Minimum lethal sets in grids and tori under 3-neighbour bootstrap percolation

Fabricio Benevides, Jean-Claude Bermond, Hicham Lesfari, Nicolas Nisse

Minimum lethal sets in grids and tori under 3-neighbour bootstrap percolation*

Fabricio Benevides[1], Jean-Claude Bermond[2], Hicham Lesfari[2], and Nicolas Nisse[2]

[1]Universidade Federal do Ceará, Fortaleza, Brazil
[2]Université Côte d'Azur, Inria, CNRS, I3S, France

March 30, 2021

Abstract

Let $r \geq 1$ be any non negative integer and let $G = (V, E)$ be any undirected graph in which a subset $D \subseteq V$ of vertices are initially *infected*. We consider the process in which, at every step, each non-infected vertex with at least r infected neighbours becomes infected and an infected vertex never becomes non-infected. The problem consists in determining the minimum size $s_r(G)$ of an initially infected vertices set D that eventually infects the whole graph G. This problem is closely related to cellular automata, to percolation problems and to the Game of Life studied by John Conway. Note that $s_1(G) = 1$ for any connected graph G. The case when G is the $n \times n$ grid, $G_{n\times n}$, and $r = 2$ is well known and appears in many puzzle books, in particular due to the elegant proof that shows that $s_2(G_{n\times n}) = n$ for all $n \in \mathbb{N}$. We study the cases of square grids, $G_{n\times n}$, and tori, $T_{n\times n}$, when $r \in \{3, 4\}$. We show that $s_3(G_{n\times n}) = \lceil \frac{n^2+2n+4}{3} \rceil$ for every n even and that $\lceil \frac{n^2+2n}{3} \rceil \leq s_3(G_{n\times n}) \leq \lceil \frac{n^2+2n}{3} \rceil + 1$ for any n odd. When n is odd, we show that both bounds are reached, namely $s_3(G_{n\times n}) = \lceil \frac{n^2+2n}{3} \rceil$ if $n \equiv 5 \pmod 6$ or $n = 2^p - 1$ for any $p \in \mathbb{N}^*$, and $s_3(G_{n\times n}) = \lceil \frac{n^2+2n}{3} \rceil + 1$ if $n \in \{9, 13\}$. Finally, for all $n \in \mathbb{N}$, we give the exact expression of $s_4(G_{n\times n})$ and of $s_r(T_{n\times n})$ when $r \in \{3, 4\}$.

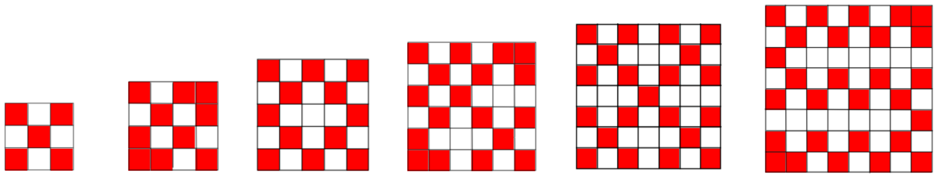
1 Introduction

Originally developed by von Neumann after a suggestion of Ulam, *cellular automata* are a dynamical system defined over graphs endowed with some homogeneous and local update rules. The notion of *bootstrap percolation* is an example of a cellular automaton which has been extensively investigated by mathematicians, physicists, computer scientists and sociologists, among others. For further applications to several other areas, we refer the reader to the survey article by Adler and Lev [AL03], and the references therein.

Several variants of classical bootstrap percolation on graphs have been considered. The particular model we are studying belongs to the class of *r-neighbour bootstrap processes* ($r \geq 1$). It was first introduced by Chalupa, Leath, and Reich [CLR79] as a monotone version of the Glauber dynamics in ferromagnetism.

Let $r \geq 1$ be a given integer and G a finite graph whose vertices (usually called *sites* in the context of percolation) can be in one of two states: *healthy* or *infected*. An initial set of infected nodes is given. At any step, any healthy vertex with at least r infected neighbours

*This work is supported by the SticAm-Sud project GALOP.



(a) $n=3$ (b) $n=4$ (c) $n=5$ (d) $n=6$ (e) $n=7$ (f) $n=8$

Figure 1: Some instances of minimum lethal sets in $G_{n\times n}$ when $r=3$. The vertices are depicted as small squares. Initially infected (resp., not infected) vertices are red (resp., white).

becomes infected while infected vertices remain infected forever. The parameter r reflects at which extent sites *resist* to the infection spread. Note that the term *bootstrap percolation* is sometimes used with the implicit assumption that the initial set of vertices infected is random. In this paper we consider the same model but use a deterministic initial set.

An initial set of infected vertices is called *lethal* if at the end of the process all the vertices are infected. A problem widely considered in the literature consists in determining the minimum size of a lethal set denote $s_r(G)$. (Knowing this value, for example, plays certain starting role in the study of the probability for a random initial set to be lethal). Computing exactly $s_r(G)$ is NP-hard and this hardness results hold even when $r=2$ and G has maximal degree d, where d is a constant not depending on the size of G (see [Che09]). The parameter $s_r(G)$ has been studied for several families of graphs including trees [Rie12], d-dimensional grids [BB06, BP98, PS20], hypercubes [BB06, MN18], expanders [COFKR14], random regular graphs [GS15].

In particular, the most known case is the square grids $G_{n\times n}$ with $r=2$ as it appears as a popular puzzle regularly in newspapers and is referenced in puzzles books [Win03, Bol06, LL11]. According to [Win03], the problem appeared for the first time in the Soviet magazine Kvant around 1986. The value $s_2(G_{n\times n})=n$ can be proved with the elegant perimeter argument. Our interest to the problem was revived, in fact, due to a problem proposed in the french newspaper “Le Monde” (Problem 1141, entitled ”Le jeu de la viralité”, April 2020) in honor to John Conway (who just passed away). This leads us to study the problem of determining the value $s_3(G_{n\times n})$ (see examples for small grids in Figure 1). To the best of our knowledge this problem was considered first in [Pet97]. The result appears also in [BP98]. In [Pet97] it is proven that $\lceil (n^2+2n)/3\rceil \leq s_3(G_{n\times n}) \leq (n^2+4n)/3+O(1)$. The lower bound uses also the perimeter argument. In [Bol06] (Problem 65, pages 171-172) Bollobás gave the same lower bound for n odd but a slightly better one for n even. He also proves that for $n\equiv 2 \pmod 6$ the lower bound is attained and in that case $s_3(G_{n\times n})=(n^2+2n+4)/3$ (see Figure 1(f) for $n=8$). However, as far as we know, no further progress has been done on the exact value of $s_3(G_{n\times n})$. The problem for square tori was considered in [Bol06, Win03, Pet97] but only for $r=2$.

Other related problems have been considered in the literature like finding the size of a largest inclusion-minimal lethal set [Mor09, Rie10]. The speed of convergence was also considered in the square grid (see [BP13, BP15]).

Our contributions. In this paper, we study the contamination process in square grids $G_{n\times n}$ and square tori $T_{n\times n}$. In Section 2, we formally define the problem and recall some known results about $s_3(G_{n\times n})$ that we use throughout the paper. Furthermore, we give the exact expressions of $s_4(G_{n\times n})$ and $s_4(T_{n\times n})$ for every $n\in\mathbb{N}^*$. Our main result is the following theorem that deals with an almost tight bound of $s_3(G_{n\times n})$.

Theorem 1 *Let $n \in \mathbb{N}^*$. Let $LB_n = \lceil \frac{n^2+2n}{3} \rceil$ if n is odd and $LB_n = \lceil \frac{n^2+2n+4}{3} \rceil$ if n is even.*

- $s_3(G_{n\times n}) = LB_n$ *if n is even or if $n \equiv 5 \mod 6$ or if $n = 2^p - 1$;*
- $LB_n \leq s_3(G_{n\times n}) \leq LB_n + 1$ *if n is odd;*
- $s_3(G_{n\times n}) = LB_n + 1$ *if $n \in \{9, 13\}$.*

Section 3 is devoted to the proof of the first two items of Theorem 1. In Section 4, we prove the last item of Theorem 1. Then, Section 5 is devoted to settle the problem when $r = 3$ in tori:

Theorem 2 *For every $n \geq 3$, $s_3(T_{n\times n}) = \lceil \frac{n^2+1}{3} \rceil$.*

We conclude in Section 6 by describing several open questions.

2 Preliminaries

2.1 Notations and Problem statement

Let $G = (V, E)$ be a graph. For a vertex $v \in V$, $N(v) = \{u \in V \mid \{u, v\} \in E\}$ is the neighbourhood of v and $d(v) = |N(v)|$ is the *degree* of v.

The 2-dimensional (square) grid graph with n rows and n columns is denoted by $G_{n\times n}$. Its vertex set is defined by $V(G_{n\times m}) = \{(i, j) \mid 1 \leq i \leq n, 1 \leq j \leq n\}$. Two vertices (i, j) and (i', j') are adjacent if and only if $|i - i'| + |j - j'| = 1$. If $1 < i, j < n$, vertex (i, j) has degree 4. The *corners* are the vertices with degree at most 2, that is, the vertices $(1, 1), (1, n), (n, 1)$ and (n, n). The *border* $\mathcal{B}$ is the set of vertices with degree at most 3.

For $n \geq 3$, let also $T_{n\times n}$ be the torus with vertex-set $\{(i, j) \mid i \in \mathbb{Z}_n$ and $j \in \mathbb{Z}_n\}$, where $\mathbb{Z}_n$ denotes the set of integers modulo n denoted $0, 1, \ldots, n - 1$. Vertex (i, j) is adjacent to the 4 vertices $(i - 1, j)$, $(i + 1, j)$ $(i, j - 1)$ and $(i, j + 1)$.

Given a graph G and a natural number $r \in \mathbb{N}^*$, we consider the following deterministic process (known as r-neighbour bootstrap percolation) that models the spread of an infection in G. Let $D_0 = D$ be a subset of initially *infected* vertices and for each step $t \geq 1$, let

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

For a set $D \subset V(G)$, let $\langle D \rangle = \bigcup_{t=0}^{\infty} D_t$ be the closure of D, i.e., the set of eventually infected vertices in the process that was started from D. A *configuration* is a pair (G, D) that consists of a graph G together with the subset D of its vertices that are initially infected. Abusing the notation, we call the *size* of the configuration as the size $|D|$ of the set D.

Any set $D \subseteq V$ is said *lethal* if $\langle D \rangle = V$. Similarly, a configuration (G, D) is lethal if D is a lethal set. Let $s_r(G)$ be the minimum size of a lethal set in G. Since $\langle V \rangle = V$, $s_r(G)$ is always well defined. A lethal set (resp. a lethal configuration) is *optimal* if it is of size $s_r(G)$. Note that $s_1(G) = 1$ for every connected graph G. The main goal of this paper is to investigate $s_3(G_{n\times n})$ and $s_3(T_{n\times n})$, i.e., focusing on square grids and tori for $r = 3$. Let us first deal with the cases $r \in \{2, 4\}$.

2.2 Cases $r \in \{2, 4\}$

For completeness, we first precisely recall the known results when $r = 2$ and give exact results in the case when $r = 4$.

The following result for $r = 2$ can be considered as folklore and appeared in many books with puzzles [Bol06, LL11, Win03]. In any grid, the lower-bound is proved using an elegant perimeter argument and an optimal lethal set is obtained by taking the n vertices of the diagonal.

Theorem 3 ([Bol06, LL11, Win03]) *Let $n \geq 1$, then $s_2(G_{n\times n}) = n$.*

The result for the torus can be found in [Bol06, Win03].

Theorem 4 (Problem 66, page 173 in [Bol06]) *Let $n \geq 1$, then $s_2(T_{n\times n}) = n - 1$.*

The case $r = 4$ was considered in [BP98] where it is only stated that $s_4(G_{n\times n}) \sim n^2/2$. However, this case is easy to solve exactly. Let $\alpha(G)$ be the maximum size of an independent set in any graph G.

Proposition 5 *For every $n \geq 3$, we have*

- $s_4(G_{n\times n}) = 4(n-1) + |V(G_{(n-2)\times(n-2)})| - \alpha(G_{(n-2)\times(n-2)}) = \lfloor \frac{n^2+4n-4}{2} \rfloor$.
- $s_4(T_{n\times n}) = |V(T_{n\times n})| - \alpha(T_{n\times n}) = n\lfloor \frac{n+1}{2} \rfloor$.

Proof. Let D be any lethal set of $G_{n\times n}$ or $T_{n\times n}$. For purpose of contradiction, let us assume that there exist $u, v \in V \setminus D$ that are adjacent. Then u should be infected before v otherwise it has at most 3 already infected neighbours, but v should also be infected before u a contradiction Hence, $V \setminus D$ must be an independent set.

In the case of a torus, any set D such that $V \setminus D$ is an independent set is a lethal set. Indeed any vertex of $V \setminus D$ has its 4 neighbours infected. Therefore, any optimal lethal set D is such that $V \setminus D$ is a minimum independent set of the torus.

In the case of a grid, any lethal set must furthermore contain all vertices of the border (since they all have degree at most 3). Finally, every set D containing all vertices of the border and such that $V \setminus D$ is an independent set is clearly a lethal set (since all vertices of $V \setminus D$ do not belong to the border and so have degree 4 in D). Note that, in this case, $V \setminus D$ is an independent set of the subgrid $G_{(n-2)\times(n-2)}$.

Finally, note that $\alpha(G_{n\times n}) = \lceil \frac{n^2}{2} \rceil$ and $\alpha(T_{n\times n}) = n\lceil \frac{n-1}{2} \rceil$ (folklore). ■

2.3 Known results for $r = 3$ that are used throughout this paper

The following lower bound has been proved in [Bol06] using the perimeter argument and noting that there are four pairs of adjacent infected vertices in $\mathcal{B}$. In particular, the notation LB_n defined below will be used throughout the paper.

Theorem 6 (Problem 65, pages 171-172 in [Bol06]) *Let $n \in \mathbb{N}^*$. It holds that:*

$$s_3(G_{n\times n}) \geq LB_n = \begin{cases} \left\lceil \frac{n^2+2n}{3} \right\rceil & \textit{if } n \textit{ is odd,} \\ \left\lceil \frac{n^2+2n+4}{3} \right\rceil & \textit{if } n \textit{ is even.} \end{cases}$$

This allows to prove the following corollary that we extensively use later.

Corollary 7 *Let $n \in \mathbb{N}$.*

$$LB_{n+3} - LB_n = \begin{cases} 2n+3 \textit{ when } n \equiv 0,4 \pmod 6 \\ 2n+4 \textit{ when } n \equiv 2 \pmod 6 \\ 2n+6 \textit{ when } n \equiv 5 \pmod 6 \\ 2n+7 \textit{ when } n \equiv 1,3 \pmod 6 \end{cases}$$

$$LB_{n+6} - LB_n = 4n + 16.$$

In [Bol06], Bollobás proved that the lower bound LB_n is indeed reached in the case $n \equiv 2 \pmod 6$ (see Figure 1(f) for $n = 8$). We rephrase his result as follows by specifying an extra property (useful later) of some optimal lethal sets.

Theorem 8 ([Bol06]) *Let $n \equiv 2 \pmod 6$, then $s_3(G_{n\times n}) = LB_n = \frac{n^2+2n+4}{3}$. Furthermore, there exists an optimal lethal set of $G_{n\times n}$ containing the vertices $(n-1,1)$, $(n,1),(n,2),(1,n-1),(n,1)$ and $(2,n)$.*

3 Various constructions and optimal results

In this section, we present several ways to use (lethal or not) configurations for smaller grids in order to obtain new lethal configurations for larger grids. Each of the different tools that we propose allow us to prove Theorem 1 (but its last item that is proved in next Section).

3.1 From n even to $n+3$ odd and optimality for $n \equiv 5 \pmod 6$

Proposition 9 *Let n be even. If D is a lethal set in $G_{n\times n}$ containing the vertices $(n-1,1),(n,2),(1,n-1)$ and $(2,n)$, then there exists a lethal configuration $(G_{(n+3)\times(n+3)}, D')$ with size $|D'| = |D| + 2n + 4$.*

Proof. From the configuration $(G_{n\times n}, D)$, let $(G_{(n+3)\times(n+3)}, D')$ be the configuration defined as follows. The restriction of D' to the subgrid $G_{n\times n}$ consisting of the first (topmost) n rows and first (leftmost) n columns of $G_{(n+3)\times(n+3)}$ will be the set D minus the vertices $(1,n)$ and $(n,1)$ (which belong to D since D is a lethal set in $G_{n\times n}$ and they are corners). Moreover, D' contains the following infected vertices: $(1,n+1)$ and $(n+1,1)$, plus the vertices $(n+2,2j+2)$ for every $0 \leq j \leq n/2$ and $(n+3,2j+1)$ for every $0 \leq j \leq n/2+1$. Symmetrically, D' contains the vertices $(2j+2,n+2)$ for every $0 \leq j \leq n/2-1$ and $(2j+1,n+3)$ for every $0 \leq j \leq n/2$. See Figure 2 for an illustration. Hence, we have $2n+6$ infected vertices in the last (bottommost) 3 rows and last (rightmost) 3 columns. Overall, $|D'| = |D| + 2n + 4$.

Now let us prove that D' is a lethal set. The vertices $(1,n)$ and $(n,1)$ will become infected at the first step because they have 3 infected neighbours initially. Therefore, every vertex of the subgrid $G_{n\times n}$ will become infected (as D is a lethal set). At the first step, all the vertices of rows and columns $n+2$ and $n+3$ are also infected plus the vertices $(n+1,2)$ and $(2,n+1)$. From these last two vertices the infection propagates along row $n+1$ and column $n+1$, until it reaches the vertex $(n+1,n+1)$. ■

By Corollary 7, we get:

Corollary 10 *Let D be a lethal set for $G_{n\times n}$ such that $\{(n-1,1),(n,2),(1,n-1),(2,n)\} \subseteq D$. If $n \equiv 0$ or $4 \pmod 6$, then $s_3(G_{(n+3)\times(n+3)}) - LB_{n+3} \leq |D| - LB_n + 1$. If $n \equiv 2 \pmod 6$, then $s_3(G_{(n+3)\times(n+3)}) - LB_{n+3} \leq |D| - LB_n$.*

Theorem 11 *Let $n \equiv 5 \pmod 6$. Then, $s_3(G_{n\times n}) = LB_n = \frac{n^2+2n+1}{3}$.*

Proof. By Theorem 8, since $n-3 \equiv 2 \pmod 6$, $s_3(G_{(n-3)\times(n-3)}) = LB_{n-3}$. Moreover, there exists an optimal lethal configuration of $G_{(n-3)\times(n-3)}$ containing the vertices in $\{(n-1,1),(n,2),(1,n-1),(2,n)\}$. The result follows from the Corollary 10. ■

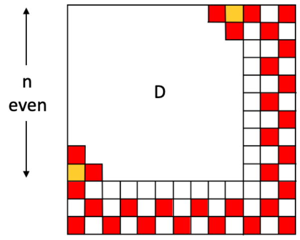


Figure 2: Illustration of Proposition 9. The vertices are depicted as small squares (with most vertices inside $G_{n\times n}$ as well as their status omitted). Initially infected (resp., not infected) vertices of D' are red (resp., white). Orange vertices are the ones that are initially infected in D but not in D'.

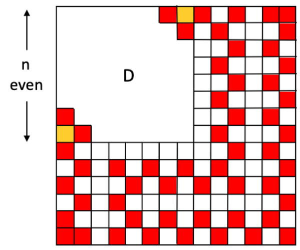


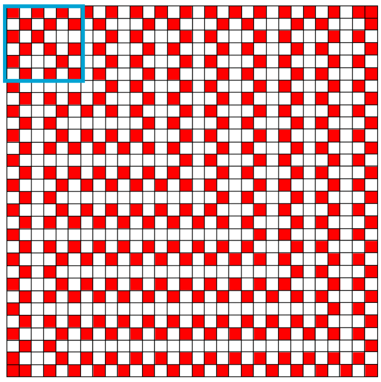
Figure 3: Illustration of Proposition 12. The vertices are depicted as small squares (with most vertices inside $G_{n\times n}$ as well as their status omitted). Initially infected (resp., not infected) vertices of D'' are red (resp., white). Orange vertices are the ones that are initially infected in D but not in D''.

3.2 From n even to $n+6$ (even) and optimality for every n even

Proposition 12 *Let n be even. If D is a lethal set in $G_{n\times n}$ such that $\{(1,n-1),(2,n),(2,2),(n-1,1),(n,2),\}\subseteq D$, then there exists a lethal configuration $(G_{(n+6)\times(n+6)},D'')$ with size $|D''|=|D|+4n+16$ and such that $\{(1,n+5),(2,n+6),(2,2),(n+5,1),(n+6,2)\}\subseteq D''$.*

Proof. From the configuration $(G_{n\times n},D)$, we first construct the configuration $(G_{(n+3)\times(n+3)},D')$ as in Proposition 9 and then the configuration $(G_{(n+6)\times(n+6)},D'')$ as follows. The restriction of D'' to the subgrid $G_{n+3\times n+3}$ consisting of the first (topmost) $n+3$ rows and first (leftmost) $n+3$ columns of $G_{(n+6)\times(n+6)}$ will be the set D' minus the vertex $(n+3,3)$. Then, D'' contains the following vertices: $(n+4,2)$ and $(n+4,4)$, $(n+5,1)$ plus the vertices $(n+5,2j+1)$ for every $2\leq j\leq n/2+2$ (note that $(n+5,3)$ is not infected) and the vertices $(n+6,2j+2)$ for every $0\leq j\leq n/2+2$. In addition, D'' contains the vertices $(2j+1,n+5)$ and $(2j+2,n+6)$ for every $0\leq j\leq n/2+1$. Finally, D'' contains the two corners $(n+6,1)$ and $(1,n+6)$. See Figures 3 for an illustration. Overall, $|D''|=|D'|+2n+12=D+4n+16$.

Now let us prove that D'' is a lethal set. The vertices $(1,n)$ and $(n,1)$ will become infected at the first step because they have 3 infected neighbours initially. Then, every vertex of the subgrid $G_{n\times n}$ will become infected (as D is a lethal set). At the first step, all the vertices of columns $n+2,n+3,n+5$ and $n+6$ become infected and all the vertices of rows $n+2,n+3,n+5$ and $n+6$ except $(n+2,3),(n+3,3),(n+5,3),(n+6,3)$. Vertices $(n+1,2)$, $(2,n+1)$ and $(n+4,5)$ are also infected at step 1. From the vertex $(2,n+1)$ the infection propagates along column $n+1$ until it reaches the vertex $(n+1,n+1)$ and then along row $n+1$ until it reaches vertex $(n+1,4)$. Then vertices $(n+2,3),(n+3,3),(n+4,3),(n+5,3),(n+6,3)$ become infected.


(a) Infection process at $t = 0$.

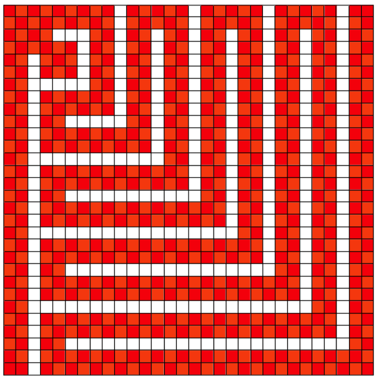

(b) Infection process at $t = 1$.

Figure 4: Construction for $n = 30$. Here we start from the optimal grid $G_{6\times 6}$ (depicted by a blue frame) obtained from the grid $G_{3\times 3}$ (Theorem 21) and apply the construction recursively. In the left part, initially infected (resp., not infected) vertices are red (resp., white). In the right part, vertices infected at step 1 are in orange and those not infected at the end of step 1 are in white. To get optimal lethal sets for the grids with n even we should also have the corners infected and to get almost optimal for the grids with n odd we should also have the vertex $(n, 3)$ infected.

From the vertex $(n+4, 5)$ the infection propagates along row $n+4$ until it reaches the vertex $(n+4, n+4)$ and then along column $n+4$ until it reaches vertex $(1, n+4)$. See an example in Figure 4. ■

Remark: We can do the proof by deleting from D' instead of vertex $(n+3, 3)$ any vertex $(n+3, 2j_0+1)$ with $1 \leq j_0 \leq n/2$. Then D'' should contain in row $n+4$ the infected vertices: $(n+4, 2j_0)$ and $(n+4, 2j_0+2)$ and in row $n+5$ all the vertices $(n+5, 2j+1)$ for every $0 \leq j \leq n/2+2$ except vertex $(n+5, 2j_0+1)$. That might be useful to diminish the propagation time.

Theorem 13 *Let n be even. Then, $s_3(G_{n\times n}) = LB_n$. Moreover, there exists an optimal lethal set which contains the vertex* $(2, 2)$.

Proof. The theorem is true for $n = 2, 4, 6$, in which cases, optimal grids can be constructed directly (for $n = 4$ and 6, see Figure 1). Then, the theorem follows by induction on n (even) using Proposition 12 and Corollary 7. ■

Theorem 14 *Let $n \equiv 1$ or $3 \pmod 6$. Then, $s_3(G_{n\times n}) \leq LB_n + 1$. Moreover, there exists a lethal set of size $LB_n + 1$ which contains the vertex* $(2, 2)$.

Proof. The theorem follows from Theorem 13 and Corollary 10. ■

3.3 From n to $2n+1$ and optimality for $n = 2^p - 1$

We give now another tool which, while rather simple, allows us to identify a new class of grids (namely, $n = 2^p - 1$) with odd side where the lower bound is tight.

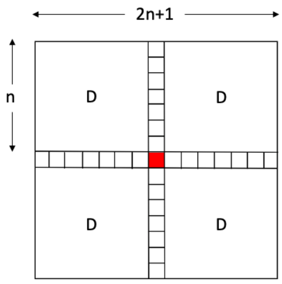


Figure 5: Illustration of the configuration $\mathcal{H}(G_{n\times n}, D)$.

For any configuration $(G_{n\times n}, D)$, let $(G_{(2n+1)\times(2n+1)}, D') = \mathcal{H}(G_{n\times n}, D)$ be the configuration defined as follows. The restriction of D' to each of the four connected components obtained from $G_{(2n+1)\times(2n+1)}$ by removing its central row and central column (i.e., the $(n+1)^{th}$ row and $(n+1)^{th}$ column) is equal to D. Finally, D' also contains the vertex $(n+1, n+1)$. See Fig. 5 for an illustration.

Lemma 15 *If $(G_{n\times n}, D)$ is a lethal configuration, then $\mathcal{H}(G_{n\times n}, D)$ is a lethal configuration.*

Proof. Since D is a lethal set for $G_{n\times n}$, each of the component of $G_{(2n+1)\times(2n+1)}$ obtained by removing the central row and the central column will be infected independently. Finally, the central row and central column will be infected using the fact that every other vertex and the central one $(n+1, n+1)$ are infected. ■

Definition 16 *Let H_1 be the configuration that consists of the grid $G_{1\times 1}$ whose single vertex is infected. For every $p > 1$, let $H_p = \mathcal{H}(H_{p-1})$.*

Proposition 17 *For every $p \geq 1$, H_p is an optimal lethal configuration for the grid $G_{2^p-1\times 2^p-1}$ with $\frac{4^p-1}{3}$ vertices initially infected.*

Proof. Since H_1 is clearly lethal, by induction on p and Lemma 15, then H_p is lethal for all p. Let D_p be the lethal set of H_p, then $|D_p| = 4|D_{p-1}|+1$ and as $|D_1|= 1$, we get $D_p = \frac{4^p-1}{3}$. Finally, the optimality comes from Theorem 6 that states that for $n = 2^p - 1, LB_n = \frac{n(n+2)}{3} = \frac{4^p-1}{3}$. ■

Theorem 18 *For every $p \in \mathbb{N}^*$, let $n = 2^p - 1$. Then, $s_3(G_{n\times n}) = LB_n = \frac{n(n+2)}{3}$.*

4 The lower bound is not always tight

In the case when n is odd such that $n \equiv 1, 3 \pmod 6$ and $n \neq 2^p - 1$, it remains to decide whether $s_3(G_{n\times n})$ equals LB_n or $LB_n + 1$. The first two values which are undetermined yet are $n = 9$ and $n = 13$. For these values, we prove that the lower bound is not tight using a Linear Program. Finally, for $n = 9$, we also give a long combinatorial proof.

4.1 Useful properties of lethal sets

First, let us present some useful properties that must be satisfied by any lethal set (or more precisely by the complement of any lethal set) of a grid.

Property 19 *Every lethal set in $G_{n\times m}$ contains every corner.*

Proof. Let u be a corner of $G_{n\times m}$ and let D be a lethal set. Since u has degree at most 2 and requires at least 3 neighbours to be infected, then $u \in D$. ■

The next property states that, for every two adjacent vertices on the border, at least one must be initially infected in order to eventually infect the whole grid.

Property 20 *Let u, v be two adjacent vertices in $\mathcal{B}$ of $G_{n\times m}$. Let D be a lethal set. Then $D \cap \{u, v\} \neq \emptyset$.*

Proof. Let D be a lethal set of $G_{n\times m}$. For purpose of contradiction, let us assume that there are two adjacent vertices u and v of the border (so they have degree at most 3) that are not in D. Then, the first vertex to be contaminated in $\{u, v\}$ would have at most two contaminated neighbours before being infected, a contradiction. ■

Property 21 *Let D be a lethal set of the grid $G_{n\times m}$. Let $H = V \setminus D$. Then, H induces an acyclic subgraph whose every connected component has at most one vertex on the border.*

Proof. For purpose of contradiction, let us first assume that H induces a subgraph containing a cycle C and let u be the first (according to $<_D$) vertex of C contaminated by D. Then, when u becomes infected, it has at most two infected neighbours, a contradiction.

Similarly, if H induces a subgraph that contains a path P (with at least two vertices) whose ends are in the border, then the first vertex to be infected in P would have at most 2 already infected neighbours, a contradiction. ■

4.2 Linear Program

We present a Mixed-Integer Linear Program (MILP) for computing $s_r(G)$ in any graph G. As initially described in section 2, we consider a *step* of the contamination process. That is, at every step, all non-infected vertices with at least r infected neighbours become infected. The question addressed in this section is as follows:

Instance : A graph $G = (V, E)$, non-negative integers r and T.
Question : What is the minimum number $s_r^T(G)$ of initially infected vertices such that the whole graph is contaminated in at most T steps?

Note that, for every $k \in \mathbb{N}$: $s_r(G) \leq k$ if and only if $s_r^{|V|-k}(G) \leq k$.

We formulate the problem as the MILP below, which computes an optimal solution for $s_r^T(G)$. The main variables are the binary variables $c_{v,t}$ for $v \in V$ and $t \in \{1, ..., T\}$, defined as follows: $c_{v,t} = 1$ if the vertex v is infected after the t^{th} step of the contamination process and 0 otherwise.

We describe hereafter the different constraints (1-6) of the MILP, starting by the objective function:

(1) Minimize the number of initially infected vertices.

(2) After T steps, all the vertices are infected.

(3) The r-neighbour contamination process.

(4) Every vertex with a degree strictly smaller than r must be initially infected (case for instance of the corners of a grid $G_{n \times n}$ when $r = 3$ (Property 19)).

(5) If two adjacent vertices have degree r, then at least one must be initially infected (case for instance of two adjacent vertices of the border of a grid $G_{n \times n}$ when $r = 3$, (Property 20)).

(6) If D is a lethal set and $v \in D$ such that $|N(v) \cap D| \geq r$, then $D \setminus \{v\}$ is a lethal set.

$$
\begin{aligned}
&\text{Minimize } \sum_{v\in V} c_{v,0} && && (1)\\
&\text{Subject to } \sum_{v\in V} c_{v,T} = |V| && && (2)\\
&c_{v,t} \le c_{v,t-1} + \frac{1}{r}\sum_{w\in N(v)} c_{w,t-1} && \forall v\in V, t\in\{1,...,T\} && (3)\\
&c_{v,0} = 1 && \forall v\in V, d(v) < r && (4)\\
&c_{u,0} + c_{v,0} \ge 1 && \forall \{u,v\}\in E, d(u)=d(v)=r && (5)\\
&c_{v,0} + \sum_{w\in S} c_{w,0} \le r && \forall v\in V, d(v)\ge r, \forall S\subseteq N(v), |S|=r && (6)\\
&c_{v,t}\in\{0,1\} && \forall v\in V, t\in\{1,...,T\} && (7)
\end{aligned}
$$

We note that the above cuts were not sufficient to make the MILP terminate (in *sufficiently reasonable time*) for $G = G_{n\times n}$ except for some small values of n. Therefore, to speedup the search, we propose further optimization cuts which hold under certain conditions on G.

Further cuts if $r \ge 3$ and G has maximum degree 4.
Let $r \ge 3$. By Property 21, if D is a lethal set, then $H = V \setminus D$ is acyclic. We introduce the next constraints (8-13) to express this property.

First, we consider the binary variables y_e for $e = \{u,v\} \in E$, defined as follows: $y_e = 1$ if and only if $c_{u,0} = 0$ and $c_{v,0} = 0$ (i.e., $y_e = 1$ if and only if e is an edge of a connected component of H).

$$
\begin{aligned}
y_e + c_{u,0} + c_{v,0} \ge 1 &\quad \forall e = \{u,v\}\in E && (8)\\
2y_e + c_{u,0} + c_{v,0} \le 2 &\quad \forall e = \{u,v\}\in E && (9)\\
y_e \in \{0,1\} &\quad \forall e = \{u,v\}\in E && (10)
\end{aligned}
$$

Then, to ensure that H is acyclic, we leverage upon an efficient formulation usually used to design a Linear Program for computing the Maximum Average Degree of a graph in polynomial time. To this end, we consider the non-negative variables $z_{e,v}$ and $z_{e,w}$ for every $e = \{v,w\} \in E$. Intuitively, each edge induced by H distributes a potential of one from each of its end-vertices, and H is acyclic if and only if no vertex receives at least one of potential.

$$
\begin{aligned}
z_{e,u} + z_{e,v} = y_e &\quad \forall e = \{u,v\}\in E && (11)\\
\sum_{\substack{e'=\{w,v\}\\ w\in N(v)}} z_{e',v} < 1 &\quad \forall v\in V && (12)\\
z_{e,u}, z_{e,v} \ge 0 &\quad \forall e = \{u,v\}\in E && (13)
\end{aligned}
$$

Further cuts if $r \ge 3$ and $G = G_{n\times n}$.
Let $r \ge 3$. By Property 21, if D is a lethal set, then $H = V \setminus D$ contains no path (of length at least 2) with both its ends in some side of the border (possibly both distinct ends in the same side). We introduce the next constraints (18-20) to express this property.

Let the parts of the border on the top, right, bottom and left of the grid $G_{n\times n}$ be denoted by the *side* $\mathcal{N}, \mathcal{E}, \mathcal{S}$ and $\mathcal{W}$, respectively. We aim at describing constraints which ensure that there is no path (of length at least two) from a side x to a side y in H, for every $x, y \in \{\mathcal{N}, \mathcal{E}, \mathcal{S}, \mathcal{W}\}$.

Let us first assume that $x \neq y$. Let G^{xy} be obtained from $G_{n\times n}$ by adding two vertices x and y to it such that x (resp., y) is adjacent to all vertices in the x (resp., y) side of $G_{n\times n}$ (here, we abuse notations by identifying the side x (resp., y) of $G_{n\times n}$ and the vertex x (resp., y) of G^{xy}).

For every edge $e \in E(G^{xy})$, we consider the binary variables y_e^{xy}, defined as follows: $y_e^{xy} = y_e$ if $e \in E(G_{n\times n})$, $y_e^{xy} = 1 - c_{v,0}$ if $e = \{x, v\}$ (or $e = \{y, v\}$) when v is not a common vertex of x and y sides, and $y^{xy}_{\{x,v\}} + y^{xy}_{\{y,v\}} = 1$ if v is a common corner of x and y sides. Now, for every vertex v in G^{xy}, we consider the non-negative real variables p_v^{xy} satisfying the constraints (14-16) (following the classical Linear Program for edge-cut).

$$p_x^{xy} = 0 \text{ and } p_y^{xy} = 1 \tag{14}$$

$$p_v^{xy} - p_w^{xy} \leq 1 - y^{xy}_{\{v,w\}} \quad \forall \{v, w\} \in E(G^{xy}) \tag{15}$$

$$p_w^{xy} - p_v^{xy} \leq 1 - y^{xy}_{\{v,w\}} \quad \forall \{v, w\} \in E(G^{xy}) \tag{16}$$

If $x = y$ (i.e., both sides are the same side), let G^{xy} be obtained from $G_{n\times n}$ by adding two vertices x and y, each of them being adjacent to all vertices of the same side $x = y$ of $G_{n\times n}$. For every edge $e \in E(G^{xy})$, we consider the binary variables y_e^{xy} defined as follows: $y_e^{xy} = y_e$ if $e \in E(G_{n\times n})$, and $y^{xy}_{\{x,v\}} + y^{xy}_{\{y,v\}} = 1 - c_{v,0}$ for every v in the $x = y$ side of $G_{n\times n}$. The remaining part is similar to what is described above.

Further optimizations. We also provided the MILP with lower and upper bounds on the expected solution. That is, we add constraints of the following form $LB \leq \sum_{v\in V} c_{v,0} \leq UB$ for some given integers LB and UB. We note that the main purpose of the previous MILP is to determine whether the lower bound LB_n is tight for the cases not covered by Theorem 1. Therefore, we added some specific constraints which reflect the properties of lethal sets of size LB_n. For instance, when $n \equiv 1$ or $3 \pmod 6$, every such lethal set D does not contain two adjacent vertices. In addition, a vertex in $V \setminus D$ cannot be surrounded by four vertices in D (Property 23). In some cases, we also imposed some further restrictions (such as, in the case when n is odd, that the vertices in the border of the grids are precisely characterized if we expect a lethal set of size LB_n) or explicitly implemented branch and bound algorithms where we specified the values of some vertices.

Overall, the MILP (these LPs) allowed us to obtain best known solutions for every n up to 20 (but 19) even when combinatorial proofs were not known to do so. So far, the case $n = 19$ is the largest size that still resists to the MILP as it provided a solution with $LB_{19}+1$ vertices initially contaminated, but was not able to terminate when requiring a solution with LB_{19} vertices. This is in contrast with the case when $n = 13$, where the MILP terminates certifying that there are no solutions using LB_{13} vertices initially contaminated. Our experiments based on the MILP allowed us as such to show that $s_3(G_{n\times n}) = LB_n + 1$ for $n \in \{9, 13\}$ (Proposition 22); but the MILP does not terminate for $n = 19$.

Proposition 22 *$s_3(G_{n\times n}) = LB_n + 1$ if $n \in \{9, 13\}$.*

Proof. The upper bounds comes Theorem 14. The fact that this is optimal results from the execution of the LP described in this section and that certified that no solutions with LB_n vertices exist. ■

4.3 Combinatorial proof for $n = 9$

We now provide below an ad-hoc combinatorial proof that $s_3(G_{9\times 9}) = LB_9 + 1$; but it seems quite tedious to generalize this proof already for $n = 13$. We first state a proposition which gives more properties of the vertices of D and $V \setminus D$ when $n \equiv 1$ or $3 \pmod 6$.

Property 23 *Let $n \equiv 1$ or $3 \pmod 6$ and let D be a lethal set of size $LB_n = (n^2+2n)/3$; then*
a) there are no two adjacent vertices in D, and
b) a vertex in $V \setminus D$ cannot have 4 neighbours in D.

Proof. We rephrase the elegant perimeter's argument used to prove Theorem 6 with a more careful analysis. Each vertex has a perimeter 4 and so the initial perimeter of a lethal set is at most $4|D|$. But, if two vertices of D are adjacent, their perimeter is 6 and not 8 and so the initial perimeter is at most $4|D| - 2$. In the process of infection each time a new vertex is infected the perimeter decreases by at least 2 and the final perimeter is $4n$. So we get $4|D| - 2 - 2(n^2 - |D|) \geq 4n$ or $|D| \geq (n^2 + 2n + 1)/3 > LB_n$ and that proves property a). If a vertex in $V \setminus D$ has 4 neighbours in D, then when this vertex is infected the perimeter decreases by 4 and not 2. So in that case we get $4|D|-2(n^2-|D|)-2 \geq 4n$ or $|D| \geq (n^2+2n+1)/3 > LB_n$ and that proves property b). ■

Proposition 24 *We have $s_3(G_{9\times 9}) = LB_9 + 1 = 34$.*

Proof. The upper bounds come from Theorem 14. To prove the proposition, by Theorem 6, it is sufficient to show that there is no lethal set for $G_{9\times 9}$ with 33 vertices.

Hence, for purpose of contradiction, let us assume that there exists a lethal set D of size 33 in the grid $G_{9\times 9}$. The basic idea of the proof is mainly to use Properties 20, 21 and 23 in order to progressively show that some vertices are forced to belong to D (vertices in red in Figure 6) or to $V \setminus D$ (vertices in yellow in Figure 6). There are few cases to be considered.

By Property 20 and 23, $D \cap \mathcal{B} = \{(1,1),(1,3),(1,5),(1,7),(1,9),\ (3,9),(5,9),\ (7,9),(9,9),$ $(9,7),(9,5),(9,3),(9,1),(7,1),(5,1),(3,1)\}$. Then by Property 23, $(2,3),(2,5),(2,7),(3,8),(5,8),$ $(7,8),(8,7),(8,5),(8,3),(7,2),(5,2),(3,2)$ are not in D. Then, Property 21 implies that $(2,2) \in D$ (otherwise there will the path $(1,2),(2,2),(2,1)$); similarly $(2,8),(8,2),(8,8) \in D$. So far, we may assume that D contains the vertices described in red and does not contain the ones in yellow as shown in Figure 6(a).

Let us now prove two claims very useful for the proof.

Claim 25 *At least one vertex in each of the pairs $\{(2,4),(2,6)\}$ $\{(4,2),(6,2)\}$, $\{(4,8),(6,8)\}$ and $\{(8,4),(8,6)\}$ belongs to D.*

Proof of Claim. Suppose it is not true and that for example $\{2,4)$, and $(2,6)\}$ are in $V \setminus D$. Then there will be the path $(1,4),(2,4),(2,5),(2,6),(1,6)$ contradicting Property 21. ⋄

Claim 26 *For each pair $\{(2,4),(4,2)\}$ $\{(6,2),(8,4)\}, \{(2,6),(4,8)\}$ and $\{(6,8),(8,6)\}$, the two vertices of this pair have the same status (either both in D or both $V \setminus D$).*

Proof of Claim. For purpose of contradiction, let us assume by symmetry that $(2,4) \in D$ and $(4,2) \notin D$ (see Figure 6(b)). By Property 23b), vertex $(3,3) \notin D$ (otherwise the vertex $(3,2)$ which belongs to $V \setminus D$ will have 4 neighbours in D. Then, Property 21 implies that vertex $(4,3) \in D$ (otherwise $V \setminus D$ would contain a 4-cycle). Moreover, by Claim 25, as $(4,2) \notin D$, then $(6,2) \in D$. Now, by Property 23a, vertices $(3,4),(4,4),(5,3)$ and $(6,3)$ are not in D. Then, Property 21 implies $(5,4) \in D$ (since otherwise we will have in $V \setminus D$ the 8-cycle $(3,2),(3,3),(3,4),(4,4),(5,4),(5,3),(5,2),(4,2))$. Then, by Property 23a), we have $(5,5),(6,4) \notin D$. Then, by Property 23b) $(7,3) \notin D$ (since otherwise $(7,2)$ would be a vertex in $V \setminus D$ with four neighbours in D). Finally, Property 21 implies $(7,4) \in D$ (otherwise $V \setminus D$ contains the 4-cycle $((7,4),(7,3),(6,3),(6,4))$) and $(8,4) \in D$ otherwise $V \setminus D$ contains a path from $(4,1)$ to $(9,4)$. But then, there are two adjacent vertices in D namely $(7,4)$ and $(8,4)$, contradicting Property 23a) (see Figure 6(b)). $\diamond$

Now, let us come back to the partial configuration described in Figure 6(a). Recall that, red vertices are known to belong to D and yellow vertices does not belong to D.

By Claim 25, at least one vertex in each of the pairs $\{(2,4),(2,6)\}$ $\{(4,2),(6,2)\}$, $\{(4,8),(6,8)\}$ and $\{(8,4),(8,6)\}$ belongs to D. We consider two cases

- Case 1: all vertices $(2,4),(2,6),(4,2),(6,2),(4,8),(6,8),(8,4),(8,6)$ belong to D (see Figure 6(c)).

  By Property 23a), this implies that vertices $(3,4),(3,6),(4,7),(6,7),(7,6),(7,4),(6,3),(4,3)$ are not in D. Then, vertices $(3,3),(3,5)(3,7),(7,3),(7,5)(7,7)$ are not in D by Property 23b). But, then there exists a 16-cycle $(3,3),(3,4),(3,5),(3,6),(3,7),(4,7),(5,7),(6,7),$ $(7,7),(7,6),(7,5),(7,4),(7,3),(6,3),(5,3),(4,3)$.

- case 2 : In at least one of the pairs $\{(2,4),(2,6)\}$ $\{(4,2),(6,2)\}$, $\{(4,8),(6,8)\}$ $\{(8,4),(8,6)\}$ one vertex belongs to D and the other not. By symmetry suppose $(2,4) \in D$ and $(2,6) \notin D$.

  By Claim 26, as $(2,4) \in D$, then $(4,2) \in D$. By Property 23a) $(3,4) \notin D$ and $(4,3) \notin D$. By Claim 26, as $(2,6) \notin D$, then $(4,8) \notin D$. Hence, by Claim 25, $(6,8) \in D$ and again by Claim 26, $(8,6) \in D$. Moreover, by Property 23a) $(6,7)$ and $(7,6)$ are not in D. Now, Property 21 implies $(3,7) \in D$, since otherwise there would be a path from $(1,6)$ to $(4,9)$ in $V \setminus D$. Then, Property 23a) implies that $(3,6)$ and $(4,7) \notin D$. Then, by Property 21, $(4,6) \in D$ again to avoid a path from $(1,6)$ to $(4,9)$ in $V \setminus D$ and then, by Property 23a) $(4,5)$ and $(5,6) \notin D$. Then, vertices $(3,5)$ and $(5,7)$ need to be in D to avoid 4-cycle in $V \setminus D$. See Figure 6(d) for the configuration reached so far. There are two subcases to be considered.

  - Case $(6,2) \in D$ (see Figure 6(e)). By Claim 26, $(8,4) \in D$ and so by Property 23a), $(6,3)$ and $(7,4) \notin D$. Then, Property 23b), $(7,3) \notin D$ (otherwise $(8,3)$ would have 4 neighbours in D). Then $(6,4)$ must be in D to avoid a 4-cycle in $V \setminus D$ and so, by Property 23a), $(5,4),(6,5) \notin D$ to avoid adjacent vertices in D. At this point, D already contains 31 vertices. Then to avoid 4-cycles in $V \setminus D$ either $(4,4) \in D$ or both $(3,3)$ and $(5,3) \in D$; similarly either $(6,6) \in D$ or both $(5,5)$ and $(7,5) \in D$. Therefore, to get $|D = 33|$ we need to have $(4,4) \in D$ and $(6,6) \in D$ and the other vertices $(5,3), 5,5), 7,5) \notin D$. But, then there is a 8-cycle in $V \setminus D$ $((5,3),(5,4),(5,5),(6,5),(7,5),(7,4),(7,3),(6,3))$, a contradiction.
  - Case $(6,2) \notin D$ (See Figure 6(f)). By Claim 26, $(8,4) \notin D$. Hence $(7,3) \in D$ to avoid a path from $(6,1)$ to $(9,4)$ in $V \setminus D$. Then, by Property 23a), $(6,3)$ and $(7,4) \notin D$. Hence, $(5,3),(7,5) \in D$ to avoid 4-cycles in $V \setminus D$, and $(6,4) \in D$ to avoid a path from $(6,1)$ to $(9,4)$ in $V \setminus D$. Moreover, by Property 23a), $(5,4)$ and $(6,5) \notin D$ to avoid adjacent vertices in D. There are already 32 vertices in D and the single remaining (undetermined yet) vertex of D is not sufficient to break all 4-cycles in $V \setminus D$, a contradiction.

$\blacksquare$

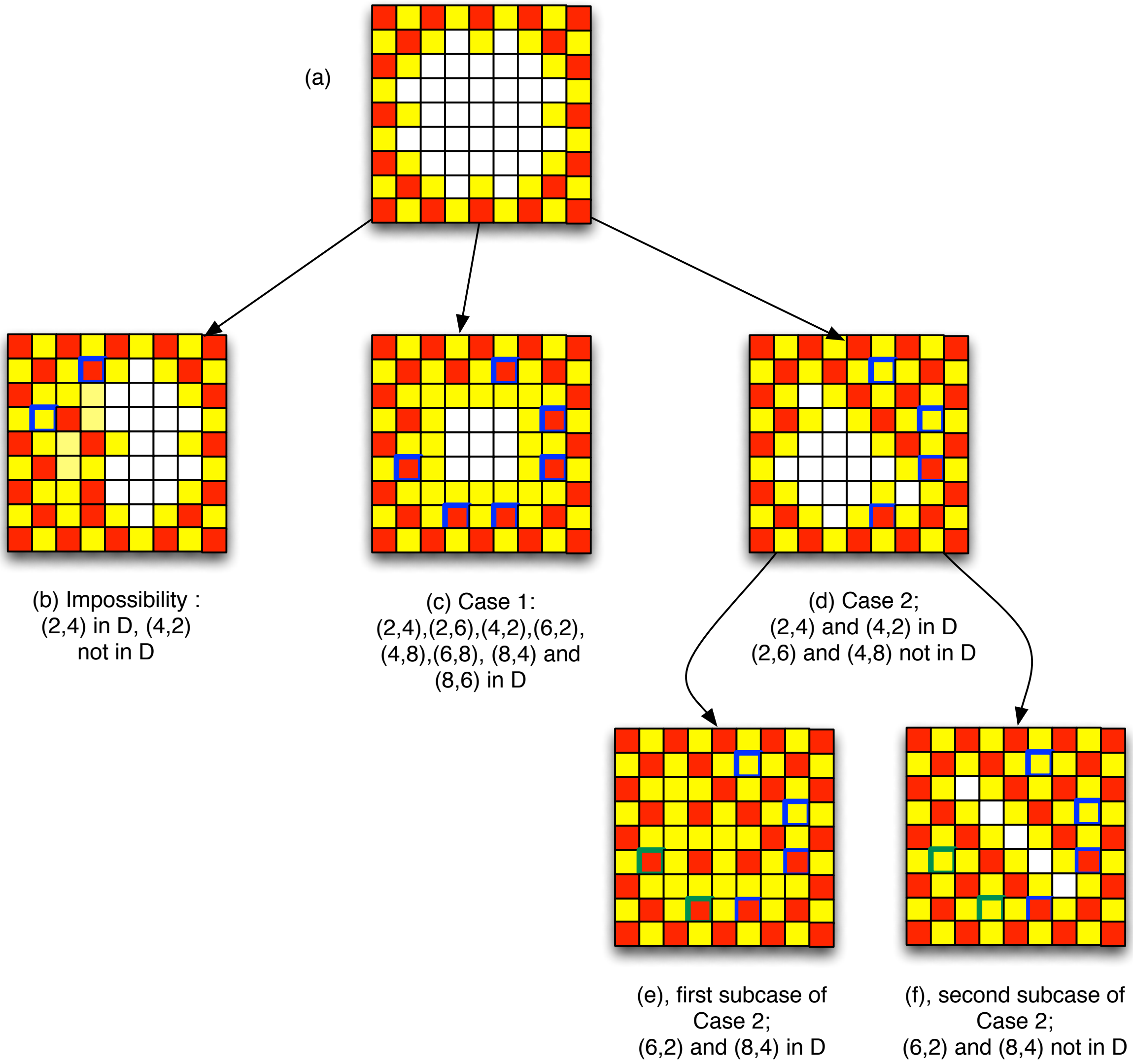
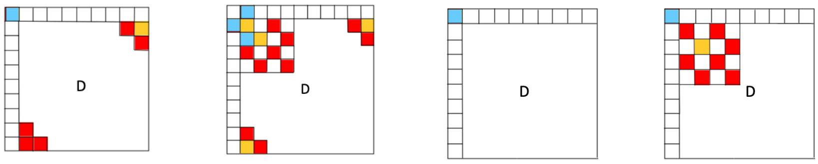


Figure 6: Illustrations of Proposition 24 ($n = 9$). Red vertices are the one that are assumed to belong to the lethal set D of size 33, yellow vertices are assumed to belong to $V \setminus D$ and white vertices are undetermined yet. Vertices (squares) surrounded by blue or green correspond to the hypotheses done in the different cases of the proof (green corresponds to the subcases). Figure (a) is a configuration that is certain if $|D| = 33$. Figure (b) is the configuration obtained if $(2,4) \in D$ and $(4,2) \notin D$ and leads to a contradiction (Claim 26). Figure (c) corresponds to the first case and leads to a contradiction. Figure (d) corresponds to the second case. Figure (e) (resp., (f)) to the subcase $(6,2) \in D$ (resp. $(6,2) \notin D$) leading to a contradiction in both subcases.

5 Tori

In this section, we focus on the square tori. We determine the exact value of $s_3(T_{n \times n})$ for every $n \geq 3$, as given in Theorem 2.

We note that Property 21 proved for the grids holds for any graph and thus, in particular for tori.



(a) $n \equiv 3$ [6] (b) $n \equiv 1, 5$ [6] (c) $n \equiv 0$ [6] (d) $n \equiv 2, 4$ [6]

Figure 7: Illustration of Theorem 29 and Theorem 30 for the torus $T_{n\times n}$. The vertices are depicted as small squares. Red squares are those of a lethal set D of $G_{(n-1)\times(n-1)}$. Orange squares are deleted from D and not infected in the torus. Blue vertices are extra infected vertices in the torus. In Figure 7(b) (resp. 7(d)), we start from the optimal grid $G_{4\times 4}$ (resp. $G_{6\times 6}$) and apply recursively the construction of proposition 12 (resp. plus proposition 9).

Property 27 *Let D be a lethal set of the torus $T_{n\times n}$. Let $H = V \setminus D$. Then, H induces an acyclic subgraph.*

Proposition 28 *Any lethal set I of $T_{n\times n}$ has size at least $\lceil \frac{n^2+c}{3} \rceil$ where $c \geq 1$ is the number of connected components of $V \setminus I$.*

Therefore, $s_3(T_{n\times n}) \geq LBT_n = \lceil \frac{n^2+1}{3} \rceil$.

Proof. Let I be any lethal set and let $H = V \setminus I$. Note that $|H| = n^2 - |I|$. Let m_{IH} be the number of edges between a vertex in I and a vertex in H and let m_H be the number of edges linking two vertices of H.

By Property 27, H must induce a forest since I is a lethal set. Hence, $m_H \leq |H| - c$ where c is the number of connected components induced by H. Moreover, since all vertices have degree 4, then $m_{IH} \leq 4|I|$. Similarly, $m_{IH} = 4|H| - 2m_H$.

Hence, $2|H| + 2c \leq 4|H| - 2m_H = m_{IH} \leq 4|I|$. Finally, $n^2 - |I| + c \leq 2|I|$. ∎

Theorem 29 *If n is odd, then $s_3(T_{n\times n}) = LBT_n$.*

Proof. As n is odd, $n-1$ is even. By Theorem 13, there exists a lethal configuration $(G_{(n-1)\times(n-1)}, D)$ of size LB_{n-1} and such that $\{(1, n-1), (1, n), (2, n), (2, 2), (n-1, 1), (n, 1), (n, 2)\} \subseteq D$. We build a lethal configuration $(T_{n\times n}, D')$ as follows.

- Let $n \equiv 3 \pmod 6$. The restriction of D' to the subgrid $G_{(n-1)\times(n-1)}$ consisting of the last (bottommost) $n-1$ rows and last (rightmost) $n-1$ columns of $G_{(n-1)\times(n-1)}$ will be the set D minus the corners $(1, n)$. Moreover, D' contains the vertex $(0, 0)$ (see Figure 7(a)). So, $|D'| = |D|$. We have $|D| = LB_{n-1} = \frac{(n-1)^2+2(n-1)+4}{3} = \frac{n^2+3}{3} = LBT_n$.
- Let $n \equiv 1, 5 \pmod 6$. The restriction of D' to the subgrid $G_{(n-1)\times(n-1)}$ consisting of the last (bottommost) $n-1$ rows and last (rightmost) $n-1$ columns of $G_{(n-1)\times(n-1)}$ will be the set D minus the four vertices $(1, n), (n, 1), (1, 1)$ and $(2, 2)$. Moreover, D' contains the three vertices $(0, 1), (1, 0)$ and $(2, 1)$ (see Figure 7(b)). So, $|D'| = |D| - 1$. We have $|D| = LB_{n-1} = \frac{(n-1)^2+2(n-1)+6}{3} = \frac{n^2+5}{3}$. So, $|D'| = \frac{n^2+2}{3} = LBT_n$.

It is easy to check that D' is lethal in both cases. ∎

Theorem 30 *If n is even, then $s_3(T_{n\times n}) = LBT_n$.*

Proof.

- Let $n \equiv 0 \pmod 6$. So $n-1 \equiv 5 \pmod 6$. By Theorem 14, there exists a lethal set D in the grid $G_{(n-1)\times(n-1)}$ of size LB_{n-1}. We construct a lethal configuration $(T_{n\times n}, D')$ as follows. The restriction of D' to the subgrid $G_{(n-1)\times(n-1)}$ consisting of the last (bottommost) $n-1$ rows and last (rightmost) $n-1$ columns of $G_{(n-1)\times(n-1)}$ will be the set D. Moreover, D' contains the vertex $(0,0)$. (see Figure 7(c)). So, $|D'| = |D| + 1$. We have $|D| = LB_{n-1} = \frac{(n-1)^2+2(n-1)+1}{3} = \frac{n^2}{3}$. So, $|D'| = \frac{n^2+3}{3} = LBT_n$.

- Let $n \equiv 2, 4 \pmod 6$. So $n-1 \equiv 1, 3 \pmod 6$. By Theorem 14, there exists a lethal set D in the grid $G_{(n-1)\times(n-1)}$ of size $LB_{n-1}+1$. We construct a lethal configuration $(T_{n\times n}, D')$ as follows.The restriction of D' to the subgrid $G_{(n-1)\times(n-1)}$ consisting of the last (bottommost) $n-1$ rows and last (rightmost) $n-1$ columns of $G_{(n-1)\times(n-1)}$ will be the set D minus the vertex $(2,2)$. Moreover, D' contains the vertex $(0,0)$ (see Figure 7(d)). So, $|D'| = |D|$. We have $|D| = LB_{n-1}+1 = \frac{(n-1)^2+2(n-1)}{3} + 1 = \frac{n^2+2}{3}$. So, $|D'| = \frac{n^2+2}{3} = LBT_n$.

It is easy to check that D' is lethal in both cases. ■

6 Further Work

The first open problem would be to completely settle the question of determining $s_3(G_{n\times n})$ (either LB_n or LB_{n+1}) for any undetermined n, i.e., for every odd $n > 13$ such that $n \not\equiv 5 \pmod 6$ and $n \neq 2^p - 1$. Note that the first undetermined value is $n = 19$ for which our Linear Program did not terminate. We can show that our results can be extended to rectangular grids and tori. Therefore, the next graph class to be considered would be d-dimensional grids for $d > 2$. Last but not least, it would be interesting to investigate further the question of the speed of the infection, i.e., determining optimal (in terms of size) lethal sets that infect the whole graph as fast (resp., as slow) as possible.

References

[AL03] Joan Adler and Uri Lev. Bootstrap percolation: visualizations and applications. *Brazilian Journal of Physics*, 33(3):641–644, 2003.

[BB06] József Balogh and Béla Bollobás. Bootstrap percolation on the hypercube. *Probability Theory and Related Fields*, 134(4):624–648, 2006.

[Bol06] Béla Bollobás. *The art of mathematics: Coffee time in Memphis.* Cambridge University Press, 2006.

[BP98] József Balogh and Gábor Pete. Random disease on the square grid. *Random Structures & Algorithms*, 13(3-4):409–422, 1998.

[BP13] Fabricio Benevides and Michał Przykucki. On slowly percolating sets of minimal size in bootstrap percolation. *The Electronic Journal of Combinatorics*, pages P46–P46, 2013.

[BP15] Fabricio Benevides and Michał Przykucki. Maximum percolation time in two-dimensional bootstrap percolation. *SIAM Journal on Discrete Mathematics*, 29(1):224–251, 2015.

[Che09] Ning Chen. On the approximability of influence in social networks. *SIAM Journal on Discrete Mathematics*, 23(3):1400–1415, 2009.

[CLR79] John Chalupa, Paul L Leath, and Gary R Reich. Bootstrap percolation on a bethe lattice. *Journal of Physics C: Solid State Physics*, 12(1):L31, 1979.

[COFKR14] Amin Coja-Oghlan, Uriel Feige, Michael Krivelevich, and Daniel Reichman. Contagious sets in expanders. In *Proceedings of the twenty-sixth annual ACM-SIAM symposium on Discrete algorithms*, pages 1953–1987. SIAM, 2014.

[GS15] Alberto Guggiola and Guilhem Semerjian. Minimal contagious sets in random regular graphs. *Journal of Statistical Physics*, 158(2):300–358, 2015.

[LL11] Anany Levitin and Maria Levitin. *Algorithmic puzzles.* OUP USA, 2011.

[MN18] Natasha Morrison and Jonathan A Noel. Extremal bounds for bootstrap percolation in the hypercube. *Journal of Combinatorial Theory, Series A*, 156:61–84, 2018.

[Mor09] Robert Morris. Minimal percolating sets in bootstrap percolation. *The Electronic Journal of Combinatorics*, 16(1):Research Paper 2,20, 2009.

[Pet97] Gabor Pete. *Disease processes and bootstrap percolation.* PhD thesis, Thesis for diploma at the Bolyai Institute, Jzsef Attila University, Szeged, 1997.

[PS20] Michał Przykucki and Thomas Shelton. Smallest percolating sets in bootstrap percolation on grids. *The Electronic Journal of Combinatorics*, pages P4–34, 2020.

[Rie10] Eric Riedl. Largest minimal percolating sets in hypercubes under 2-bootstrap percolation. *The Electronic Journal of Combinatorics*, 17(1):v17i1r80–pdf, 2010.

[Rie12] Eric Riedl. Largest and smallest minimal percolating sets in trees. *The Electronic Journal of Combinatorics*, pages P64–P64, 2012.

[Win03] Peter Winkler. *Mathematical puzzles: a connoisseur's collection.* CRC Press, 2003.