound in Theorem 5.1 holds with $c_r = e^{-\frac{r-2}{r-1}}$.

Next let us prove that there exists $C_r > 0$ so that $f_r^{GW}(b) \leq C_r e^{\frac{b}{r-1}}$ when b is sufficiently large. We shall do this by first considering a sequence of offspring distributions which, as we show, have critical probability 0.

For each $r \geq 2$, define an offspring distribution ξ_r as follows. For every $k \geq r$, set $\mathbb{P}(\xi_r = k) = \frac{r-1}{k(k-1)}$. Note that for any r, $\mathbb{E}(\xi_r) = \infty$. In Lemma 5.13 below, we show that, given $b > r$ sufficiently large, the distribution ξ_r can be 'pruned' to obtain the appropriate critical probability and mean b.

Claim 5.12. *For each $r \geq 2$, and for all $x \in [0,1]$, $G^r_{\xi_r}(x) = 1$.*

Proof. We apply induction on r. First, for $r = 2$, by the definition of the function $G^r_\xi(x)$,

$$\begin{aligned} G^2_{\xi_2}(x) &= \sum_{k\geq 2} \frac{1}{k(k-1)} \left(kx^{k-2} - (k-1)x^{k-1}\right) \\ &= 1 + \sum_{k\geq 3} \frac{1}{k-1} x^{k-2} - \sum_{k\geq 2} \frac{1}{k} x^{k-1} \\ &= 1, \end{aligned}$$

as claimed. Turning to the induction step, assume that the Claim holds for $r \geq 2$: $G^r_{\xi_r}(x) = 1$ for $x \in [0,1)$. Then, for $x \in [0,1)$,

$$\begin{aligned} G^{r+1}_{\xi_{r+1}}(x) &= \sum_{k\geq r+1} \frac{r}{k(k-1)} g^{r+1}_k(x) \\ &= \sum_{k\geq r+1} \frac{r}{k(k-1)} \left(g^r_k(x) + \binom{k}{r} x^{k-r-1}(1-x)^r\right) \qquad \text{(by (5.12))} \\ &= \frac{r}{r-1}\left(\sum_{k\geq r} \frac{r-1}{k(k-1)} g^r_k(x) - \frac{1}{r} g^r_r(x)\right) \\ &\quad + \sum_{k\geq r+1} \frac{1}{r-1}\binom{k-2}{r-2} x^{k-r-1}(1-x)^r \\ &= \frac{r}{r-1} G^r_{\xi_r}(x) - \frac{1}{r-1}\left(g^r_r(x) - \frac{1-x-(1-x)^r}{x}\right) \\ &= \frac{r}{r-1} - \frac{1}{r-1}\left(\frac{1-(1-x)^r}{x} - \frac{1-x-(1-x)^r}{x}\right) \qquad \text{(by (5.11))} \\ &= \frac{r}{r-1} - \frac{1}{r-1} = 1, \end{aligned}$$

so our claim holds for $r+1$, completing the proof. □

By (5.9), an immediate corollary of Claim 5.12 is that, for every $r \geq 2$, the Galton–Watson tree T_{ξ_r} satisfies $p_c(T_{\xi_r}, r) = 0$.

LEMMA 5.13. *For every $r \geq 2$, there is a constant C_r such that if $b \geq (r-1)\log(4er)$, then there is an offspring distribution $\eta_{r,b}$ with $\mathbb{E}(\eta_{r,b}) = b$ and*

$$p_c(T_{\eta_{r,b}}, r) \leq C_r e^{-\frac{b}{r-1}}.$$

PROOF. If b is sufficiently large, the distribution $\eta_{r,b}$ is constructed by restricting the support of the distribution ξ_r to a finite set of integers and redistributing the remaining measure suitably. Note that for $m \geq r$ we have

$$\mathbb{P}(\xi_r \leq m) = \sum_{k=r}^{m} \mathbb{P}(\xi_r = k) = (r-1)\sum_{k=r}^{m}\left(\frac{1}{k-1} - \frac{1}{k}\right) = 1 - \frac{r-1}{m}. \quad (5.25)$$

Also, using the convention that $H_0 = 0$,

$$\sum_{k=r}^{m} k\mathbb{P}(\xi_r = k) = (r-1)\sum_{k=r}^{m}\frac{1}{k-1} = (r-1)\left(H_{m-1} - H_{r-2}\right)$$

is the part of the expected value contributed by the $(m-r+1)$ smallest possible values of ξ_r. Given b and r, let $k_0 = \max\{m : (r-1)\left(H_{m-1} - H_{r-2}\right) \leq b\}$. Then,

$$b < (r-1)\left(H_{k_0} - H_{r-2}\right) < (r-1)H_{k_0} \leq (r-1)(\log k_0 + 1),$$

so $k_0 > e^{\frac{b}{r-1}-1} \geq 4r$ for $b \geq (r-1)\left(\log(4r)+1\right) = (r-1)\log(4er)$.

Let $k_1 = k_0 - 2r > r$. Then by equation (5.25) we have

$$A = 1 - \sum_{k=r}^{k_1} \mathbb{P}(\xi_r = m) = \frac{r-1}{k_1} = \frac{r-1}{k_0 - 2r}.$$

Define $K = b - \sum_{k=r}^{k_1} k\mathbb{P}(\xi_r = k)$, roughly thought of as the unallocated portion of the expected value. Then K can be bounded from below by

$$K \geq \sum_{k=k_1+1}^{k_0} k\mathbb{P}(\xi_r = k) = (r-1)\left(H_{k_0-1} - H_{k_1-1}\right) \geq (r-1)\frac{2r}{k_0}.$$

Since $b < \sum_{k=r}^{k_0+1} k\mathbb{P}(\xi_r = k)$, we have that

$$K < \sum_{k=k_1+1}^{k_0+1} k\mathbb{P}(\xi_r = k) = (r-1)\left(H_{k_0} - H_{k_1-1}\right) \leq (r-1)\frac{2r+1}{k_0 - 2r}.$$

Thus, it follows that $K/A \leq 2r+1$ and for $k_0 > 4r$,

$$K/A \geq 2r\left(\frac{r-1}{k_0}\right)\left(\frac{k_0-2r}{r-1}\right) = 2r\left(\frac{k_0-2r}{k_0}\right) > r.$$

This implies that, for $b > (r-1)\log(4er)$, there exists $\alpha \in (0,1)$ such that $\frac{K}{A} = \alpha r + (1-\alpha)(2r+1)$ and hence,

$$\sum_{k=r}^{k_1} k\mathbb{P}(\xi_r = k) + \alpha A r + (1-\alpha)A(2r+1) = b.$$

This is used to define the pruned offspring distribution $\eta_{r,b}$ as follows,

$$\mathbb{P}(\eta_{r,b} = k) = \begin{cases} \mathbb{P}(\xi_r = k) & \text{for } r < k \leq k_1,\ k \neq 2r+1 \\ \mathbb{P}(\xi_r = r) + \alpha A & \text{for } k = r, \text{ and} \\ \mathbb{P}(\xi_r = 2r+1) + (1-\alpha)A & \text{for } k = 2r+1. \end{cases}$$

Note that since $k_0 > 4r$, $k_1 = k_0 - 2r > 2r$.

This pruning $\eta_{r,b}$ of the distribution of ξ_r is used to give an upper bound on $f_r^{GW}(b)$. Recall that for every $k \geq r$, the functions $g_k^r(x)$, given by Definition 5.8, are non-negative and by equation (5.14), $g_k^r(x) \leq g_r^r(x)$. By Claim 5.12, $G_{\xi_r}^r(x) = 1$ which shows that,

$$G_{\eta_{r,b}}^r(x) \leq G_{\xi_r}^r(x) + \alpha A g_r^r(x) + (1-\alpha)A g_{2r+1}^r(x) \leq 1 + A g_r^r(x).$$

Therefore, since $g_r^r(x)$ is decreasing and $g_r^r(0) = r$, we have $\max_{x\in[0,1]} G_{\eta_{r,b}}^r(x) \leq 1 + A g_r^r(0) = 1 + Ar$, and so by (5.10)

$$p_c(T_{\eta_{r,b}}, r) \leq Ar = \frac{r(r-1)}{k_0 - 2r} < \frac{r(r-1)}{e^{\frac{b-r+1}{r-1}} - 2r} < 2er(r-1)e^{-\frac{b}{r-1}}$$

for $b > (r-1)\log(4er)$. □

Thus the upper bound in Theorem 5.1 holds with $C_r = 2er(r-1)$ for $b \geq (r-1)\log(4er)$, and it is trivially true for some C_r for smaller b.

5.3.2. Bounds for $p_c(T_\xi, r)$.

5.3.2.1. *Bounds based on higher moments.* In this section, we shall prove a lower bound on the critical probability $p_c(T_\xi, r)$ based on the $(1+\alpha)$-moments of the offspring distribution ξ for all $\alpha \in (0, r-1)$, using a modification of the proof of Lemma 5.11 and some properties of the gamma and beta functions.

Recall that the gamma function is given, for z with $\Re(z) > 0$, by $\Gamma(z) = \int_0^\infty t^{z-1}e^{-t}\,dt$, and for all $n \in \mathbb{Z}^+$, satisfies $\Gamma(n) = (n-1)!$ (for more on the gamma function see the work of Artin [**7**]). The beta function is given, for $\Re(x), \Re(y) > 0$, by $\mathrm{B}(x,y) = \int_0^1 t^{x-1}(1-t)^{y-1}\,dt$ and satisfies $\mathrm{B}(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}$. We shall use the following bound on the ratio of two values of the gamma function obtained by Gautschi [**31**]. For $n \in \mathbb{N}$ and $0 \le s \le 1$,

$$\left(\frac{1}{n+1}\right)^{1-s} \le \frac{\Gamma(n+s)}{\Gamma(n+1)} \le \left(\frac{1}{n}\right)^{1-s}. \tag{5.26}$$

The proof of the lower bound on $p_c(T_\xi, r)$ in Theorem 5.2 is first given for the case $\alpha \in (0, r-1) \setminus \mathbb{N}$. For $\alpha \in \{1, 2, \dots, r-2\}$, we then deduce the result by a continuity argument.

Proof of Theorem 5.2. Fix $r \ge 2$, $\alpha \in (0, r-1)$ with $\alpha \notin \mathbb{N}$ and an offspring distribution ξ. Set $t = \lfloor \alpha \rfloor$ and $\varepsilon = \alpha - t$ so that $\varepsilon \in (0,1)$ and t is an integer with $t \in [0, r-2]$. For the upper bound, from (5.14) and the definition of the beta function, for every $k \ge r$

$$\begin{aligned}
\int_0^1 \frac{g_r^r(x) - g_k^r(x)}{(1-x)^{\alpha+2}}\,dx &= \sum_{i=r}^{k-1} \binom{i}{r-1} \int_0^1 x^{i-r}(1-x)^{r-2-\alpha}\,dx \\
&= \sum_{i=r}^{k-1} \binom{i}{r-1} \mathrm{B}(i-r+1, r-1-\alpha) \\
&= \sum_{i=r}^{k-1} \frac{i!}{(r-1)!(i-r+1)!} \frac{(i-r)!\Gamma(r-1-\alpha)}{\Gamma(i-\alpha)} \\
&= \sum_{i=r}^{k-1} \frac{i(i-1)\dots(i-t)\Gamma(i-t)}{(i-r+1)\Gamma(i-t-\varepsilon)} \\
&\qquad \cdot \frac{\Gamma(r-1-t-\varepsilon)}{(r-1)(r-2)\dots(r-1-t)\Gamma(r-1-t)}.
\end{aligned} \tag{5.27}$$

Let $c_1 = c_1(r, \alpha) = \frac{\Gamma(r-1-t-\varepsilon)}{(r-1)(r-2)\cdots(r-1-t)\Gamma(r-1-t)}$. Note that by inequality (5.26), for $t < r-2$,

$$\frac{\Gamma(r-1-t-\varepsilon)}{\Gamma(r-1-t)} \leq \frac{1}{(r-2-t)^{\varepsilon}}$$

and so

$$c_1 \leq \frac{1}{(r-2-t)^{t+1+\varepsilon}} = (r-2-t)^{-(\alpha+1)}.$$

Note that this upper bound is finite for all $\varepsilon \in (0,1]$ which will be crucial in our continuity argument. On the other hand, if $t = r-2$, then

$$c_1 = \frac{\Gamma(1-\varepsilon)}{(r-1)!} = \frac{\Gamma(2-\varepsilon)}{(1-\varepsilon)(r-1)!} \geq \frac{1}{2(r-1)!(1-\varepsilon)}$$

which tends to ∞ as $\varepsilon \to 1$, e.g., as $\alpha \to r-1$.

Thus, continuing equation (5.27), applying inequality (5.26) again yields

$$\begin{aligned}
&\sum_{i=r}^{k-1} \frac{i(i-1)\cdots(i-t)\Gamma(i-t)}{(i-r+1)\Gamma(i-t-\varepsilon)} \cdot \frac{\Gamma(r-1-t-\varepsilon)}{(r-1)(r-2)\cdots(r-1-t)\Gamma(r-1-t)} \\
&\quad \leq c_1 \sum_{i=r}^{k-1} \frac{i}{i-r+1}(i-1)(i-2)\cdots(i-t)(i-t)^{\varepsilon} \\
&\quad \leq r c_1 \sum_{i=r}^{k-1} i^{t+\varepsilon} \\
&\quad \leq r c_1 k^{1+t+\varepsilon} = r c_1 k^{1+\alpha}.
\end{aligned}$$

Thus, taking the expectation over k with respect to ξ,

$$\int_0^1 \frac{g_r^r(x) - G_\xi^r(x)}{(1-x)^{2+\alpha}}\, dx \leq r c_1 \mathbb{E}(\xi^{1+\alpha}). \tag{5.28}$$

Let us now bound our integral from below by some function of p_c. Again, for an offspring distribution ξ let $M = \max_{x\in[0,1]} G_\xi^r(x)$. Recall that we have $p_c = p_c(T_\xi, r) = 1 - \frac{1}{M}$. Recall also that, since $g_r^r(x)$ is decreasing and continuous, $g_r^r(0) = r$, $g_r^r(1) = 1$ and $G_\xi^r(x) \leq g_r^r(x)$, we have $M \in [1, r]$ and there is a unique $y \in [0,1]$ with $g_r^r(1-y) = M$. Thus $M = 1 + y + \ldots + y^{r-1}$ and so (recall (5.23))

$$p_c = 1 - \frac{1}{M} = \frac{y(1-y^{r-1})}{1-y^r} \geq \frac{r-1}{r} y, \tag{5.29}$$

using $1-y^r \le \frac{r(1-y^{r-1})}{r-1}$. A lower bound on the integral in question is given by

$$\begin{aligned}
\int_0^1 \frac{g_r^r(x)-G_\xi^r(x)}{(1-x)^{2+\alpha}}\,dx &\ge \int_0^{1-y}\frac{g_r^r(x)-M}{(1-x)^{2+\alpha}}\,dx\\
&= \int_0^{1-y} -\frac{(M-1)}{(1-x)^{2+\alpha}} + \sum_{i=0}^{t}\frac{1}{(1-x)^{\alpha+1-i}} + \sum_{i=t+1}^{r-2}(1-x)^{i-\alpha-1}\,dx\\
&= \left[-\frac{(M-1)}{(\alpha+1)(1-x)^{1+\alpha}} + \sum_{i=0}^{t}\frac{1}{(\alpha-i)(1-x)^{\alpha-i}} - \sum_{i=t+1}^{r-2}\frac{(1-x)^{i-\alpha}}{i-\alpha}\right]_0^{1-y}\\
&= -\frac{(M-1)}{(\alpha+1)}\left(\frac{1}{y^{1+\alpha}}-1\right) + \sum_{i=0}^{t}\frac{1}{\alpha-i}\left(\frac{1}{y^{\alpha-i}}-1\right) + \sum_{i=t+1}^{r-2}\frac{1-y^{i-\alpha}}{i-\alpha}\\
&= \frac{1}{y^\alpha}\left(\frac{M-1}{\alpha+1}\left(\frac{y^{\alpha+1}-1}{y}\right) + \sum_{i=0}^{t}\frac{y^i-y^\alpha}{\alpha-i} + \sum_{i=t+1}^{r-2}\frac{y^\alpha-y^i}{i-\alpha}\right)\\
&= \frac{1}{y^\alpha}\left(\frac{(1+y+\cdots+y^{r-2})(y^{\alpha+1}-1)}{(\alpha+1)} + \sum_{i=0}^{t}\frac{y^i-y^\alpha}{\alpha-i} + \sum_{i=t+1}^{r-2}\frac{y^\alpha-y^i}{i-\alpha}\right)\\
&= \frac{1}{y^\alpha}\left(\frac{-1}{\alpha+1}+\frac{1}{\alpha}+\sum_{i=1}^{t}\left(\frac{y^i}{\alpha-i}-\frac{y^i}{\alpha+1}\right) - \frac{y^{t+1}}{\alpha+1} + \sum_{i=0}^{r-t-4}\frac{y^{\alpha+1+i}-y^{t+2+i}}{\alpha+1}\right.\\
&\qquad\left. + \sum_{i=r-t-3}^{r-2}\frac{y^{\alpha+1+i}}{\alpha+1} - \sum_{i=0}^{t}\frac{y^\alpha}{\alpha-i} + \sum_{i=t+1}^{r-2}\frac{y^\alpha-y^i}{i-\alpha}\right)\\
&\ge \frac{1}{y^\alpha}\left(\frac{1}{\alpha(\alpha+1)} - \frac{y^{t+1}}{\alpha+1} - \sum_{i=0}^{t}\frac{y^\alpha}{\alpha-i}\right).
\end{aligned}$$

Set $c_2 = c_2(\alpha) = \sum_{i=0}^{t}\frac{1}{\alpha-i} + \frac{1}{\alpha+1}$ and consider separately two different cases. For the first, if $y^\alpha c_2 \ge \frac{1}{2\alpha(\alpha+1)}$ then since $\mathbb{E}(\xi^{\alpha+1}) \ge 1$,

$$y^\alpha \ge \frac{1}{2\alpha(\alpha+1)c_2} \ge \frac{1}{2\alpha(\alpha+1)c_2}\mathbb{E}(\xi^{1+\alpha})^{-1}.$$

Thus, if $c_2' = \left(\frac{1}{2\alpha(\alpha+1)c_2}\right)^{1/\alpha}$, then $y \ge c_2'\mathbb{E}(\xi^{1+\alpha})^{-1/\alpha}$.

In the second case, if $y^\alpha < \frac{1}{2\alpha(\alpha+1)c_2}$, then since $y^{t+1} \le y^\alpha$, we have

$$\int_0^1 \frac{g_r^r(x)-G_\xi^r(x)}{(1-x)^{2+\alpha}}\,dx \ge \frac{1}{y^\alpha}\frac{1}{2\alpha(\alpha+1)}. \tag{5.30}$$

Combining equation (5.30) with equation (5.28) yields

$$y^\alpha \geq \frac{1}{2\alpha(\alpha+1)} \frac{1}{rc_1} \mathbb{E}(\xi^{1+\alpha})^{-1}$$

and setting $c_1' = (2\alpha(\alpha+1)rc_1)^{-1/\alpha}$ gives $y \geq c_1' \mathbb{E}(\xi^{1+\alpha})^{-1/\alpha}$.

Finally, set $c_{r,\alpha} = \frac{r-1}{r} \min\{c_1', c_2'\}$ so that by inequality (5.29) we obtain,

$$p_c(T_\xi, r) \geq \frac{r-1}{r} y \geq c_{r,\alpha} \mathbb{E}(\xi^{1+\alpha})^{-1/\alpha}.$$

For every $n \in \{1, 2, \ldots, r-2\}$, note that $\lim_{\alpha \to n^-} c_{r,\alpha} > 0$ and, by monotone convergence theorem, there is a constant $c_{r,n} > 0$ so that

$$p_c(T_\xi, r) \geq c_{r,n} \mathbb{E}(\xi^{1+n})^{-1/n}.$$

This completes the proof of the lower bound on $p_c(T_\xi, r)$.

Note that in the above proof, as $\alpha \to (r-1)^-$, we have $c_1(r, \alpha) \to \infty$ and hence $\lim_{\alpha \to (r-1)^-} c_{r,\alpha} = 0$, so the proof does not directly extend to the case $\alpha = r-1$. We deal with this problem for $r = 2$ in Theorem 5.3 where an essentially sharp lower bound on $p_c(T_\xi, 2)$ is given based on the second moment of ξ.

The upper bound in Theorem 5.2 follows from (5.10) and (5.19) which show that for any $r \geq 2$ there is a constant $c_r > 0$ such that for any $k \geq r$,

$$\max_{x \in [0,1]} g_k^r(x) - 1 \leq \frac{c_r}{k^{r/(r-1)}}.$$

Thus the upper bound follows immediately from inequality (5.10). $\square$

5.3.2.2. *Bounds for* $p_c(T_\xi, 2)$. In this section we focus on 2-neighbour bootstrap percolation on Galton–Watson trees. This specific problem is easier to tackle analytically which gives us an opportunity to obtain sharp bounds on $p_c(T_\xi, 2)$. To simplify notation, we write G_ξ for G_ξ^2.

Proof of Theorem 5.3. First we prove the rather easy bound given in (5.2). By the definition of function $G_\xi(x)$ we see that for each $k \geq 2$ we have

$$G_\xi(x) \geq \mathbb{P}(\xi = k) g_k^2(x) = \mathbb{P}(\xi = k) \left(kx^{k-2} - (k-1)x^{k-1}\right).$$

Now, $g_2^2(x) = 2-x$ so it attains its maximum in the interval $[0,1]$ at $x = 0$ with $g_2^2(0) = 2$, while for $k \geq 3$ the functions $g_k^2(x)$ are maximized at $x_k = \frac{k(k-2)}{(k-1)^2}$, with $g_k^2(x_k) = \frac{k^{k-1}(k-2)^{k-2}}{(k-1)^{2k-3}}$. Thus formula (5.2) follows immediately from (5.9).

Considering the maximum value of the function $g_k^2(x)$,

$$\frac{k^{k-1}(k-2)^{k-2}}{(k-1)^{2k-3}} = \left(\frac{k(k-2)}{(k-1)^2}\right)^{k-1}\left(\frac{k-1}{k-2}\right) = \left(1-\frac{1}{(k-1)^2}\right)^{k-1}\left(\frac{k-1}{k-2}\right).$$

One can show that for $k \geq 3$ and $t \geq 1$,

$$\left(1-\frac{1}{(k-1)^2}\right)^t \leq 1-\frac{t}{(k-1)^2}+\frac{t(t-1)}{2(k-1)^4}. \tag{5.31}$$

Indeed, inequality (5.31) follows from the following argument. Clearly, for t independent Bernoulli variables $X_1,\dots,X_t$ such that for all $1 \leq i \leq t$ we have $\mathbb{P}(X_i = 1) = \frac{1}{(k-1)^2}$, we have $\mathbb{P}(\max\{X_1,\dots,X_t\} = 1) = 1-\left(1-\frac{1}{(k-1)^2}\right)^t$. Also, by inclusion-exclusion formula, $\mathbb{P}(\max\{X_1,\dots,X_t\} = 1) \geq t\mathbb{P}(X_1 = 1) - \binom{t}{2}\mathbb{P}(X_1 = 1)^2$, which implies inequality (5.31).

In particular, setting $t = k-1$ in this inequality yields

$$\left(1-\frac{1}{(k-1)^2}\right)^{k-1} \leq 1-\frac{1}{(k-1)}+\frac{(k-2)}{2(k-1)^3} = \frac{(k-2)}{(k-1)}\left(1+\frac{1}{2(k-1)^2}\right)$$

and hence for $k \geq 3$, and all $x \in [0,1]$, $g_k^2(x) \leq 1+\frac{1}{2(k-1)^2}$. The maximum value for $g_2^2(x)$ is $g_2^2(0) = 2 > 1+\frac{1}{2}$, but it is certainly true that for all $k \geq 2$, $g_k^2(x) \leq 1+\frac{1}{2(k-1)^2-(k-1)} = 1+\frac{1}{(k-1)(2k-3)}$. Hence

$$G_\xi(x) \leq 1+\mathbb{E}\left(\frac{1}{(\xi-1)(2\xi-3)}\right)$$

which with (5.10) yields the upper bound given by inequality (5.3). Note that the first bound in inequality (5.3) is essentially sharp as demonstrated by the $(b+1)$-regular tree T_b for which $p_c(T_b,2) \sim \frac{1}{2b^2}$.

Now let us prove bound (5.4). To simplify notation, for every k, let $(\xi)_k = \xi(\xi-1)(\xi-2)\dots(\xi-k+1)$ denote the k-th falling factorial. The goal is to approximate $G_\xi(x)$ by a polynomial of degree 2 whose maximum value can be easily calculated.

Consider the Taylor series for $G_\xi(x)$ about $x = 1$. For this, note that

$$\begin{aligned}
G_\xi(1) &= \sum_{k\geq 2} \mathbb{P}(\xi = k) = 1,\\
G'_\xi(1) &= \sum_{k\geq 2} \mathbb{P}(\xi = k)(-1) = -1,\\
G''_\xi(1) &= \sum_{k\geq 2} \mathbb{P}(\xi = k)(-(k-2)(k+1)) = \sum_{k\geq 2} \mathbb{P}(\xi = k)(-k(k-1)+2)\\
&= -\mathbb{E}((\xi)_2) + 2.
\end{aligned}$$

Note that for all $m \geq 1$, $G_\xi^{(m)}(1) < 0$, where it exists.

Set $P_2(x) = 1 - (x-1) - \frac{(\mathbb{E}(\xi)_2 - 2)}{2}(1-x)^2 = 2 - x - \frac{(\mathbb{E}(\xi)_2-2)}{2}(1-x)^2$. It is shown below that for all $x \in [0,1]$, $P_2(x) \leq G_\xi(x)$. Note that

$$P_2(x) = \sum_{k\geq 2} \mathbb{P}(\xi = k)\left(g_2^2(x) - \frac{(k^2-k-2)}{2}(1-x)^2\right).$$

Recall that, by equation (5.13), for all x, $g_{k+1}^2(x) - g_k^2(x) = -kx^{k-2}(1-x)^2$. Thus,

$$\begin{aligned}
g_{k+1}^2(x) &+ \frac{((k+1)^2-(k+1)-2)}{2}(1-x)^2\\
&\quad - \left(g_k^2(x) + \frac{(k^2-k-2)}{2}(1-x)^2\right)\\
&= -kx^{k-2}(1-x)^2 + \frac{2k}{2}(1-x)^2\\
&= k(1-x)^2(1-x^{k-2}).
\end{aligned} \tag{5.32}$$

Considering $G_\xi(x) - P_2(x)$, note that for $k = 2$,

$$g_k^2(x) - g_2^2(x) + \frac{(k^2-k-2)}{2}(1-x)^2 = 0.$$

For $k \geq 3$, by (5.32),

$$g_k^2(x) - g_2^2(x) + \frac{(k^2-k-2)}{2}(1-x)^2 = \sum_{i=2}^{k-1} i(1-x)^2(1-x^{i-2}) \geq 0.$$

Hence,

$$G_\xi(x) - P_2(x) = \sum_{k\geq 2} \mathbb{P}(\xi = k)\left(g_k^2(x) - g_2^2(x) + \frac{(k^2-k-2)}{2}(1-x)^2\right) \geq 0$$

and so for all x, $G_\xi(x) \geq P_2(x)$.

Now, $P_2(x)$ is a parabola which attains its maximum value at $x = 1 - \frac{1}{\mathbb{E}(\xi)_2 - 2}$ with

$$\begin{aligned} P_2\left(1 - \frac{1}{\mathbb{E}(\xi)_2 - 2}\right) &= 1 + \frac{1}{\mathbb{E}(\xi)_2 - 2} - \frac{1}{2}(\mathbb{E}(\xi)_2 - 2)\frac{1}{(\mathbb{E}(\xi)_2 - 2)^2} \\ &= 1 + \frac{1}{2(\mathbb{E}(\xi)_2 - 2)}. \end{aligned}$$

This immediately implies a lower bound for the critical probability for T_ξ,

$$p_c(T_\xi, 2) \geq 1 - \frac{1}{1 + \frac{1}{2\mathbb{E}(\xi)_2 - 4}} = 1 - \frac{2\mathbb{E}(\xi)_2 - 4}{2\mathbb{E}(\xi)_2 - 3} = \frac{1}{2\mathbb{E}(\xi)_2 - 3}.$$

□

5.3.3. Examples. The $(b+1)$-regular tree shows that one cannot hope for a stronger bound based on the second moment of ξ than the one given by inequality (5.4). What is more, this bound turns out to be an accurate estimate of the critical probability in a number of natural offspring distributions. A few such examples are examined here for comparison. For simplicity, we consider only $r = 2$, and we continue to write G_ξ for G_ξ^2. In what follows, the notation $o_b(1)$ is used to denote a function tending to 0 as $b \to \infty$.

5.3.3.1. 2 *or* a *children.* For $a \in \mathbb{N}$ and b with $a \geq b > 2$, consider trees denoted $T_{\xi_{b,a}}$ with offspring distribution $\mathbb{P}(\xi_{b,a} = 2) = \frac{a-b}{a-2}$ and $\mathbb{P}(\xi_{b,a} = a) = \frac{b-2}{a-2}$. Note that the branching number of $T_{\xi_{b,a}}$ is $\mathrm{br}(T_{\xi_{b,a}}) = \mathbb{E}(\xi_{b,a}) = b$. We do not present a complete proof of the following theorem. However, sharp lower bounds on $p_c(T_{\xi_{b,a}}, 2)$ follow from Theorem 5.3.

THEOREM 5.14. *The critical probability in 2-neighbour bootstrap percolation on* $T_{\xi_{b,a}}$ *is*

$$p_c(T_{\xi_{b,a}}, 2) = \max\left\{1 - \frac{a-2}{2(a-b)}, \frac{1+o_b(1)}{2ab}\right\},$$

with the first quantity being always greater for $a \geq 2b-1$ *and the second for* $a \leq 2b-2$*.*

$\square$

The random variable $\xi_{b,a}$ is supported on only two values and so clearly $\mathbb{E}((\xi_{b,a})_2)$ is finite and the assumptions of Theorem 5.3 are satisfied. We have

$$\begin{aligned}\mathbb{E}((\xi_{b,a})_2) &= \mathbb{P}(\xi_{b,a} = a)a(a-1) + \mathbb{P}(\xi_{b,a} = 2)2 \\ &= \frac{(b-2)a(a-1) + 2(a-b)}{a-2} \\ &< \frac{(b-2)a(a-1)}{a-2} + 2.\end{aligned}$$

Thus, inequality (5.4) yields a lower bound on the critical probability given by

$$p_c(T_{\xi_{b,a}}, 2) > \frac{1}{2\left(\frac{(b-2)a(a-1)}{a-2} + 2\right) - 3} = \frac{1}{2\frac{(b-2)a(a-1)}{a-2} + 1} = \frac{1 + o_b(1)}{2ab},$$

agreeing asymptotically with the correct value for $a \leq 2b-2$.

For $a \geq 2b-1$ we have in fact $p_c(T_{\xi_{b,a}}, 2) = 1 - \frac{1}{2\mathbb{P}(\xi_{b,a}=2)}$. The value of the critical probability, in this case, tells us what prevents $T_{\xi_{b,a}}$ from percolating when we have $p < p_c(T_{\xi_{b,a}}, 2)$. Since $\frac{a-b}{a-2} > \frac{1}{2}$, after deleting all vertices of degree $a+1$, the tree almost surely contains infinite components, with all vertices having degree at most 3, with branching number $c = 2\frac{a-b}{a-2} > 1$. Every initially healthy doubly infinite path contained in such subtree is an infinite healthy 1-fort in $T_{\xi_{b,a}}$. The critical probability for such paths to occur is $1/c$ and so if $1 - p > 1/c$ then $T_{\xi_{b,a}}$ almost surely does not percolate. Note that exactly the same arguments can be used to prove the first lower bound in inequality (5.2).

5.3.3.2. *Shifted Poisson.* A natural offspring distribution for a Galton–Watson tree is a Poisson distribution. Since any distribution ξ with $\mathbb{P}(\xi \leq 1) > 0$ has critical probability 1, consider a Poisson distribution shifted by 2. That is, for each $b > 2$, let ξ_{Po}^{b} be the offspring distribution with the property that, for each $k \geq 2$,

$$\mathbb{P}(\xi^b_{Po} = k) = e^{-(b-2)}\frac{(b-2)^{k-2}}{(k-2)!}.$$

Then, $\mathbb{E}(\xi^b_{Po}) = b$ and the function $G_{\xi^b_{Po}}(x)$ is given by

$$\begin{aligned} G_{\xi^b_{Po}}(x) &= \sum_{k\geq 2} e^{-(b-2)}\frac{(b-2)^{k-2}}{(k-2)!}(kx^{k-2} - (k-1)x^{k-1}) \\ &= e^{-(b-2)(1-x)}(2 + (b-3)x - (b-2)x^2). \end{aligned}$$

Here, the critical probability can be given precisely since the function $G_{\xi^b_{Po}}$ attains its (global) maximum value when $x = \frac{b-5+\sqrt{(b+3)(b-1)}}{2(b-2)}$, which belongs to $[0,1]$ when $b \geq 7/3$; the maximum value is

$$\exp\left(-\frac{1}{2}(b+1-\sqrt{(b+3)(b-1)})\right)\left(\frac{-2+\sqrt{(b+3)(b-1)}}{b-2}\right).$$

Thus, with a little bit of calculation, one can show that, for $b \geq 7/3$,

$$p_c(T_{\xi^b_{Po}}, 2) = 1 - \frac{(b-2)e^{\frac{b+1-\sqrt{(b+3)(b-1)}}{2}}}{-2+\sqrt{(b+3)(b-1)}} = \frac{1}{2b^2} + \frac{1}{3b^3} + O\left(\frac{1}{b^4}\right).$$

Indeed, we have

$$\sqrt{(b+3)(b-1)} = b + 1 - \frac{2}{b} + \frac{2}{b^2} - \frac{4}{b^3} + O\left(\frac{1}{b^4}\right),$$

and so

$$(b-2)e^{\frac{b+1-\sqrt{(b+3)(b-1)}}{2}} = b - 1 - \frac{5}{2b} + \frac{13}{6b^2} + O\left(\frac{1}{b^3}\right).$$

Thus,

$$\begin{aligned} 1 - \frac{(b-2)e^{\frac{b+1-\sqrt{(b+3)(b-1)}}{2}}}{-2+\sqrt{(b+3)(b-1)}} &= 1 - \frac{b-1-\frac{5}{2b}+\frac{13}{6b^2}+O\left(\frac{1}{b^3}\right)}{b-1-\frac{2}{b}+\frac{2}{b^2}+O\left(\frac{1}{b^3}\right)} \\ &= 1 - 1 + \frac{\frac{1}{2b}-\frac{1}{6b^2}+O\left(\frac{1}{b^3}\right)}{b-1-\frac{2}{b}+\frac{2}{b^2}+O\left(\frac{1}{b^3}\right)} \\ &= \frac{1}{2b^2} + \frac{1}{2b^3} - \frac{1}{6b^3} + O\left(\frac{1}{b^4}\right) \\ &= \frac{1}{2b^2} + \frac{1}{3b^3} + O\left(\frac{1}{b^4}\right). \end{aligned}$$

One can apply Theorem 5.3 to the distribution ξ^b_{Po} since $\mathbb{E}((\xi^b_{Po})_2) = b^2 - 2$. Thus, (5.4) yields

$$p_c(T_{\xi^b_{Po}}, 2) \geq \frac{1}{2b^2 - 7} = \frac{1 + o_b(1)}{2b^2}$$

which is asymptotically correct.

5.3.3.3. *Shifted geometric distribution.* Consider now a shifted geometric distribution. For $b > 2$, let ξ^b_g be defined by

$$\mathbb{P}(\xi^b_g = k + 2) = \frac{1}{b-1}\left(\frac{b-2}{b-1}\right)^k, \qquad k \geq 0.$$

Then, $\mathbb{E}(\xi^b_g) = b$ and the function $G_{\xi^b_g}$ is given by

$$G_{\xi^b_g}(x) = \frac{2(b-1) - (2b-3)x}{((b-1) - (b-2)x)^2},$$

and attains its maximum when $x = \frac{(2b-5)(b-1)}{(b-2)(2b-3)}$ with value $\frac{(2b-3)^2}{4(b-1)(b-2)}$. Thus, if $b \geq 5/2$,

$$p_c(T_{\xi^b_g}, 2) = 1 - \frac{4(b-1)(b-2)}{(2b-3)^2} = \frac{1}{(2b-3)^2}.$$

On the other hand we see that $\mathbb{E}((\xi^b_g)_2) = 2(b-1)^2$; thus (5.4) yields

$$p_c(T_{\xi^b_g}, 2) \geq \frac{1}{4(b-1)^2 - 3} = \frac{1 + o_b(1)}{4b^2},$$

again agreeing asymptotically with the true value.

5.4. Final remarks and open problems

In chapters 4 and 5 we study general infinite trees and show that for any $b \geq r$ and any $\varepsilon > 0$ there exists a tree with bounded degree, branching number $\mathrm{br}(T) = b$ and critical probability $p_c(T, r) < \varepsilon$. We then show that, by equation (5.24), given an offspring distribution ξ with $\mathbb{P}(\xi < r) = 0$, for a Galton–Watson tree T_ξ we almost surely have

$$p_c(T_\xi, r) \geq \exp\left(-\frac{\mathbb{E}(\xi) - 1}{r - 1} - \mathbb{E}(H_{\xi - r})\right).$$

Using the concavity of the logarithm function and, setting $\mathrm{br}(T_\xi) = \mathbb{E}(\xi) = b$, this bound was simplified to $p_c(T_\xi, r) \geq c_r \frac{e^{-\frac{b}{r-1}}}{b}$, as stated in Theorem 5.1.

However, the bound $\mathbb{E}(H_{\xi-r}) \leq \log b$ is very weak unless the distribution ξ is strongly concentrated around its mean. When ξ is concentrated though, we already know that $p_c(T_\xi, r)$ is large, e.g., by Theorems 5.2 and 5.3, as well as by the results for regular trees in [**13**] and [**27**]. With this in mind we conjecture that the family of offspring distributions $\eta_{r,b}$ constructed in the proof of Lemma 5.13 minimizes $p_c(T_\xi, r)$ up to a factor depending on r only.

Conjecture 5.15. *The upper bound in Theorem 5.1 is essentially sharp, i.e., for $r \geq 2$ there are constants c_r and C_r such that if $b \geq r$ then*

$$c_r e^{-\frac{b}{r-1}} \leq f_r^{GW}(b) \leq C_r e^{-\frac{b}{r-1}}.$$

The second conjecture we state in this section is an extension of Theorem 5.2 which says that for $\alpha \in (0, r-1)$ we have $p_c(T_\xi, r) \geq c_{r,\alpha} \left(\mathbb{E}(\xi^{1+\alpha})\right)^{-1/\alpha}$. For $r = 2$ and $\alpha > 1$ such bound does not hold as is seen by taking $\xi = b$ constant, i.e., a regular tree T_b, when $p_c(T_b, 2) \sim \frac{1}{2b^2}$. However, Theorem 5.2 does hold for $r = 2$ and $\alpha = 1$ as shown in Theorem 5.3. Moreover, turning to Lemma 5.10 we observe that $p_c(T_b, r) \sim c_r b^{-\frac{r}{r-1}}$. This motivates the following conjecture, extending Theorem 5.2 to $\alpha = r-1$ for all $r \geq 3$.

Conjecture 5.16. *For each $r \geq 3$ there exists a constant $c_r > 0$ such that for any offspring distribution ξ we have*

$$p_c(T_\xi, r) \geq c_r \left(\mathbb{E}(\xi^r)\right)^{-1/(r-1)}.$$

In Theorems 5.2 and 5.3, we give upper bounds on $p_c(T_\xi, r)$ based on the $\left(\frac{r}{r-1}\right)$-th negative moments of ξ. However, the example of the $\xi_{b,a}$ offspring distribution in Theorem 5.14 immediately shows that negative moments are not enough to tightly bound the critical probability from above. This motivates the following question.

Question 5.17. *What other characteristics of the distribution ξ lead to upper bounds on $p_c(T_\xi, r)$?*

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