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How Many Lions Can One Man Avoid?

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Abstract

A pride of lions are prowling among the vertices and edges of an $n \times n$ grid. If their paths are known in advance, is it possible to design a safe path for a man that avoids all lions, assuming that man and lion move at the same speed? In their recent paper [4], Dumitrescu et al. employed probabilistic arguments to show that $O(\sqrt{n})$ lions can always be avoided. They raised the question if it is also possible to avoid $O(n)$ lions. Using a proof technique quite different from theirs, we give a positive answer. Even $\lfloor \frac{n}{2} \rfloor$ lions can be avoided in dimension 2. However, there is no escaping from, by order of magnitude, $\Theta(\frac{n^{d-1}}{\sqrt{d}})$ lions on the d-dimensional grid.

Introduction

Pursuit-evasion problems have a long history in mathematics and computer science, and many different models have been studied. At SoCG'07, Dumitrescu et al. [4] introduced a variant that has, apparently, not received much attention before.

Let G denote the $n \times n$ grid with vertex set V. A path π visiting $p \in V$ at time $t \in \{0, \ldots, T-1\}$ may visit a direct neighbor q of p at time $t+1$, or remain at p. Two paths π_1, π_2 are said to avoid each other if they never occupy the same vertex at the same time t and, in their transition from t to $t+1$, never traverse the same grid edge from opposite sides. Now the problem is the following. What is the maximum number $k = k(n)$ such that for all possible sets of k "lion" paths with arbitrary length T in G one can construct a "man" path that avoids them all?

This problem differs from the classical man-and-lion problem introduced by Gale, see *e.g.* Alonso et al. [1], and from cop-and-robber games investigated by Nowakowski and Winkler [8], in that they consider the online situation where the lions can adapt their paths to the escape maneuvers of their prey. The problem at hand also differs from the classical graph search problems surveyed by, *e.g.* Bienstock [2] where the man would be allowed infinite speed. In particular, it is not clear how to adapt, to our problem, the proof of LaPaugh's [6] result that a searchable graph can be searched in a monotonic way.

To the best of our knowledge, only Petrov [9] studies a model similar to ours for the graph formed by the edges of a tetrahedon. Otherwise, he assumes that lions are arbitrarily fast.

Looking at these differences to the other models, our setting may appear much less exciting. We hasten to argue why we do not think so. Instead of the path of one man, let us consider the set $W(t)$ of all vertices where this man could be at time t. That is, $W(0)$ equals V minus the lions' start positions, and $W(t+1)$ consists of all vertices p of V that

- belong to $W(t)$ and are not visited by a lion at time $t+1$, or

- are not occupied by a lion at time $t+1$, and have a direct neighbor q in $W(t)$ that is not visited at time $t+1$ by a lion coming directly from p.

Now let us side with the lions! We may consider $W(t)$ as the set of locations that are, at time t, contaminated by some evil force that spreads one step per time unit in each direction not blocked by a lion. The lions' task is to fight contamination. A lion clears a contaminated vertex by visiting it. Once the lion is gone, the vertex may become recontaminated, according to the rules stated above.

With this interpretation, our problem can be stated as follows. How many lions are needed to clear an initially contaminated $n \times n$ grid, in the model introduced above?

Clearly, n lions are able to clear the grid, by performing a left-to-right sweep in column formation. More generally, $O(n)$ lions are sufficient to clear any planar graph over n^2 vertices. Namely, due to Lipton and Tarjan [7] there exists a $c \cdot n$ vertex separator where one group of lions can be positioned, while the remaining subgraphs are recursively cleared one by one.

One could think it obvious that n lions are necessary to clear a 2-dimensional $n \times n$ grid, on the belief that a line sweep is the only way to do so. By the same reasoning, one could conjecture that it takes n^{d-1} lions to decontaminate a d-dimensional grid of size n, because a hyperplane sweep seems the only possible way to do so.

It turns out that the two-dimensional situation is not at all obvious, whereas in higher dimensions the above conjecture is wrong.

As to *two-dimensional grids*, Dumitrescu et al. [4] have employed probabilistic arguments in proving that $O(\sqrt{n})$ lions are not able to clear an $n \times n$ grid. They raised the question if the same result can be shown for a linear number of lions.

We answer this question in the affirmative, by proving that even $\lfloor \frac{n}{2} \rfloor$ lions cannot clear an $n \times n$ grid. Our proofs in dimension 2 and in higher dimensions are based on an isoperimetric inequality for grid vertex sets by Bollobás and Leader [3]. A direct proof of this inequality in dimension 2 is included in Section 2. We use this inequality in proving the following dynamic saturation property. If the set of cleared vertices has reached a critical size then its boundary contains, for each lion that clears a vertex in its next move, at least one vertex that is about to be recontaminated. Consequently, the set of cleared vertices cannot increase in size.

As to *d-dimensional grids*, we first demonstrate, in Section 3, how 8 lions, rather than $n^{d-1} = 3^2 = 9$, can clear the $3 \times 3 \times 3$ grid. This is a simple counterexample to the above conjecture. More generally, we prove that the minimum number of lions needed to clear an d-dimensional grid of size n

equals the number of grid vertices of L_1-distance $\lfloor \frac{d(n-1)}{2} \rfloor$ from the origin, up to a constant factor. Since no closed formula for this number seems to be known, we employ a folk-theorem that establishes an asymptotic estimate by means of the central limit theorem. As a consequence, we obtain that the d-dimensional grid of size n can be cleared by $\Theta(\frac{n^{d-1}}{\sqrt{d}})$ many lions.

We consider these combinatoric results as prerequisites for the design of efficient algorithms that might help to deploy forces in tasks like fire fighting.

1 Definitions

Following [3], we define $[n] := \{0, \ldots, n-1\}$. Let $G_n^d := (V_n^d, E_n^d)$ denote the d-dimensional $(n \times \ldots \times n)$-grid with vertex set $V_n^d := [n]^d$ and edge set $E_n^d := \{\{v, w\} \mid |v - w| = 1\}$ where $|.|$ denotes the L_1-distance, which is defined as the sum of the absolute values of all coordinate differences.

In the following we will often omit the indices d and n. For any vertex $v \in V$ we denote its *neighborhood* by $\mathcal{N}(v) := \{w \in V \mid w = v \vee \{v, w\} \in E\}$. A *path* in G over the time set $\{0, \ldots, T\}$ is a function $\pi : \{0, \ldots, T\} \to V$ such that every non-constant step of the path uses an edge in G, i.e., $\forall t \in \{0, \ldots, T-1\} : \pi(t+1) \in \mathcal{N}(\pi(t))$.

Given two paths π_1, π_2 over $\{0, \ldots, T\}$, we say that they *avoid* each other if they do not meet at any time $t \in \{0, \ldots, T\}$ and if the two paths never traverse the same edge in the same time step. Expressed in a more formal way this means

$$\begin{aligned} &\forall t \in \{0, \ldots, T\} : \quad \pi_1(t) \neq \pi_2(t) \\ &\quad \wedge \quad \forall t \in \{0, \ldots, T-1\} : \quad \{\pi_1(t), \pi_1(t+1)\} \neq \{\pi_2(t), \pi_2(t+1)\}. \end{aligned}$$

Avoidance question in G_n^d. Given k paths over $\{0, \ldots, T\}$ in G_n^d, does there exist another path over the same time set which avoids them? We say that G_n^d has *avoidance number* $k_d(n)$, if any $k_d(n)$ paths in G_n can be avoided over an arbitrary long time set $\{0, \ldots, T\}$ and if there exist $k_d(n)+1$ paths which cannot be avoided.

Let us now consider k arbitrary paths $\pi_1, \ldots, \pi_k : \{0, \ldots, T\} \to V$. We call a vertex $v \in G_n$ *cleared* at time $t \in \{0, \ldots, T\}$ if there does not exist any path $\rho : \{0, \ldots, t\} \to V$ with $\rho(t) = v$ which avoids $\{\pi_1|_{\{0,\ldots,t\}}, \ldots, \pi_k|_{\{0,\ldots,t\}}\}$, see Figure 1 for an example. Let $\mathcal{C}(t)$ denote the set of cleared vertices at time t.

As in the Introduction, we can also define vertex sets $W(t)$ in the following way. $W(0)$ is the set of all grid vertices minus the lions' start positions $\{\pi_1(0), \ldots, \pi_k(0)\}$. The set $W(t+1)$ consists of all vertices $p \notin \{\pi_1(t+1), \ldots, \pi_k(t+1)\}$ for which a neighbor $q \in \mathcal{N}(p) \cap W(t)$ exists such that for no j, where $1 \le j \le k$, the conditions $\pi_j(t) = p$ and $\pi_j(t+1) = q$ hold; this includes the case $p = q$.

With these notations the following facts are obvious.

Lemma 1 *1. For all t we have $[n]^d = W(t) \cup \mathcal{C}(t)$ and $W(t) \cap \mathcal{C}(t) = \emptyset$.*

2. $k_d(n) + 1$ is the smallest number of lions whose paths can achieve that $\mathcal{C}(T) = [n]^d$ holds at some time T.

As Dumitrescu et al. [4] observed for $d = 2$, it is easy to verify that

$$k_d(n) + 1 \le n^{d-1}$$

holds, by sweeping the grid with a hyperplane manned with n^{d-1} lions.

There are different types of cleared vertices depending on their neighborhood. A cleared vertex $v \in \mathcal{C}(t)$ is a cleared *interior* vertex if all of its neighbors are also cleared, i.e. $\mathcal{N}(v) \subseteq \mathcal{C}(t)$. Otherwise it is a cleared *boundary* vertex. More generally, for any vertex set $C \subset [n]^d$ we define the set of *boundary vertices* as $\partial C := \{v \in C \mid \mathcal{N}(v) \cap \overline{C} \neq \emptyset\}$ where $\overline{C} := [n]^d \setminus C$ denotes the complement of C.

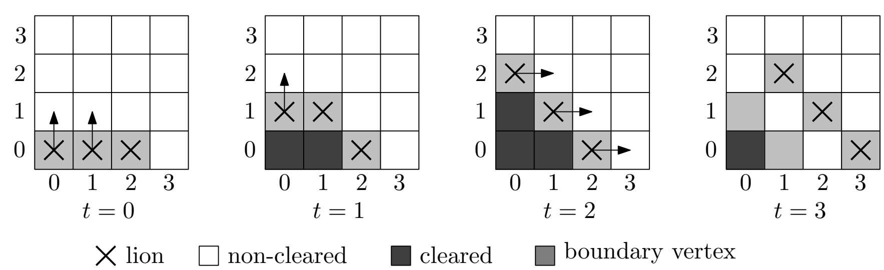

Figure 1: Three lions try to decontaminate a 2-dimensional 4×4-grid. (In this illustration the vertices are cells, and edges exist between neighbor cells.)

2 Results in dimension 2

In this section we study the 2-dimensional case and prove the following result.

Theorem 2 *$n/2$ lions are not capable of cleaning a 2-dimensional grid of size n. In other words, $k_2(n) \ge n/2$.*

In the following the variable k always denotes the number of lions. As a first step we prove the following simple lemma.

Lemma 3 *The number of cleared vertices cannot increase by more than k within one time step.*

Proof. Let $\mathcal{L}(t) := \{\pi_1(t), \ldots, \pi_k(t)\}$ denote the set of vertices which are occupied by lions at time t. The set of newly cleared vertices equals

$$\mathcal{C}(t+1) \setminus \mathcal{C}(t) \;=\; \mathcal{L}(t+1) \setminus \mathcal{C}(t). \tag{1}$$

This shows $|\mathcal{C}(t+1) \setminus \mathcal{C}(t)| \leq |\mathcal{L}(t+1)| \leq k$. Hence, we have

$$\begin{aligned} |\mathcal{C}(t+1)| &= |\mathcal{C}(t+1) \cap \mathcal{C}(t)| + |\mathcal{C}(t+1) \setminus \mathcal{C}(t)| \\ &\leq |\mathcal{C}(t)| + k. \end{aligned}$$

The number of cleared vertices can increase by at most k. □

Next, we show a slightly more involved statement which is an important step of the proof.

Lemma 4 *If there are more than $2k-1$ boundary vertices, then the amount of cleared vertices cannot increase in the following step.*

$$|\partial C(t)| \geq 2k \;\;\Rightarrow\;\; |\mathcal{C}(t+1)| \leq |\mathcal{C}(t)|.$$

Proof. We assume $|\partial C(t)| \geq 2k$. We want to prove that in the time step from t to $t+1$ there are not more vertices cleared than recontaminated by the lions, i.e.,

$$|\mathcal{C}(t+1) \setminus \mathcal{C}(t)| \;\overset{?}{\leq}\; |\mathcal{C}(t) \setminus \mathcal{C}(t+1)|. \tag{2}$$

The set of newly cleared vertices is described in (1). The set of recontaminated vertices, $\mathcal{C}(t) \setminus \mathcal{C}(t+1)$, is more difficult to describe. Clearly, a vertex has to be a boundary vertex at time t to become recontaminated. And it must not be occupied by a lion at time $t+1$. We call the vertices of $\partial C(t) \cap \mathcal{L}(t+1)$ the ones which are *kept by arriving or remaining lions*, and we denote the set by $\mathcal{K}_{ar}$. For instance in Figure 1 at time $t = 1$, the vertex $(0,1)$ is kept by a leaving lion and vertex $(2,0)$ is kept by a remaining lion.

However, there is one other way how the lions can keep a boundary vertex cleared. Let v be a boundary vertex with i non-cleared neighbors. If there are at least i lions located on v at time t and these lions move in such a way that they use every edge leading to a non-cleared neighbor, then v remains cleared. Those vertices are *kept by leaving lions*; we denote the vertex set by $\mathcal{K}_l$. For example the vertex $(0,0)$ is kept by a leaving lion in the first step of Figure 1.

The sets $\mathcal{K}_l$ and $\mathcal{K}_{ar}$ need not be disjoint. However, every boundary vertex which is not kept by arriving lions nor kept by leaving lions is recontaminated. Hence the set of recontaminated vertices equals

$$\mathcal{C}(t) \setminus \mathcal{C}(t+1) \;=\; \partial C(t) \setminus (\mathcal{K}_{ar} \cup \mathcal{K}_l)\,. \tag{3}$$

Clearly, every lion can contribute only once to $\mathcal{K}_l$ which implies $|\mathcal{K}_l| \leq k$. On the other hand, a lion moves either to a contaminated or to a cleared vertex. In the first case it can contribute at most once to the set of newly cleared vertices. In the second case it can contribute at most once to $\mathcal{K}_{ar}$. This implies $|\mathcal{C}(t+1) \setminus \mathcal{C}(t)| + |\mathcal{K}_{ar}| \leq k$. We plug everything together and get

$$\begin{aligned}
|\mathcal{C}(t) \setminus \mathcal{C}(t+1)| &\overset{(3)}{=} |\partial C(t) \setminus (\mathcal{K}_{ar} \cup \mathcal{K}_l)| \\
&\geq \underbrace{|\partial C(t)|}_{\geq 2k} - \underbrace{|\mathcal{K}_l|}_{\leq k} - \underbrace{|\mathcal{K}_{ar}|}_{\leq k - |\mathcal{C}(t+1) \setminus \mathcal{C}(t)|} \\
&\geq |\mathcal{C}(t+1) \setminus \mathcal{C}(t)|.
\end{aligned}$$

This proves (2), and the proof of the lemma is completed. □

Observe that both Lemma 3 and Lemma 4 hold for arbitrary graphs.

Next, we will prove that every set $C \subset V_n^2$ of approximately $n^2/2$ cleared vertices has at least n boundary vertices. This isoperimetric inequality is by Bollobás and Leader [3]. For convenience, we include a direct proof in dimension 2. Its Lemma 5 and an analogue to Lemma 6 were also used by Galtier [5].

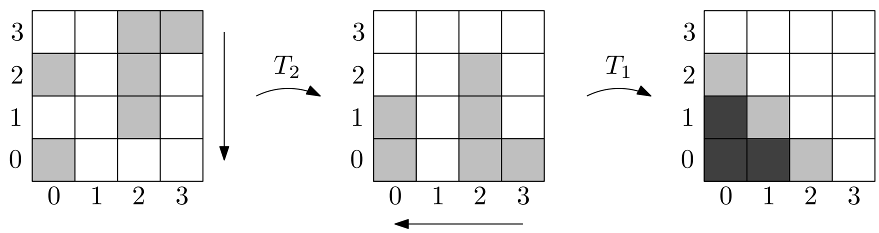

Figure 2: The fall-down transformation does not increase the number of boundary cells (=vertices).

We introduce the *fall-down transformation*[1] which enables us to concentrate on situations where the cleared vertices are spread in a monotone way, cf. Figure 2. The idea is to turn on a kind of gravity which tows all cleared vertices downward towards the 0-level of a particular coordinate i, and to execute this transformation for every coordinate $i \in \{1, \ldots, d\}$.

More formally, let $C \subseteq [n]^d$ be an arbitrary subset of the grid-vertices. Let $i \in \{1, \ldots, d\}$ be arbitrary, and let

$$n_{i,C}(v_1, \ldots, v_{i-1}, v_{i+1}, \ldots, v_d) := |\{(v_1, \ldots, v_{i-1}, a, v_{i+1}, \ldots, v_d) \in C \mid a \in [n]\}|$$

[1]Bollobás and Leader [3] call those transformations compressions and Galtier [5] called it "pushing" process.

denote the number of vertices of C in the column over the vertex $(v_1, \dots, v_{i-1}, 0, v_{i+1}, \dots, v_d)$. For simplicity, we will often omit the C in $n_{i,C}(V)$. The *fall-down transformation with respect to coordinate* i is defined by

$$T_i(C) := \{(v_1, \dots, v_d) \mid v_i < n_i(v_1, \dots, v_{i-1}, v_{i+1}, \dots, v_d)\}\,.$$

The general *fall-down transformation* is a concatenation of all such transformations,

$$T : \mathcal{P}([n]^d) \to \mathcal{P}([n]^d), \quad T(C) := T_1 \circ T_2 \circ \ldots \circ T_d(C).$$

Note that changing the order in this concatenation can alter the result but not the monotonicity of the result. A set $C \subseteq [n]^d$ is said to be *i-monotone*, $i \in \{1, \dots, d\}$, if

$$\begin{aligned} &\forall (v_1, \dots, v_{i-1}, v_i, v_{i+1}, \dots, v_d) \in C : v_i > 1 \\ &\ \Rightarrow\ (v_1, \dots, v_{i-1}, v_i - 1, v_{i+1}, \dots, v_d) \in C. \end{aligned}$$

The set C is *monotone* if it is i-monotone for every $i \in \{1, \dots, d\}$.

Lemma 5 *The result of the fall-down transformation is monotone.*

Proof. By definition it is clear that the result of each T_i is i-monotone.

It remains to show that for every $i, j \in \{1, \dots, d\}$, $i \neq j$, and for every $C \subseteq [n]^d$ which is j-monotone the transformed set $T_i(C)$ is still j-monotone. To this end, let us assume that $C \subseteq [n]^d$ is j-monotone, $i \neq j$.

Let $v = (v_1, \dots, v_d) \in [n]^d$ be an arbitrary vertex satisfying $v_j > 0$. Then, we have

$$\begin{aligned} &n_i(v_1, \dots, v_{i-1}, v_{i+1}, \dots, v_d) \qquad (4)\\ &\quad = \ |\{(v_1, \dots, v_{i-1}, a, v_{i+1}, \dots, v_{j-1}, v_j, v_{j+1}, \dots, v_d) \in C \mid a \in \{1, \dots, d\}\}| \\ &\quad \leq \ |\{(v_1, \dots, v_{i-1}, a, v_{i+1}, \dots, v_{j-1}, v_j - 1, v_{j+1}, \dots, v_d) \in C \mid a \in \{1, \dots, d\}\}| \\ &\quad = \ n_i(v_1, \dots, v_{i-1}, v_{i+1}, \dots, v_{j-1}, v_j - 1, v_{j+1}, \dots, v_d) \end{aligned}$$

because the j-monotonicity of C implies that for every $(v_1, \dots, v_{i-1}, a, v_{i+1}, \dots, v_d) \in C$ also the vertex $(v_1, \dots, v_{i-1}, a, v_{i+1}, \dots, v_{j-1}, v_j - 1, v_{j+1}, \dots, v_d)$ belongs to C.

We want to prove

$$\forall (v_1, \dots, v_d) \in T_i(C) : \ \ v_j > 0 \ \Rightarrow\ (v_1, \dots, v_{j-1}, v_j - 1, v_{j+1}, \dots, v_d) \in T_i(C).$$

We assume that the preconditions are fulfilled. By (4) we can conclude

$$\begin{aligned} v_i &\overset{v \in T_i(C)}{\leq} n_i(v_1, \dots, v_{i-1}, v_{i+1}, \dots, v_{j-1}, v_j, v_{j+1}, \dots, v_d) \\ &\overset{(4)}{\leq} n_i(v_1, \dots, v_{i-1}, v_{i+1}, \dots, v_{j-1}, v_j - 1, v_{j+1}, \dots, v_d). \end{aligned}$$

By definition of $T_i(C)$ this proves $(v_1, \ldots, v_{j-1}, v_j - 1, v_{j+1}, \ldots, v_d) \in T_i(C)$. □

For lack of space, the proof of the following lemma has been moved to the Appendix.

Lemma 6 *The number of boundary vertices does not increase by the fall-down transformation.*

Now, all we need to conclude that $n/2$ lions are not enough to decontaminate the 2-dimensional $n \times n$ grid is the following statement.

Lemma 7 *Any vertex set $C \subset V_n^2$ satisfying $n^2/2 - n/2 < |C| < n^2/2 + n/2$ has at least n boundary vertices.*

Proof. Due to Lemma 6 it suffices to prove the claim for monotone sets $C \subset V_n^2$. Note that in the two-dimensional setting, $n_1(j)$ denotes the number of vertices of C in the j-th row and $n_2(i)$ denotes the number of vertices of C in the i-th column. Because of the monotonicity we have

$$n_1(0) \geq n_1(1) \geq \ldots \geq n_1(n-1) \text{ and } n_2(0) \geq n_2(1) \geq \ldots \geq n_2(n-1).$$

And clearly $\sum_{j=0}^{n-1} n_1(j) = \sum_{i=0}^{n-1} n_2(i) = |C|$ holds.

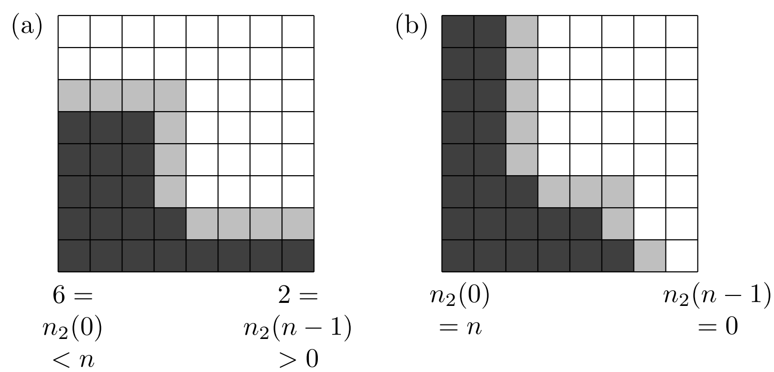

Figure 3: Two simple cases with at least n boundary vertices.

Consider Figure 3.(a). If all the columns are neither completely full nor totally empty, i.e. $n_2(0) < n$ and $n_2(n-1) > 0$, then every column contains at least one boundary vertex, and the proof is completed. Otherwise, we have either $n_2(0) = n$ or $n_2(n-1) = 0$.

We consider the first case, $n_2(0) = n$. Note that in this case $n_2(n-1) = 0$ would imply that all the rows are neither completely empty nor completely full and the proof would be completed, cf. Figure 3.(b). Hence, it suffices to consider $n_2(0) = n$ and $n_2(n-1) > 0$.

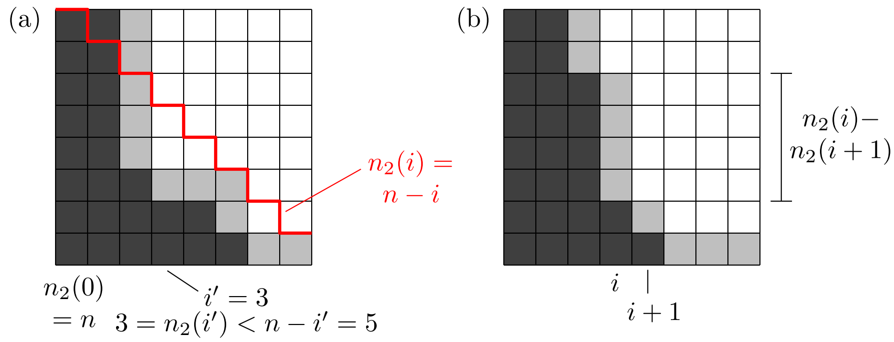

Figure 4: (a) There exists a column satisfying $n_2(i') < n - i'$. (b) Column i contains at least $n_2(i) - n_2(i+1)$ boundary vertices.

Consider Figure 4.(a). There must be a column i' satisfying $n_2(i') < n - i'$. Otherwise we had

$$\begin{aligned} |C| \;&\geq\; \sum_{i=0}^{n-1}(n-i) \;=\; n^2 - \sum_{i=0}^{n-1} i \;=\; n^2 - \frac{n(n-1)}{2} \\ &=\; n^2 - \frac{n^2}{2} + \frac{n}{2} \;=\; \frac{n^2}{2} + \frac{n}{2}. \end{aligned}$$

For such a column i' we have

$$\sum_{i=0}^{i'-1} n_2(i) - n_2(i+1) \;=\; n_2(0) - n_2(i') \;\geq\; n - (n - i') + 1 \;=\; i' + 1.$$

However, each column $i \in \{0, \ldots, i'-1\}$ contains at least $n_2(i) - n_2(i+1)$ boundary vertices, see Figure 4.(b). Hence all these columns contain at least $i' + 1$ boundary vertices. And the remaining columns $i'+1, \ldots, n-1$ contain at least $n - i' - 1$ boundary vertices. This completes the proof for the case $n_2(n) > 0$. The case $n_2(n-1) = 0$ can be treated analogously. □

Finally, we are able to prove Theorem 2.

Proof. If $k = \lfloor n/2 \rfloor$ lions were able to clear G_n^2, they would have to extend the set of cleared vertices until $|\mathcal{C}(T)| = n^2$. By Lemma 3 we know that $|\mathcal{C}(t+1)| - |\mathcal{C}(t)| \leq k \leq n/2$ for every t. Hence, there had to be a time t such that $n^2/2 - n/4 \leq |\mathcal{C}(t)| \leq n^2/2 + n/4$ and $|\mathcal{C}(t+1)| > |\mathcal{C}(t)|$. But, by Lemma 7, there would be at least n boundary vertices, and Lemma 4 shows that $|\mathcal{C}(t+1)| \leq |\mathcal{C}(t)|$, a contradiction. □

3 Results for higher dimensions

As mentioned in the introduction, one could conjecture $k_d(n) = n^{d-1} - 1$. However, this does not even hold for $d = 3$, see Figure 5. Note that the moving lion might need several steps to reach its destination. This is no problem because the remaining lions stay at their current positions and protect the cleared vertices.

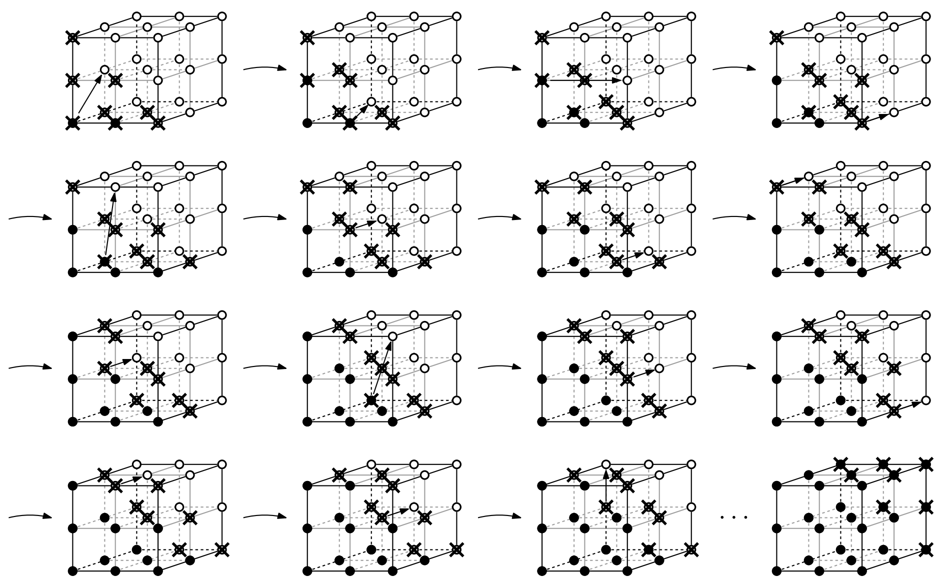

Figure 5: Eight lions (rather than $n^{d-1} = 9$) suffice to clear the $3\times3\times3$-grid.

The idea of this strategy is motivated by a result by Bollabás and Leader [3] based on the following *simplicial order* on $[n]^d$. For every two vertices $v, w \in [n]^d$ we have

$$\begin{aligned} v < w \quad :\Leftrightarrow \quad & |v| < |w| \ \vee \\ & (|v| = |w| \wedge \exists j \in [n] : \ (v_j > w_j \wedge \forall i < j : v_i = w_i)) \end{aligned}$$

Let $v^1 := 0 := (0, \ldots, 0)$, $v^2 := (1, 0, \ldots, 0)$, $v^3 := (0, 1, 0, \ldots, 0)$, $\ldots$ denote the vertices in simplicial order. And for every $i \in \{0, \ldots, n^d\}$ let $A_i := \{v^1, \ldots, v^i\}$ be the set of the first i vertices with respect to the simplicial order. Then, $|\partial A_i|$ denotes the number of boundary vertices of A_i. With this notation it is not difficult to prove the following upper bound on $k_d(n)$ by generalizing the strategy from Figure 5.

Lemma 8 $k_d(n) < \max_{m \in \{0,1,\ldots,n^d\}} |\partial A_m|$.

Proof. Let $k^* := \max_{m \in \{0,1,\ldots,n^d\}} |\partial A_m|$. Now let k^* lions sweep $[n]^d$ in simplicial order. At the beginning, let the first lion occupy the first vertex $v^1 = 0$, the second one stays at the second vertex v^2, and so on. The vertex v^{k^*} is occupied by the last lion.

Note that $\partial A_{i+1} \setminus \partial A_i = \{v^{i+1}\}$ for every $i < n^d$ and $\partial A_{n^d} \setminus \partial A_{n^d-1} = \emptyset$. This will make sure that within our strategy the boundary vertices are always occupied by lions.

Now we assume that the vertices in $\mathcal{C}(t) = A_i$ are cleared already. In the first step, we have $i = k^*$. Next, the vertex v^{i+1} has to be cleared. There is at least one lion which is currently located on a vertex w not belonging to ∂A_{i+1}, because there are never two lions on the same vertex, $|\partial A_{i+1}| \leq k^*$, and the vertex $v^{i+1} \in \partial A_{i+1}$ is not yet occupied by any lion. On the other hand, by definition of the sets A_i, we have $\partial A_{i+1} \subseteq \partial A_i \cup \{v^{i+1}\}$.

If the lion vertex $w \notin \partial A_{i+1}$ does not belong to ∂A_i either, we can move its lion to v^{i+1}. This might take several steps but no cleared vertices become recontaminated, because the remaining lions stay on their current positions and protect ∂A_i. Otherwise w belongs to $\partial A_i \setminus \partial A_{i+1}$. In this case, v^{i+1} must be the only neighbor of w which does not belong to A_i. Hence, we can move the lion from w along the edge to v^{i+1} to extend the set of cleared vertices to A_{i+1}. Again, no cleared vertex is recontaminated in this move.

The same procedure works in all the following steps. This shows that k^* lions can clear the grid, hence the upper bound is proved. □

To obtain an upper bound on the right hand side of the inequality in Lemma 8, let us first make another definition. Let $b(r, n, d)$ denote the number of vertices with L_1-distance r from vertex 0 in the d-dimensional $n \times \ldots \times n$-grid. For $r \leq d(n-1)$ the value of $b(r, n, d)$ can be computed recursively by $b(r, n, d) = \sum_{i=\max(0,r-n+1)}^{r} b(i, n, d-1)$. As start of the recursion, we can use $b(r, n, 1) = 1$ for $0 \leq r \leq n-1$ and $b(r, n, 1) = 0$ otherwise.

Lemma 9 *$b(r, n, d)$ is increasing in r for $0 \leq r \leq \frac{d(n-1)}{2}$.*

Proof. We use induction on d. For $d = 1$, we obtain $b(r, n, 1) = 1$ for $0 \leq r \leq \frac{n-1}{2}$.

So, let us assume, we already showed that $b(r, n, d)$ is increasing in r in the range of $0 \leq r \leq \frac{d(n-1)}{2}$. Due to the symmetry $b(r, n, d) = b(d(n-1)-r, n, d)$, this also means that $b(r, n, d)$ decreases monotonously in r in the range of $\frac{d(n-1)}{2} \leq r \leq d(n-1)$. The symmetry $b(r, n, d) = b(d(n-1)-r, n, d)$ holds, because all grid points with distance r from the origin have distance $d(n-1)-r$ from the grid point $(n-1, \ldots, n-1)$ and vice versa.

We want to prove the statement for dimension $d+1$. For $0 \leq r \leq n-2$, increasing r by 1 increases $b(r, n, d+1)$ by a nonnegative summand, so the monotonicity holds.

For the remaining range $n-1 \leq r \leq \frac{(d+1)(n-1)}{2} - 1$ we obtain $b(r+1, n, d+1) - b(r, n, d+1) = b(r+1, n, d) - b(r-n+1, n, d) =: x(r, n, d)$. We will prove the monotonicity by showing $x(r, n, d) \geq 0$.

If $r + 1 \leq \frac{d(n-1)}{2}$, then $r - n + 1$ as well as $r + 1$ are in the increasing part of $v \mapsto b(v, n, d)$, so $x(r, n, d) \geq 0$ and the monotonicity holds. For

$r+1 \geq \frac{d(n-1)}{2}$, the term $x(r,n,d)$ is monotonously decreasing in r, since $r+1$ is in the decreasing part of $v \mapsto b(v,n,d)$, while $r-n+1 \leq \frac{d(n-1)}{2} - \frac{n+1}{2}$ is still in the increasing part. But even if we chose $r = \lfloor \frac{(d+1)(n-1)}{2} \rfloor - 1$, which is the maximum value for r, we can still show $x(r,n,d) \geq 0$.

If d is odd or n is odd, we obtain $x(r,n,d) = b(\frac{d(n-1)}{2} + \frac{n}{2} - \frac{1}{2}, n, d) - b(\frac{d(n-1)}{2} - \frac{n}{2} - \frac{1}{2}, n, d)$, which equals $b(\frac{d(n-1)}{2} - \frac{n}{2} + \frac{1}{2}, n, d) - b(\frac{d(n-1)}{2} - \frac{n}{2} - \frac{1}{2}, n, d)$ due to the symmetry. This shows that the monotonicity of $b(.,.,d)$ implies the monotonicity of $b(.,.,d+1)$ within the range needed for Lemma 9. Accordingly, if d is even and n is even, we obtain $x(r,n,d) = b(\frac{d(n-1)}{2} + \frac{n}{2} - 1, n, d) - b(\frac{d(n-1)}{2} - \frac{n}{2} - 1, n, d) \geq 0$. □

Lemma 10 *$k_d(n) \leq 2b(\lfloor \frac{(n-1)d}{2} \rfloor, n, d)$.*

Proof. By Lemma 8, we only have to find an upper bound to $\max_{m \in \{0,1,\ldots,n^d\}} |\partial A_m|$. Assume, vertex v^m has L_1-distance r from 0. Then the simplicial order guarantees that all boundary vertices of A_m have either distance $r-1$ or distance r from 0.

Hence, $\max_{m \in \{0,1,\ldots,n^d\}} |\partial A_m| \leq 2 \max_{r \in \{0,\ldots,(n-1)d\}} b(r,n,d)$. Since the layer containing the vertices with L_1-distance $\lfloor \frac{(n-1)d}{2} \rfloor$ from the origin contains the most vertices by Lemma 9, we are done. □

The following fact is based on Bollabás and Leader [3].

Lemma 11 *For every given size $m \in \{0,\ldots,n^d\}$ the set A_m attains the minimum number of boundary vertices, i.e.*

$$\forall C \subseteq [n]^d : \ |C| = m \ \Rightarrow \ |\partial C| \geq |\partial A_m|.$$

Proof. For every $A \subseteq [n]^d$ and every $r \in \{0,\ldots,n(d-1)\}$ one defines the *r-neighborhood* of A as

$$\mathcal{N}_r(A) \ := \ \{v \in [n]^d \mid \exists w \in A : \ |v-w| \leq r\}.$$

Then, Theorem 8 in [3] states that every $C \subseteq [n]^d$ of $m := |C|$ vertices satisfies $\mathcal{N}_1(C) \geq \mathcal{N}_1(A_m)$. This can be translated into our Lemma 11 as follows.

Remember that for every set $C \subset [n]^d$, the set $\overline{C} := [n]^d \setminus C$ denotes the complement of C. Then, we have $\partial C = \mathcal{N}_1\left(\overline{C}\right) \setminus \overline{C}$. Furthermore, if v^R denotes the reflection of $v \in [n]^d$ defined by $v^R := (n-1-v_1, n-1-v_2, \ldots, n-1-v_d)$ and C^R denotes $\{v^R \mid v \in C\}$, we have $v < w \Leftrightarrow v^R > w^R$ and this implies $\overline{A_m} = A^R_{nd-m}$.

Now let $C \subseteq [n]^d$ be an arbitrary set of size m. We obtain

$$\begin{aligned} |\mathcal{N}_1\left(\overline{C}\right)| &\overset{\text{Thm. 8 [3]}}{\geq} |\mathcal{N}_1(A_{nd-m})| = |\mathcal{N}_1(A_{nd-m})^R| \\ &= |\mathcal{N}_1(A^R_{nd-m})| = |\mathcal{N}_1(\overline{A_m})|. \end{aligned} \tag{5}$$

This implies

$$\begin{aligned}|\partial C| &= |\mathcal{N}_1(\overline{C}) \setminus \overline{C}| = |\mathcal{N}_1(\overline{C})| - (nd - m) \\ &\overset{(5)}{\geq} |\mathcal{N}_1(\overline{A_m})| - (nd - m) = |\mathcal{N}_1(\overline{A_m}) \setminus \overline{A_m}| = |\partial A_m|.\end{aligned}$$

□

Lemma 12 $k_d(n) + 1 \geq \lfloor \frac{1}{6} b(\lfloor \frac{(n-1)d}{2} \rfloor, n, d) \rfloor$.

Proof. We call the vertices with L_1-distance $\lfloor \frac{(n-1)d}{2} \rfloor$ from the origin the *middle layer* of the grid. Let us consider the paths of $k_d(n)+1$ lions successfully cleaning the grid. By Lemma 3, the number of cleared vertices increases by at most $k_d(n) + 1$ within each step. Consequently, there must be some moment t such that $\frac{n^d}{2} - (k_d(n) + 1) \leq |\mathcal{C}(t)| \leq \frac{n^d}{2}$ and $|\mathcal{C}(t + 1)| > |\mathcal{C}(t)|$. Thanks to Lemma 4, we obtain

$$k_d(n) + 1 \geq \frac{1}{2} |\partial \mathcal{C}(t)|.$$

Thus we have to lower bound the number of boundary vertices of a subset of the grid with size $|\mathcal{C}(t)|$. By Lemma 11, the fewest boundary vertices for such a set are obtained by the set $A_{|\mathcal{C}(t)|}$. Thus, $k_d(n) + 1 \geq \frac{1}{2} |\partial A_{|\mathcal{C}(t)|}|$.

Let us assume there exist n, d such that $k_d(n)+1 < \lfloor \frac{1}{6} b(\lfloor \frac{(n-1)d}{2} \rfloor, n, d) \rfloor$. Then both nodes $v^{\lceil \frac{n^d}{2} \rceil - (k_d(n)+1)}$ and $v^{\lfloor \frac{n^d}{2} \rfloor}$ are contained in the middle layer. We want to estimate the number of boundary vertices of $A_{|\mathcal{C}(t)|}$ contained in the middle layer. Let us first consider the situation for the set $A_{\lfloor \frac{n^d}{2} \rfloor}$, which contains half the number of all grid vertices. If $(n - 1)d$ is even, half of the vertices of the middle layer are contained in $A_{\lfloor \frac{n^d}{2} \rfloor}$. If $(n-1)d$ is odd, $A_{\lfloor \frac{n^d}{2} \rfloor}$ contains all vertices of the middle layer and no vertex of the neighboring layer with distance $\lceil \frac{(n-1)d}{2} \rceil$ from the origin. In both cases, there are at least $\lfloor \frac{1}{2} b(\lfloor \frac{(n-1)d}{2} \rfloor, n, d) \rfloor$ boundary vertices of $A_{\lfloor \frac{n^d}{2} \rfloor}$ in the middle layer of the grid. We define $b := b(\lfloor \frac{(n-1)d}{2} \rfloor, n, d)$.

Since $A_{\lfloor \frac{n^d}{2} \rfloor}$ and $A_{|\mathcal{C}(t)|}$ differ in at most $k_d(n) + 1$ middle layer vertices, we conclude that $A_{|\mathcal{C}(t)|}$ contains at least $\lfloor \frac{1}{2} b \rfloor - (k_d(n)+1)$ boundary vertices in the middle layer. Hence,

$$k_d(n) + 1 \geq \frac{1}{2} |\partial A_{|\mathcal{C}(t)|}| \geq \frac{1}{2} \left\lfloor \frac{b}{2} \right\rfloor - \frac{1}{2}(k_d(n) + 1) > \frac{1}{2} \left\lfloor \frac{b}{2} \right\rfloor - \frac{1}{2} \left\lfloor \frac{b}{6} \right\rfloor \geq \left\lfloor \frac{b}{6} \right\rfloor$$

To verify the last inequality, we notice that the value of $\frac{1}{2} \left\lfloor \frac{b}{2} \right\rfloor - \frac{3}{2} \left\lfloor \frac{b}{6} \right\rfloor$ depends only on b mod 6, hence it is sufficient to check the cases $0 \leq b \leq 5$. What we obtained is a contradiction to our assumption $k_d(n) + 1 < \lfloor \frac{b}{6} \rfloor$. □

We can combine Lemma 10 and Lemma 12 to

Theorem 13 $k_d(n) \in \Theta(b(\lfloor\frac{(n-1)d}{2}\rfloor, n, d))$.

How does the size of the middle layer $b(\lfloor\frac{(n-1)d}{2}\rfloor, n, d)$ grow? Unfortunately, we are not aware of a closed formula for $b(\lfloor\frac{(n-1)d}{2}\rfloor, n, d)$ in general. But the following Theorem describes an asymptotic estimate.

Theorem 14 $b(\lfloor\frac{(n-1)d}{2}\rfloor, n, d) \in \Theta(\frac{n^{d-1}}{\sqrt{d}})$

Proof. Let us consider d independent and identically distributed random variables $X_1, \ldots, X_d$ each of which can take any integer value from 0 to $n-1$ with equal probability. Each X_i has expectation $(n-1)/2$ and variance $(n^2-1)/12$. Therefore, the random variable $S_d^n := X_1 + \ldots + X_d$ has expectation $d(n-1)/2$ and variance $d(n^2-1)/12$. By the central limit theorem, the distribution of $\frac{S_d^n - d(n-1)/2}{\sqrt{d(n^2-1)/12}}$ converges towards the standard normal distribution. This means, that the probability of the event $S_d^n = \lfloor d(n-1)/2 \rfloor$ asymptotically behaves like $\frac{1}{\sqrt{2\pi}} \int_{-1/(2\sqrt{d(n^2-1)/12})}^{1/(2\sqrt{d(n^2-1)/12})} \exp(-t^2/2)\mathrm{d}t$. For increasing n and/or d, the integration domain shrinks around 0, hence the integrand stays in an interval $[1-\varepsilon, 1]$ where $\varepsilon \searrow 0$. The probability lies in the interval $\left[(1-\varepsilon)\sqrt{\frac{6}{\pi d(n^2-1)}}, \sqrt{\frac{6}{\pi d(n^2-1)}}\right]$. Multiplying this by n^d, which is the number of all vertices in the grid, leads to the fact that the number of vertices in the middle layer asymptotically behaves like $\Theta(n^{d-1}/\sqrt{d})$. □

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4 Appendix

Lemma 2.5 *The number of boundary vertices does not increase by the fall-down transformation.*

Proof. Obviously it suffices to prove the statement for each T_i. First, we figure out how many boundary vertices exist in each column of $T_i(C)$ where $i \in \{1, \dots, d\}$ and $C \subseteq [n]^d$ are arbitrary. Let $v \in [n-1]^d$ be an arbitrary vertex. We consider the column on top of $(v_1, \dots, v_{i-1}, 0, v_i, \dots, v_{d-1})$, i.e. the set

$$\{(v_1, \dots, v_{i-1}, a, v_i, \dots, v_{d-1}) \mid a \in [n]\}.$$

It contains $n_i(v) = n_{i,T_i(C)}(v) = n_{i,C}(v)$ many vertices of $T_i(C)$ and the same number of vertices of C.

It is not difficult to see that the number of boundary-vertices of $T_i(C)$ in this column equals

$$\max\left(\max_{w \in \mathcal{N}(v)} n_i(v) - n_i(w),\ \chi_{1 \leq n_i(v) \leq n-1}\right) \tag{6}$$

where

$$\chi_{1 \leq n_i(v) \leq n-1} := \begin{cases} 1 & \text{if } 1 \leq n_i(v) \leq n-1 \\ 0 & \text{otherwise} \end{cases}.$$

First, let us consider the case where this number equals zero. Then, either we have $n_i(v) = 0$ or we have $n_i(v) = n$ and also $n_i(w) = n$ for every $w \in \mathcal{N}(v)$. In both cases the column of v does not contain any boundary vertices of C either.

Now suppose the number does not equal zero, but still the maximum is attained by $\chi_{1 \leq n_i(v) \leq n-1}$. In this case the column of v is neither full nor empty, neither with respect to $T_i(C)$ nor with respect to C. Hence, there must also exist at least one boundary vertex of C in this column.

Finally, suppose the maximum is attained by $\max_{w \in \mathcal{N}(v)} n_i(v) - n_i(w)$. And let w be the neighbor vertex which maximizes $n_i(v) - n_i(w)$. In this case we must have $n_i(v) > n_i(w)$. The column of w contains exactly $n_i(w)$ vertices of C and the column of v contains exactly $n_i(v)$ vertices of C. Thus, at least for $n_i(v) - n_i(w)$ vertices of C in the v-column the corresponding neighbor in the w-column does not belong to C. They are boundary vertices of C.

We have shown that for each column the number of boundary vertices of C cannot be less than the number of boundary vertices of $T_i(C)$. This proves the claim. □