A SHARPER THRESHOLD FOR BOOTSTRAP PERCOLATION IN TWO DIMENSIONS

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Abstract. Two-dimensional bootstrap percolation is a cellular automaton in which sites become 'infected' by contact with two or more already infected nearest neighbors. We consider these dynamics, which can be interpreted as a monotone version of the Ising model, on an $n \times n$ square, with sites initially infected independently with probability p. The critical probability p_c is the smallest p for which the probability that the entire square is eventually infected exceeds $1/2$. Holroyd determined the sharp first-order approximation: $p_c \sim \pi^2/(18 \log n)$ as $n \to \infty$. Here we sharpen this result, proving that the second term in the expansion is $-(\log n)^{-3/2+o(1)}$, and moreover determining it up to a poly$(\log \log n)$-factor.

1. Introduction

Bootstrap percolation is a cellular automaton in which, given a (typically random) initial set of 'infected' vertices in a graph G, new vertices are infected at each time step if they have at least r infected neighbours. In this paper we shall study two-neighbour bootstrap percolation on the square grid $[n]^2$. We shall determine the second term of the critical threshold for percolation up to a poly$(\log \log n)$-factor, and hence confirm a conjecture of Gravner and Holroyd [23].

We begin by defining the bootstrap process, which was introduced by Chalupa, Leath and Reich [17] in 1979. Given a graph G, let $V(G)$ denote its vertex set, and given $v \in V(G)$, let $N(v)$ denote the neighbourhood of v. Now, given an integer $r \in \mathbb{N}$, and a set of initially infected vertices $A \subset V(G)$, define A_t recursively by $A_0 = A$, and

$$A_{t+1} \;=\; A_t \cup \big\{ v \in V(G) : |N(v) \cap A_t| \geqslant r \big\}$$

for each $t \geqslant 0$. We say that the vertices of A_t have been infected by time t. Let $[A] = \bigcup_t A_t$ denote the closure of A under the r-neighbour bootstrap process, and say that the set A *percolates* if the entire vertex set is eventually infected, i.e., if $[A] = V(G)$.

We shall be interested in the case where A is a random subset of $V(G)$ in which each vertex is included independently with probability p. It is clear that the probability of percolation is strictly increasing in p, and so we define the critical probability, $p_c(G, r)$ as follows:

$$p_c(G,r) \;:=\; \inf\Big\{ p \,:\, \mathbb{P}\big(A \text{ percolates in the } r\text{-neighbour process on } G\big) \geqslant 1/2 \Big\}.$$

Our aim is to give sharp bounds on $p_c(G, r)$.

Bootstrap percolation has been extensively studied, both by mathematicians (see, for example [2, 6, 15, 25, 32]) and by physicists (see the survey [1] and the references therein).

The process may be thought of as a monotone version of the Ising model. We focus on the graph $G = [n]^d$ with vertex set $\{1, \ldots, n\}^d$ and an edge between vertices u and v if and only if $\|u - v\|_1 = 1$. Aizenman and Lebowitz [2] determined the asymptotic behaviour of $p_c([n]^d, 2)$ up to multiplicative constants, and Cerf and Cirillo [15] (in the crucial case $d = r = 3$) and Cerf and Manzo [16] proved the corresponding result for all $r \leqslant d$. The first sharp threshold for bootstrap percolation was proved by Holroyd [25], who showed that

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

This was the first result of its type, and has prompted a flurry of generalizations. Sharp thresholds have since been determined for $p_c([n]^d, r)$ for all fixed d and r [6, 8], and in high dimensions (i.e., $d = d(n) \to \infty$ sufficiently fast) when $r = \Theta(d)$ [5], and when $r = 2$ [7]. Some of the techniques from these papers have been used to prove results about the Glauber dynamics of the Ising model [20, 31]. The bootstrap process has also been studied on trees [9, 12, 19], on the random regular graph [10, 28], and on $G_{n,p}$ [29].

In this paper we shall study the two-neighbour bootstrap process on the graph $G = [n]^2$ in more detail. One of the most striking facts about the result (1) stated above is that it contradicted estimates of $\lim_{n\to\infty} p_c \log n$ given by simulations - in fact, such estimates were out by a factor of more than two. (See, for example, [22] or [24] for a discussion of the reasons behind these discrepancies.) Gravner and Holroyd [22] gave a rigorous (partial) explanation for this phenomenon, by giving the following improvement of (1):

$$p_c([n]^2, 2) \;\leqslant\; \frac{\pi^2}{18 \log n} - \frac{c}{(\log n)^{3/2}},$$

where $c > 0$ is a small constant. In [23], the same authors proved an almost matching lower bound for a simpler model (called 'local' bootstrap percolation), and conjectured that the upper bound is essentially sharp for the usual bootstrap process.

Conjecture 1 (Gravner and Holroyd [23])**.** *For every $\varepsilon > 0$, if n is sufficiently large then*

$$p_c([n]^2, 2) \;\geqslant\; \frac{\pi^2}{18 \log n} - \frac{1}{(\log n)^{3/2-\varepsilon}}.$$

In this paper we shall prove Conjecture 1 in a slightly stronger form. To be precise, we shall prove the following theorem.

Theorem 1. *There exist constants $C > 0$ and $c > 0$ such that*

$$\frac{\pi^2}{18 \log n} - \frac{C(\log\log n)^3}{(\log n)^{3/2}} \;\leqslant\; p_c([n]^2, 2) \;\leqslant\; \frac{\pi^2}{18 \log n} - \frac{c}{(\log n)^{3/2}}$$

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

Note that the upper bound follows from the result of [22] stated above, and so we shall need to prove only the lower bound. We remark that our result corrects predictions (from simulations) of the power of $\log n$ in the second term (see [23] for details).

The proof of Theorem 1 will use many of the tools and techniques of [25], together with some of the ideas of [23], and some new ideas. In particular, we shall bound the probability of percolation by the expected number of 'good' and 'satisfied' hierarchies (see Lemma 7, below). We will define a hierarchy as in [25] (see Section 3), except that our hierarchies will be much finer, each step being of order $1/\sqrt{p}$, instead of $1/p$. This means that we will have far too many hierarchies; however, almost all of these have many 'large' seeds, and we shall show that these contribute a negligible amount to the sum. In order to do so, we shall need a better bound on the probability that a seed is internally spanned than the straightforward bound that sufficed in [25]. Fortunately, the bound we need follows easily from the simple (folklore) fact that a spanning set for a rectangle R must contain no fewer than $\phi(R)/2$ elements, where $\phi(R)$ denotes the semi-perimeter of R (see Lemmas 2 and 3). Surprisingly, it appears that our proof does not extend directly to the "modified" bootstrap percolation model; it is the analogous bound for seeds that is missing in this case (see Section 5 for more information).

We finish this section by making a few definitions which we shall use throughout the proof. First, we say a set S is *spanned* by a set A if $S \subset [A]$, and that S is *internally spanned* by A if $S \subset [A \cap S]$. We write $A \sim \text{Bin}(S, p)$ to indicate that A is a random subset of S, with each element chosen independently with probability p, and write $\mathbb{P}_p$ for the corresponding probability measure. Let $I(S)$ denote the event that S is internally spanned by A. Thus $\mathbb{P}_p\big(I(S)\big)$ is the probability that the set S is internally spanned by a random set $A \sim \text{Bin}(S, p)$.

Next, define two functions, β and g, by

$$\beta(u) \;:=\; \frac{u + \sqrt{u(4-3u)}}{2} \qquad \text{and} \qquad g(z) \;:=\; -\log\left(\beta\left(1 - e^{-z}\right)\right).$$

We remark that β is increasing on $[0, 1]$, and so g is decreasing on $(0, \infty)$, and that $g(z) \leqslant 2e^{-z}$ when z is large (see Proposition 3 of [6]). Note that $\beta(u) \sim \sqrt{u}$ as $u \to 0$, and so $g(z) \sim -\log\sqrt{z}$ as $z \to 0$.

A *rectangle* is a set of the form

$$R = [(a, b), (c, d)] \;:=\; \big\{(x, y) \,:\, a \leqslant x \leqslant c,\, b \leqslant y \leqslant d\big\} \subset \mathbb{Z}^2,$$

the dimensions of R are $\dim(R) = (c-a+1, d-b+1)$, the long and short side-lengths of R are respectively $\text{sh}(R) = \min\{c-a+1, d-b+1\}$ and $\text{lg}(R) = \max\{c-a+1, d-b+1\}$, and the semi-perimeter of R is $\phi(R) = \text{sh}(R) + \text{lg}(R)$.

We say that a rectangle $R = [(a, b), (c, d)]$ is *crossed from left-to-right* by $A \subset R$ if

$$R \;\subset\; \Big[A \cup \big\{(x, y) \in \mathbb{Z}^2 \,:\, x \leqslant a-1\big\}\Big],$$

i.e., if R is spanned by A together with the set of all sites to the left of R. Note that this is equivalent to there being no 'double gap' (i.e., no adjacent pair of empty columns) in R, and the final column being occupied.

For each $p \in (0, 1)$, let $q = -\log(1-p)$, so that $p \sim q$ as $p \to 0$. To motivate this definition (and the definition of $g(z)$, above), note (from Lemma 8 of [25]) that for any rectangle R with dimensions (a,b), if $A \sim \mathrm{Bin}(R,p)$ then

$$\mathbb{P}(A \text{ crosses } R \text{ from left-to-right}) \;\leqslant\; e^{ag(bq)}.$$

We shall use the notation $f(\mathbf{x}) = O\big(h(\mathbf{x})\big)$ throughout to mean that there exists an absolute constant $C > 0$, independent of all other variables (unless otherwise stated), such that $f(\mathbf{x}) \leqslant Ch(\mathbf{x})$ for all $\mathbf{x} = (x_1, \dots, x_k)$. If the constant C depends on some other parameter y, then we shall write $f(\mathbf{x}) = O_y\big(h(\mathbf{x})\big)$. Finally, given a directed tree, let $\vec{\Gamma}(v)$ denote the set of out-neighbours of a vertex v.

The rest of the paper is organised as follows. In Section 2 we give an upper bound on the probability that a sufficiently small rectangle (a seed) is internally spanned. In Section 3 we recall from [25] the notion of a hierarchy, which is fundamental to the proof of Theorem 1, together with some important lemmas from [23] and [25]. In Section 4 we prove Theorem 1, and in Section 5 we mention some open questions.

2. A lemma on seeds

In this section we shall prove the following lemma, which bounds the probability that a small rectangle is internally spanned. Recall that $q = -\log(1-p)$.

Lemma 2. *There exists $c > 0$ such that, for any $p > 0$ and any rectangle R with $\dim(R) = (a,b)$ and $a \le b$, if $ap \le c$ then*

$$\mathbb{P}_p\big(I(R)\big) \;\leqslant\; 3^{\phi(R)} \exp\Big(- \phi(R) g(aq) \Big).$$

We begin by recalling a lovely and well-known exercise for high school students (see [13] or [33], for example). Lemma 2 follows from it almost immediately.

Lemma 3. *If $A \subset R$ percolates then $|A| \geqslant \phi(R)/2$.*

We also make a simple observation.

Observation 4. *If $z > 0$ is sufficiently small then*

$$\log(1/\sqrt{z}) \,-\, \sqrt{z} \;\leqslant\; g(z) \;\leqslant\; \log(1/\sqrt{z}) \,+\, z.$$

Proof. We use the estimates $z - z^2 \leqslant 1 - e^{-z} \leqslant z$, and $\sqrt{u} \leqslant \beta(u) \leqslant \sqrt{u} + u$, which are valid for small z and u. It follows that

$$g(z) \;\geqslant\; -\log \beta(z) \;\geqslant\; -\log(\sqrt{z} + z) \;=\; -\log\sqrt{z} - \log(1+\sqrt{z}) \;\geqslant\; -\log\sqrt{z} - \sqrt{z}.$$

The proof of the upper bound is similar. □

We can now easily deduce Lemma 2.

Proof of Lemma 2. Let $m = |A \cap R|$. By Lemma 3, if A internally spans R then $m \geqslant (a+b)/2$. There are at most $\binom{ab}{m}$ ways to choose the set A, given m. Thus

$$\mathbb{P}_p\big(I(R)\big) \;\leqslant\; \sum_{m \geqslant (a+b)/2} \binom{ab}{m} p^m \;\leqslant\; (6aq)^{(a+b)/2},$$

since $\varepsilon := aq$ is sufficiently small, and $p \sim q$. But $\log(1/\sqrt{aq}) \leqslant g(aq) + \sqrt{aq}$, by Observation 4, so

$$(aq)^{(a+b)/2} \leqslant \exp\Big(-(a+b)g(aq) + (a+b)\sqrt{aq}\Big).$$

The result now follows, since $aq = \varepsilon$, and $\sqrt{6}e^{\sqrt{\varepsilon}} < 3$ if ε is sufficiently small. □

3. Hierarchies

In this section we shall recall some important definitions and lemmas from [23] and [25]; for the proofs, we refer the reader to those papers. In particular, we define a hierarchy as in Section 9 of [25].

Definition. A *hierarchy* $\mathcal{H}$ for a rectangle $R \subset [n]^2$ is an oriented rooted tree $G_{\mathcal{H}}$, with all edges oriented away from the root ('downwards'), together with a collection of rectangles $(R_u \subset [n]^2 : u \in V(G_{\mathcal{H}}))$, one for each vertex of $G_{\mathcal{H}}$, satisfying the following criteria.

(a) The root of $G_{\mathcal{H}}$ corresponds to R.
(b) Each vertex has at most 2 neighbours below it.
(c) If $u \to v$ in $G_{\mathcal{H}}$ then $R_u \supset R_v$.
(d) If $\vec{\Gamma}(u) = \{v, w\}$ then $[R_v \cup R_w] = R_u$.

A vertex u with $\vec{\Gamma}(u) = \emptyset$ is called a *seed*. Given two rectangles $S \subset R$, we write $D(S, R)$ for the event (depending on the set $A \subset R$) that

$$R = [(A \cup S) \cap R],$$

i.e., the event that R is internally spanned by $A \cup S$.

We say a hierarchy *occurs* (or is *satisfied* by a set $A \subset R$) if the following events all occur *disjointly*.

(e) For each seed u: R_u is internally spanned by A.
(f) For each pair (u, v) satisfying $\vec{\Gamma}(u) = \{v\}$: $D(R_v, R_u)$.

Given two rectangles $S \subset R$, with dimensions (a_1, a_2) and (b_1, b_2) respectively, define

$$d_j(S, R) := \frac{b_j - a_j}{b_j}$$

for $j = 1, 2$, and let $d(S, R) = \max\{d_1(S, R), d_2(S, R)\}$.

The following definition is slightly different to that in [25], and is motivated by the method of [23] (see also Lemma 9 below). This definition is necessary because in order to prove a sharper result, we need to take a finer hierarchy. In our application we shall take $T = \sqrt{q}$ and $Z = \log^3(1/q)/\sqrt{q}$.

Definition. A hierarchy is *good* for $(T, Z) \in \mathbb{R}^2$ if is satisfies the following.

(g) If $\vec{\Gamma}(u) = \{v\}$ and $|\vec{\Gamma}(v)| = 1$ then $T \leqslant d(R_v, R_u) \leqslant 2T$.
(h) If $\vec{\Gamma}(u) = \{v\}$ and $|\vec{\Gamma}(v)| \neq 1$ then $d(R_v, R_u) \leqslant 2T$.
(i) If $|\vec{\Gamma}(u)| \geqslant 2$ and $v \in \vec{\Gamma}(u)$, then $d(R_v, R_u) \geqslant T$.
(j) u is a leaf if, and only if, $\mathrm{sh}(R_u) \leqslant Z$.

Before continuing, we make a simple observation about the height, $h(\mathcal{H})$ of a hierarchy $\mathcal{H}$, by which we mean the maximum distance in $G_{\mathcal{H}}$ of a leaf from the root.

Lemma 5. *Let R be a rectangle, let $Z > 1 > T > 0$, and let $\mathcal{H}$ be a hierarchy for R which is good for (T, Z). Then*

$$h(\mathcal{H}) \leqslant \frac{8}{T} \log\left(\frac{\phi(R)}{Z}\right) + 1.$$

Proof. Consider a path P of length $h(\mathcal{H})$ from the root to a leaf u. Let w be the neighbour of u in $G_{\mathcal{H}}$, and note that $\mathrm{sh}(R_w) > Z$. Note also that in every two steps backwards along P, at least one of the dimensions of the corresponding rectangle increases by a factor of at least $1 + T$. Hence one of the dimensions goes up by this factor at least $(h(\mathcal{H}) - 1)/4$ times (on the path from w to the root), and so

$$Z(1 + T)^{(h(\mathcal{H})-1)/4} \leqslant \phi(R).$$

The result follows by rearranging and using the inequality $\log(1 + T) \geqslant T/2$, which is valid for all $T \in (0, 1)$. $\square$

The following key lemma about hierarchies was proved in [25]. Although our definition of hierarchy is slightly different, the proof in our case is identical.

Lemma 6 (Proposition 32 of [25])**.** *Let $Z > 1 > T > 0$, let R be a rectangle, and suppose A internally spans R. Then there exists a hierarchy $\mathcal{H}$ for R, which is good for (T, Z), and which is satisfied by A.*

We can now easily deduce, as in Section 10 of [25], our basic bound on the probability of percolation. Given a rectangle R and a pair $(T, Z) \in \mathbb{R}^2$, we write $\mathcal{H}(R, T, Z)$ for the collection of hierarchies for R which are good for (T, Z).

Recall that $\mathbb{P}_p\big(I(R)\big)$ and $\mathbb{P}_p\big(D(S, R)\big)$ denote the probabilities, given $A \sim \mathrm{Bin}(R, p)$, of the events "$R$ is internally spanned by A" and "R is internally spanned by $A \cup S$" respectively.

Lemma 7. *Let R be a rectangle in $[n]^2$, let $Z > 1 > T > 0$, let $p > 0$ and let $A \sim \mathrm{Bin}(R, p)$. Then*

$$\mathbb{P}\Big([A] = R\Big) \leqslant \sum_{\mathcal{H} \in \mathcal{H}(R,T,Z)} \left(\prod_{\vec{\Gamma}(u)=\{v\}} \mathbb{P}_p\big(D(R_v, R_u)\big) \right) \prod_{\text{seeds } u} \mathbb{P}_p\big(I(R_u)\big).$$

(Above and in subsequent usage, the first product is over all pairs of vertices (u, v) of $\mathcal{H}$ that satisfy the given condition $\vec{\Gamma}(u) = \{v\}$, and the second product is over all seeds u of $\mathcal{H}$.)

Proof of Lemma 7. By Lemma 6, if A internally spans R then there exists a hierarchy in $\mathcal{H}(R, T, Z)$ which is satisfied by A. Hence the probability that A internally spans R is bounded above by the expected number of such hierarchies. Since the events "R_u is internally spanned by A" and $D(R_v, R_u)$ (see (e) and (f) above) are all monotone, and all occur disjointly, the result follows by the van den Berg-Kesten Lemma. $\square$

We recall the following lemma of Aizenman and Lebowitz [2], which is a standard tool for proving lower bounds on $p_c([n]^d, 2)$.

Lemma 8. *Suppose A internally spans $[n]^2$. Then, for all $1 \leqslant L \leqslant n$, there exists a rectangle R, internally spanned by A, with*

$$L \;\leqslant\; \mathrm{long}(R) \;\leqslant\; 2L.$$

We recall also the following bound on $\mathbb{P}_p\big(D(R,R')\big)$ from [23].

Lemma 9 (Lemma 5 of [23])**.** *Let $R \subset R'$ be rectangles of dimensions (a,b) and $(a+s,b+t)$ respectively. Then*

$$\mathbb{P}_p\big(D(R,R')\big) \;\leqslant\; \exp\Big(- sg(bq) - tg(aq) + 2\big(g(bq) + g(aq)\big) + stqe^{2g(bq)+2g(aq)} \Big).$$

The following observation is also from [23].

Observation 10 (Lemma 10 of [23])**.** *Let $a \leqslant B/q$. Then $e^{2g(aq)} \leqslant \dfrac{4B}{aq}$.*

We shall need a couple more definitions in order to rewrite Lemmas 7 and 9 in a more useful form. Let

$$W_g(\mathbf{a},\mathbf{b}) \;:=\; \inf_{\gamma\,:\,\mathbf{a}\to\mathbf{b}} \int_\gamma \Big(g(y)\,dx \;+\; g(x)\,dy \Big),$$

where the infimum is taken over all piecewise linear, increasing paths from $\mathbf{a}$ to $\mathbf{b}$ in $\mathbb{R}^2$ (see Section 6 of [25]). Now, for any two rectangles $R \subset R'$, define

$$U(R,R') \;=\; W_g\big(q\dim(R), q\dim(R')\big).$$

The following observation is immediate from the definition.

Observation 11 (Proposition 13 of [25])**.** *Let $R \subset R'$ be rectangles of dimensions (a,b) and $(a+s,b+t)$ respectively. Then*

$$sg(bq) + tg(aq) \;\geqslant\; \frac{1}{q}U(R,R').$$

Let $N(\mathcal{H})$ denote the number of vertices in a hierarchy $\mathcal{H}$, and $M(\mathcal{H})$ for the number of vertices of $\mathcal{H}$ which have outdegree two. The following technical lemma was proved in [25].

Lemma 12 (Lemma 37 of [25])**.** *Let $\mathcal{H}$ be a hierarchy for the rectangle R. Then there exists a rectangle $S \subset R$, called the 'pod' of $\mathcal{H}$, such that*

$$\dim(S) \;\leqslant\; \sum_{\text{seeds } u} \dim(R_u)$$

and

$$\sum_{\vec{\Gamma}(v)=\{w\}} U(R_w,R_v) \;\geqslant\; U(S,R) \;-\; M(\mathcal{H})qg(Zq).$$

We shall use the following observation to bound $U(S,R)$ from below, and again later in the proof of Theorem 1.

Observation 13. *There exists $C > 0$ such that, for every $0 < a < \infty$, we have*
$$\int_0^a g(z)\,dz \;\leqslant\; \frac{a}{2}\log\frac{1}{a} \,+\, Ca.$$

Proof. Let $\varepsilon > 0$ be such that Observation 4 holds when $z < \varepsilon$. Then, if $a < \varepsilon$ we have
$$\int_0^a g(z)\,dz \;\leqslant\; \frac{1}{2}\int_0^a -\log z + 2z\,dz \;\leqslant\; \frac{a}{2}\log\frac{1}{a} \,+\, a \,+\, a^2,$$
as required. Moreover, since g is decreasing, we have
$$\int_\varepsilon^a g(z)\,dz \;\leqslant\; ag(\varepsilon),$$
and so the observation follows. □

Finally, we shall use the following lemma, which follows from Lemma 16 of [25] (see also Lemma 7 of [23]). Recall that we use the notation $O(\cdot)$ to denote the existence of an absolute constant, independent of all variables, such that if we multiply the function in the brackets by this constant then the bound holds.

Lemma 14. *Let $q > 0$ and $S \subset R$, with $\dim(S) = (a,b)$ and $\dim(R) = (A,B)$, where $A \leqslant B$. If $b \leqslant A$, then*
$$\frac{1}{q}U(S,R) \;\geqslant\; \frac{2}{q}\int_0^{Aq} g(z)\,dz \,+\, \big(B-A\big)g(Aq) \,-\, \frac{\phi(S)}{2}\log\frac{2}{\phi(S)q} \,-\, O\big(\phi(S)\big).$$
If $b > A$, then
$$\frac{1}{q}U(S,R) \;\geqslant\; (A-a)g(bq) \,+\, \big(B-b\big)g(Aq).$$

Proof. By Lemma 16 of [25], the path integral is minimized by paths which follow the main diagonal as closely as possible. Assuming for simplicity that $a \leqslant b$, by following the piecewise linear path $(a,b) \to (b,b) \to (A,A) \to (A,B)$ we obtain
$$\frac{1}{q}U(S,R) \;\geqslant\; (b-a)g(bq) \,+\, \frac{2}{q}\int_{bq}^{Aq} g(z)\,dz \,+\, \big(B-A\big)g(Aq).$$
Now, by Observation 13, we have
$$\frac{2}{q}\int_0^{bq} g(z)\,dz \;\leqslant\; b\log\frac{1}{bq} \,+\, O(b),$$
and by Observation 4, $g(bq) \geqslant \frac{1}{2}\log(1/bq) - O(1)$. Hence
$$(b-a)g(bq) \,-\, \frac{2}{q}\int_0^{bq} g(z)\,dz \;\geqslant\; -\frac{a+b}{2}\log\frac{1}{bq} \,-\, O(b),$$
as required. The inequality for $b > A$ can be obtained by following the path $(a,b) \to (A,b) \to (A,B)$, and applying Lemma 16 of [25]. □

4. The proof of Theorem 1

In this section we shall put together the pieces and prove Theorem 1. Recall that, given $p > 0$, we define $q = -\log(1-p) \sim p$.

Proposition 15. *Let $C > 0$ and $\varepsilon > 0$ be constants, let $p = p(C, \varepsilon) > 0$ be sufficiently small, and let R be a rectangle with dimensions (a, b), where*

$$\frac{\varepsilon}{q} \leqslant a \leqslant b \leqslant \frac{C}{q} \log\left(\frac{1}{q}\right).$$

Let $A \sim \mathrm{Bin}(R, p)$. Then

$$\mathbb{P}_p\Big([A] = R\Big) \leqslant \exp\left(-\left[\frac{2}{q}\int_0^{aq} g(z)dz + (b-a)g(aq)\right] + \frac{O_C(1)}{\sqrt{q}}\left(\log\frac{1}{q}\right)^3\right).$$

We remark that the constant implicit in the $O_C(1)$ term depends on the constant C, but not on the variables p, a and b (and also not on the constant ε).

Proof. We begin by defining some of the parameters we shall use. First, set $B = C\log(1/q)$, so that $a \leqslant b \leqslant B/q$, set $T = \sqrt{q}$, and set

$$Z = \frac{1}{\sqrt{q}}\left(\log\frac{1}{q}\right)^3.$$

<u>Claim</u>: Let $S = S(\mathcal{H})$ denote the pod of a hierarchy $\mathcal{H}$, given by Lemma 12. Then

$$\mathbb{P}_p\Big([A] = R\Big) \leqslant \sum_{\mathcal{H} \in \mathcal{H}(R,T,Z)} \exp\left[-\frac{1}{q}U(S,R) + O_C\left(N(\mathcal{H})\left(\log\frac{1}{q}\right)^2\right)\right] \prod_{\text{seeds } u} \mathbb{P}_p\big(I(R_u)\big).$$

In order to prove the claim, first note that by Observation 11 and Lemma 12, the pod $S \subset R$ of $\mathcal{H}$ satisfies

$$\sum_{\vec{\Gamma}(u_i) = \{v_i\}} s_i g(b_i q) + t_i g(a_i q) \geqslant \frac{1}{q}\sum_{\vec{\Gamma}(u) = \{v\}} U(R_v, R_u) \geqslant \frac{1}{q}U(S,R) - M(\mathcal{H})g(Zq),$$

where (a_i, b_i) and $(a_i + s_i, b_i + t_i)$ are the dimensions of R_{v_i} and R_{u_i} respectively.

Now, by the definition of a hierarchy, we have $s_i \leqslant 2Ta_i$ and $t_i \leqslant 2Tb_i$ for every pair (u_i, v_i) with $\vec{\Gamma}(u_i) = \{v_i\}$. Recall that $g(z)$ is decreasing, so

$$\max\{g(Zq), g(a_i q), g(b_i q)\} \leqslant g(q) \leqslant \log\frac{1}{q},$$

by Observation 4, and that $a_i, b_i \leqslant B/q$. By Observation 10, it follows that $s_i e^{2g(a_i q)} \leqslant 4Bs_i/a_i q \leqslant 8BT/q$, and similarly for b_i. Thus

$$g(Zq) + 2g(b_i q) + 2g(a_i q) + s_i t_i q e^{2g(b_i q) + 2g(b_i q)} \leqslant 5\log\frac{1}{q} + O\left(\frac{B^2T^2}{q}\right),$$

and hence, since $T^2 = q$, $B = O_C(\log(1/q))$ and $M(\mathcal{H}) \leqslant N(\mathcal{H})$,

$$\mathcal{M}(\mathcal{H})g(Zq) + \sum_{\vec{\Gamma}(u)=\{v\}} \Big(2g(bq) + 2g(aq) + stqe^{2g(bq)+2g(aq)}\Big) \;=\; O_C\left(N(\mathcal{H})\left(\log\frac{1}{q}\right)^2\right).$$

Hence, by Lemma 9, we have

$$\prod_{\vec{\Gamma}(u)=\{v\}} \mathbb{P}_p\big(D(R_v,R_u)\big) \;\leqslant\; \exp\left[-\frac{1}{q}U(S,R) + O_C\left(N(\mathcal{H})\left(\log\frac{1}{q}\right)^2\right)\right],$$

and so the claim follows by Lemma 7.

Our problem now is that there are too many hierarchies: there could be as many as $2^{1/\sqrt{q}}$ vertices in $G_{\mathcal{H}}$, and for each vertex u we have many choices for the rectangle R_u. However, most of these hierarchies have many seeds, and those with many *large* seeds have rather small weight in the sum. This turns out to be the key idea in the proof.

Indeed, let us define a *large seed* to be one with $\phi(R_u) \geqslant Z/3$, and note that every (non-seed) vertex of $\mathcal{H}$ lies above at least one large seed. Let the number of large seeds in a hierarchy $\mathcal{H}$ be denoted $m = m(\mathcal{H})$. Observe that, by Lemma 5, $\mathcal{H}$ has height at most $(10/\sqrt{q})\log(1/q)$, and hence that the number of vertices $N(\mathcal{H})$ in $G_{\mathcal{H}}$ satisfies

$$N(\mathcal{H}) \;\leqslant\; 2m \cdot h(\mathcal{H}) \;=\; O\left(\frac{m}{\sqrt{q}}\log\frac{1}{q}\right). \tag{2}$$

Therefore, the number of hierarchies with m large seeds is at most

$$\left(\frac{B}{q}\right)^{4N(\mathcal{H})} \;\leqslant\; \exp\left(O(1)\frac{m}{\sqrt{q}}\left(\log\frac{1}{q}\right)^2\right). \tag{3}$$

Now, for each hierarchy $\mathcal{H}$, define

$$X \;=\; X(\mathcal{H}) \;:=\; \sum_{\text{seeds } u} \phi(R_u),$$

and note that $X(\mathcal{H}) \geqslant \dfrac{m(\mathcal{H})Z}{3}$, and that $\phi\big(S(\mathcal{H})\big) \leqslant X(\mathcal{H})$, by Lemma 12. By Lemma 2, for every seed R_u we have

$$\mathbb{P}_p\big(I(R_u)\big) \;\leqslant\; 3^{\phi(R_u)}\exp\Big(-\phi(R_u)g(Zq)\Big),$$

since $\mathrm{sh}(R_u) \leqslant Z = o(1/q)$ as $q \to 0$, and $g(z)$ is decreasing in z. Thus

$$\prod_{\text{seeds } u} \mathbb{P}_p\big(I(R_u)\big) \;\leqslant\; \prod_{\text{seeds } u} 3^{\phi(R_u)}\exp\Big(-\phi(R_u)g(Zq)\Big) \;\leqslant\; 3^X\exp\Big(-Xg(Zq)\Big). \tag{4}$$

We split into two cases. The first is easier to handle, and we shall not have to approximate too carefully; in the second the calculation is much tighter.

<u>Case 1</u>: $\lg(S) > a$.

We have $a < \phi(S) \leqslant X$, by Lemma 12, and $\frac{1}{q}U(S,R) \geqslant (b-X)g(aq)$, by Lemma 14. Hence, by the claim, (2) and (4),

$$\mathbb{P}\big([A]=R\big) \;\leqslant \sum_{\mathcal{H}\in\mathcal{H}(R,T,Z)} 3^X \exp\left(-(b-X)g(aq) \,+\, O_C\left(\frac{m}{\sqrt{q}}\left(\log\frac{1}{q}\right)^3\right) \,-\, Xg(Zq)\right).$$

Now, by Observation 4, and since $X \geqslant mZ/3$ and $a/Z \geqslant q^{-1/3}$, we have

$$X\big(g(Zq)-g(aq)\big) \;\geqslant\; \frac{X}{7}\log\left(\frac{1}{q}\right) \;=\frac{1}{o(1)}\,mZ \;=\; \frac{1}{o(1)}\,\frac{m}{\sqrt{q}}\left(\log\frac{1}{q}\right)^3$$

as $q \to 0$. Using (3), it follows that

$$\mathbb{P}\big([A]=R\big) \;\leqslant\; \sum_{\mathcal{H}} \exp\left(-bg(aq) \,-\, \frac{X}{8}\log\frac{1}{q}\right) \;\leqslant\; \frac{1}{q}\exp\left(-\frac{2}{q}\int_0^{aq} g(z)\,dz \,-\, bg(aq)\right),$$

as required. The final inequality follows from Observation 13, since

$$\frac{2}{q}\int_0^{aq} g(z)\,dz \;\leqslant\; a\log\left(\frac{1}{aq}\right) \,+\, O(a) \;= o\left(X\log\frac{1}{q}\right)$$

as $q \to 0$ (recall that $aq \geqslant \varepsilon$ and $a < X$). Note also that $\sum_{m>1/q} e^{-mZ} \leqslant e^{-q^{-3/2}}$.

<u>Case 2</u>: $\lg(S) \leqslant a$.

By Lemma 14, and since $\phi(S) \leqslant X$, we have

$$\frac{1}{q}U(S,R) \;\;\geqslant\;\; \frac{2}{q}\int_0^{aq} g(z)\,dz \,+\, \big(b-a\big)g(aq) \,-\, \frac{X}{2}\log\frac{1}{Xq} \,-\, O(X).$$

Hence, by the claim, (2) and (4), we have

$$\mathbb{P}_p\Big([A]=R\Big) \;\leqslant \sum_{\mathcal{H}\in\mathcal{H}(R,T,Z)} 3^X \exp\bigg[-\frac{2}{q}\int_0^{aq} g(z)\,dz \,-\, \big(b-a\big)g(aq) \,+\, \frac{X}{2}\log\frac{1}{Xq}$$
$$+\, O(X) \,+\, O_C\left(\frac{m}{\sqrt{q}}\left(\log\frac{1}{q}\right)^3\right) \,-\, Xg(Zq)\bigg].$$

By Observation 4, this is at most

$$\sum_{\mathcal{H}} \exp\left[-\frac{2}{q}\int_0^{aq} g(z)\,dz \,-\, \big(b-a\big)g(aq) \,-\, \frac{X}{2}\log\frac{X}{C'Z} \,+\, O_C\left(\frac{m}{\sqrt{q}}\left(\log\frac{1}{q}\right)^3\right)\right],$$

for some constant $C' > 0$. Now, note that $\dfrac{X}{2}\log\dfrac{X}{C'Z}$ is increasing in X, and recall that $X \geqslant \dfrac{mZ}{3}$ and $Z = \dfrac{1}{\sqrt{q}}\left(\log\dfrac{1}{q}\right)^3$. Thus

$$\begin{aligned} -\frac{X}{2}\log\frac{X}{C'Z} + O_C\left(\frac{m}{\sqrt{q}}\left(\log\frac{1}{q}\right)^3\right) \;&\leqslant\; -\frac{mZ}{6}\log\frac{m}{3C'} + O_C\left(\frac{m}{\sqrt{q}}\left(\log\frac{1}{q}\right)^3\right) \\ &\leqslant\; \frac{O_C(1)}{\sqrt{q}}\left(\log\frac{1}{q}\right)^3 - \frac{m}{\sqrt{q}}\left(\log\frac{1}{q}\right)^3. \end{aligned}$$

Hence, using (3), and summing over m, we obtain

$$\mathbb{P}_p\Big([A] = R\Big) \;\leqslant\; \exp\left[-\frac{2}{q}\int_0^{aq} g(z)\,dz - \big(b-a\big)g(aq) + \frac{O_C(1)}{\sqrt{q}}\left(\log\frac{1}{q}\right)^3\right],$$

as required. □

Before deducing Theorem 1 from Proposition 15, we need to recall the following fact from [25], and to make an easy observation.

Lemma 16 (Proposition 5 of [25])**.**

$$\int_0^\infty g(z)\,dz \;=\; \frac{\pi^2}{18}.$$

The following observation follows almost immediately from Lemma 16.

Observation 17. *Let $p > 0$ be sufficiently small, and let $a, b \in \mathbb{R}$, with $a \leqslant b$ and $b \geqslant B/2p$, where $B = 10\log(1/p)$. Then*

$$\frac{2}{q}\int_0^{aq} g(z)dz + (b-a)g(aq) \;\geqslant\; \frac{2\lambda}{q} - 1,$$

where $\lambda = \pi^2/18$.

Proof. If $a \leqslant B/4p$, then this follows since $\int_{aq}^\infty g(z)\,dz = O(g(aq))$, uniformly over $a \in (0,\infty)$, and so

$$(b-a)g(aq) - \frac{2}{q}\int_{aq}^\infty g(z)\,dz \;\geqslant\; \left(\frac{B}{4p}\right)g(aq) - O\left(\frac{g(aq)}{q}\right) \;>\; 0.$$

If $a \geqslant B/4p$ then it holds because $g(z) \leqslant 2e^{-z}$ for z large, and so

$$\frac{2}{q}\int_{aq}^\infty g(z)\,dz \;\leqslant\; \frac{4}{q}e^{-aq} \;\leqslant\; \frac{4}{q}e^{-B/5} \;\leqslant\; 1,$$

as required. □

Finally, we deduce Theorem 1 from Proposition 15.

Proof of Theorem 1. Let $C > 0$ be a large constant to be chosen later, let $n \in \mathbb{N}$, and let

$$p \; < \; \frac{\pi^2}{18 \log n} \; - \; \frac{C (\log\log n)^3}{(\log n)^{3/2}}.$$

Note that $q = -\log(1-p) < p + p^2$, and so q also satisfies this inequality (possibly with a slightly different constant C).

Let $A \sim \mathrm{Bin}([n]^2, p)$, and suppose that A percolates. Then, by Lemma 8, there exists a rectangle $R \subset [n]^2$, which is internally spanned by A, and with $B/2p \leqslant \mathrm{lg}(R) \leqslant B/p$, where $B = 10\log(1/p)$. Let $\dim(R) = (a,b)$, and assume without loss of generality that $a \leqslant b$. There are at most $n^2(B/p)^2$ potential such rectangles, and each is internally spanned with probability at most

$$\mathbb{P}_p\Big([A \cap R] = R \Big) \; \leqslant \; \exp\left(- \left[\frac{2}{q} \int_0^{aq} g(z) dz \, + \, (b-a) g(aq) \right] \, + \, \frac{O(1)}{\sqrt{q}} \left(\log \frac{1}{q} \right)^3 \right),$$

if $\mathrm{sh}(R) \geqslant 1/q$, by Proposition 15, and with probability at most

$$e^{-bg(aq)} \; \leqslant \; e^{-B/10p} \; = \; p^{1/p} \; \leqslant \; \left(\frac{1}{n} \right)^{100}$$

if C is sufficiently large, and $\mathrm{sh}(R) \leqslant 1/q$.

By Observation 17, and using the identity $\frac{1}{a-b} = \frac{1}{a} + \frac{b}{a(a-b)}$, this gives, as $n \to \infty$,

$$\begin{aligned}
\mathbb{P}\Big([A] = [n]^2 \Big) \; & \leqslant \; n^2 (B/p)^2 \exp\left(- \frac{2\lambda}{q} \, + \, \frac{O(1)}{\sqrt{q}} \left(\log \frac{1}{q} \right)^3 \right) \\
& \leqslant \; n^2 (B/p)^2 \exp\left(-2\log n \, - \, \frac{C}{\lambda} (\log\log n)^3 \sqrt{\log n} \, + \, \frac{O(1)}{\sqrt{q}} \left(\log \frac{1}{q} \right)^3 \right) \\
& \leqslant \; n^2 (\log n)^3 \exp\left(\, - \, 2 \log n \, - \, (\log\log n)^3 \sqrt{\log n} \right) \; \to \; 0
\end{aligned}$$

if C is sufficiently large, as required. □

5. Extensions and open questions

In this paper we have studied bootstrap percolation on one particular graph, the two-dimensional grid with nearest-neighbour bonds. It is natural to ask whether our method can be applied to bootstrap percolation on other graphs; here we shall discuss two such possible generalizations.

The most obvious (and most extensively studied) generalization is to consider bootstrap percolation in d dimensions (i.e., on the graph $[n]^d$), with nearest neighbour interaction and threshold $2 \leqslant r \leqslant d$ (as studied in, for example, [2, 5, 6, 7, 16, 32]). The sharp metastability thresholds for these models (with d fixed, and as $n \to \infty$) will be determined in [8], and it is likely that the methods of this paper (and those of [22]) could be adapted to give improved bounds in the case of $r = 2$ and general d.

Problem 1. *Give better bounds on the second term in the asymptotic expansion of* $p_c([n]^d, 2)$ *as* $n \to \infty$.

The case $r \geqslant 3$ is more complicated, and the following problem is likely to be difficult.

Problem 2. *Give good bounds on the second term in the asymptotic expansion of* $p_c([n]^3, 3)$ *as* $n \to \infty$.

A second natural generalization is to consider bootstrap percolation in two dimensions, but with a different update rule. For example, in the 'modified' bootstrap process (see [26]), a vertex is infected if at least one of its neighbours in *each* dimension is already infected; in the 'k-cross' process (see [27, 14]), a vertex v is infected if at least k vertices in the cross-shaped set

$$\bigcup_{0 \neq j \in [-k+1, k-1]} \big\{ v + (0,j), v + (j,0) \big\}$$

are previously infected; and in the Froböse process (introduced by Froböse [21] in 1989) a site of $[n]^2$ is infected if it has one already-infected neighbour in each dimension, along with the next-nearest neighbour in the corner between them. In general (see [18]), one could consider an arbitrary neighbourhood $N(v)$ of each vertex v, an arbitrary (monotone) family $\mathcal{A}(v)$ of subsets of $N(v)$, and say that v becomes infected if the already-infected subset of its neighbours is in $\mathcal{A}(v)$.

Holroyd [25] (see also [26]) determined the sharp threshold for the modified and Froböse models, and Holroyd, Liggett and Romik [27] did so for the k-cross process for all fixed $k \in \mathbb{N}$. Moreover, Duminil-Copin and Holroyd [18] have recently shown, for a large family of such models (including all of the examples above, and other similar models), that there exists a sharp metastability threshold. It is not unreasonable to hope that our method (together with that of [22]) might yield improved bounds on the critical probability for a more general collection of bootstrap processes, of the type considered in [18]. Indeed, for two of the processes described above this is the case.

Let $p_c^{(\mathrm{F})}([n]^2)$ denote the critical probability for percolation in the Froböse process on $[n]^2$, and let $p_c^{(+)}([n]^2, k)$ denote the critical probability for percolation in the k-cross process. The upper bounds in the following theorem were proved by Gravner and Holroyd [22] (for the Froböse model) and by Bringmann and Mahlburg [14] (for the k-cross process). The lower bounds follow by the methods of this paper.

Theorem 18.

$$p_c^{(\mathrm{F})}([n]^2) \;=\; \frac{\pi^2}{6 \log n} \;-\; \frac{1}{(\log n)^{3/2 + o(1)}}.$$

as $n \to \infty$. *Let* $k \in \mathbb{N}$, *and let* $\lambda_k = \pi^2 / 3k(k+1)$. *Then*

$$p_c^{(+)}([n]^2, k) \;=\; \frac{\lambda_k}{\log n} \;-\; \frac{1}{(\log n)^{3/2 + o(1)}}.$$

In fact the bounds we prove (and those from [22, 14]) are a little stronger than those stated above; they are like the bounds in Theorem 1.

Sketch of proof of Theorem 18. For the first part, it suffices to show that (in the Froböse process) on $R = [m] \times [n]$, all spanning sets have size at least $m + n - 1$. The theorem then follows in exactly the same way as Theorem 1.

We shall give two proofs that if $[A] = R$ then $|A| \geqslant m + n - 1$. The first is standard, using Proposition 30 of [25] (see also [3], or Lemma 12 of [4]) and induction on $\phi(R)$. For the second, consider the (bipartite) graph G whose vertices are the rows and columns of R, with an edge from row x to column y if and only if $(x, y) \in A$.

To prove that G has at least $m + n - 1$ edges, we shall show that it is connected. Indeed, if G is not connected then exists a set of rows X and a set of columns Y such that $A \subset S = (X \cap Y) \cup (X^c \cap Y^c)$. But then $[S] = S \neq R$, so A does not percolate, as required.

For the second part, we need the following idea from [27]: first couple the k-cross process with an 'enhanced process' (see [27], Section 5) in which the closed sets are rectangles. In the enhanced process the minimum number of sites required to infect an $[m] \times [n]$ rectangle is about $(m + n)/k$, which is also the typical number required. (To prove this, apply the standard proof, by induction on $m + n$.) The result now follows by the proof of Theorem 1. $\square$

Gravner and Holroyd [22] also improved the upper bounds for the modified process. However, the proof of Theorem 1 does not work for the modified process, since we do not have a result analogous to Lemma 2. In particular, it is possible to internally span an $m \times n$ rectangle with $\max\{m, n\}$ infected sites, but the proportion of such minimal-size sets which percolate is very small.

Let $p_c^{(\mathrm{M})}([n]^d)$ denote the critical probability for percolation in the modified bootstrap process on the graph $[n]^d$, i.e., the infimum over p such that the probability of percolation is at least $1/2$. We have the following conjecture; it is the analogue of Conjecture 1 for the modified process.

Conjecture 2. *As $n \to \infty$,*

$$p_c^{(\mathrm{M})}([n]^2) \;=\; \frac{\pi^2}{6 \log n} \;-\; \frac{1}{(\log n)^{3/2 + o(1)}}.$$

Given a rectangle R, we say that a set $A \subset R$ is a *minimal percolating set* if A spans R, but no proper subset of A does so (see [30], for example). Given $m \geqslant n$ and $x \geqslant 0$, let $F(m, n, x)$ denote the number of minimal percolating sets of size $m + x$ in modified bootstrap percolation on $R = [m] \times [n]$. We remark that Conjecture 2 would follow from the method of this paper, together with following bound:

$$F(m, n, x) \;\leqslant\; n^{m - n + 2x + o(n)}.$$

We remark that even if we restrict ourselves to 'threshold' models, in which a vertex is infected if at least r elements of its neighbourhood are infected, we still run into similar problems. Indeed, consider the model in which a vertex is infected if at least four of its eight neighbours (including diagonals) are infected. A typical seed R is shaped like an octagon, and the number of infected sites used to fill R (in the random process) is roughly

$\phi(R)$ (which we define to be the number of external vertices plus the number of external edges), while the minimal number required to span R is only $\phi(R)/2$.

Finally, returning to the standard bootstrap process, recall that Theorem 1 determines the second term of $p_c([n]^2, 2)$ up to a poly$(\log \log n)$-factor. We conjecture that this error term can be removed.

Conjecture 3. *As $n \to \infty$,*

$$p_c([n]^2, 2) \;=\; \frac{\pi^2}{18 \log n} \;-\; \Theta\left(\frac{1}{(\log n)^{3/2}} \right).$$

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