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Maximal induced paths and minimal percolating sets in hypercubes

Research Article

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Abstract: For a graph G, the *r-bootstrap percolation* process can be described as follows: Start with an initial set A of "infected" vertices. Infect any vertex with at least r infected neighbours, and continue this process until no new vertices can be infected. A is said to *percolate in* G if eventually all the vertices of G are infected. A is a *minimal percolating set* in G if A percolates in G and no proper subset of A percolates in G.
An induced path, P, in a hypercube Q_n is *maximal* if no induced path in Q_n properly contains P. Induced paths in hypercubes are also called *snakes*.
We study the relationship between maximal snakes and minimal percolating sets (under 2-bootstrap percolation) in hypercubes. In particular, we show that every maximal snake contains a minimal percolating set, and that every minimal percolating set is contained in a maximal snake.

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1. Introduction

The problem of finding longest *induced paths* (often called *snakes* in the literature) in hypercubes has been studied since 1958 [5]. Definite values for the lengths of longest snakes in n-dimensional hypercubes are known only for dimensions $n \leq 7$ [1]. Several properties of maximal snakes have been found useful in establishing better bounds on the lengths of longest snakes in hypercubes [1, 2].

The notion of *r-bootstrap percolation* in graphs has been studied since 1979 [3]. Riedl considers the 2-bootstrap percolation process in hypercubes; in particular, he studies *minimal percolating sets* (under 2-bootstrap percolation) in hypercubes and provides an expression for the size of largest minimal percolating sets in hypercubes [4].

In this paper we show the relationship between maximal snakes and minimal percolating sets (under 2-bootstrap percolation) in hypercubes. In particular we show that every maximal snake contains a minimal percolating set, and that every minimal percolating set is contained in a maximal snake.

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2. Notation

Most of the definitions and notation in this section are directly from [2] and [4].

We will label the vertices of an n-dimensional hypercube, $Q_n = (V_n, E)$ by the 2^n distinct n-bit labels such that the labels on two vertices differ in exactly one bit position if and only if the two vertices are neighbours in Q_n. The rightmost bit in a label will be called bit number 0 and the leftmost bit will be called bit number $(n-1)$. $\mathbf{[n]}$ denotes the set $\{0, \ldots, n-1\}$. For any vertex $v \in V_n$, for each $i \in \mathbf{[n]}$, $(v)_i$ will denote the bit in bit number i of the label for v. For each $i \in \mathbf{[n]}$, l_i^n denotes the label that has all zeroes except a 1 as bit number i. $\mathbf{0}^n$ denotes the label with all zeroes. U^n will denote the set $\{l_i^n \mid i \in \mathbf{[n]}\}$, i.e., the set of all vertices at unit distance from $\mathbf{0}^n$. For a bit b in a label, $\bar{b}$ will denote the bit complement of b. We will use an asterisk to denote a wildcard in labels. A sequence of k asterisks in a label will be denoted by $(*)_k$. Thus an n-bit label with one asterisk denotes two vertices; moreover, these two vertices are adjacent, i.e., they are a 1-subcube of Q_n. In general, for each k, $0 \leq k \leq n$, a label with k asterisks denotes a k-dimensional subcube. For example, the label $(*)_2 01$ is a 2-dimensional subcube of Q_4 such that all the vertices in the subcube have 1 for bit number 0 and 0 for bit number 1. For a subcube S of Q_n, $dim(S)$ will denote the dimension of S. When vertices u and v differ in bit position d, we will denote this as $u \overset{d}{\longleftrightarrow} v$. For any two vertices $x, y \in Q_n$, $Ham(u, v)$ denotes the Hamming distance between x and y.

For a path $P = v_0, v_1, \ldots, v_l$, $\hat{P}$ will denote the path $v_1, \ldots, v_{l-1}$, i.e., the path P without its endpoints. For a path P, we will use P to denote the sequence of vertices as well as the set of vertices.

An *n-snake* is an induced path in the n-dimensional, hypercubical, undirected graph. A *maximal n-snake*, P, is an n-snake such that no other n-snake properly contains P.

The r-bootstrap percolation process in $G = (V, E)$ is described as follows: Let $A \subseteq V$ be a set of "infected" vertices. Let $A_0 = A$. Then, let A_t be the set of vertices in A_{t-1} union the set of vertices which have at least r neighbours in A_{t-1}. The set $\langle A \rangle = \cup_i A_i$ is the set of vertices infected by A. A set A is said to *percolate* in G if $\langle A \rangle = V$. A percolating set A is said to be *minimal* if for all $v \in A$, $A \backslash v$ does not percolate in G.

In the case $r = 2$ and $G = Q_n = (V_n, E)$, the progress of the percolation process can be described as follows: Given a set $A \subseteq V_n$, let $\mathbf{A}_0 = \bigcup_{u \in A} \{ \{u\} \}$, i.e., the set of all the 0-subcubes represented by the vertices in A. Then, choose a sequence of sets of subcubes $\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_k$ so that $\mathbf{A}_t$ is identical to $\mathbf{A}_{t-1}$ except that two subcubes $B, C \in \mathbf{A}_{t-1}$ that are within distance 2, in Q_n, of each other are replaced by the subcube $\langle B \cup C \rangle$, and so that $\mathbf{A}_k$ is a set of subcubes all of which are distance at least 3, in Q_n, from each other. Clearly, then, A percolates in Q_n if $\mathbf{A}_k = \{V_n\}$. $\mathbf{A}_0, \ldots, \mathbf{A}_k$ is called an *execution path* of the percolation process. In the rest of the paper, unless specified otherwise, "distance" will refer to "distance in Q_n", and by "percolating" we will mean 2-percolating.

3. Maximal snakes percolate

Theorem 3.1. *Every maximal n-snake is a percolating set.*

Proof. The set of maximal n-snakes that have $\mathbf{0}^n$ as one of the end points, and l_0^n as the next vertex is equal to the set of all maximal n-snakes up to isomorphism [2]. Thus, without loss of generality, let P be a maximal n-snake $v_0, v_1, \ldots, v_k$ where $v_0 = \mathbf{0}^n$ and $v_1 = l_0^n$. Since the snake is maximal, none of the vertices $l_i^n, 1 \leq i < n$ are on the snake (since $\mathbf{0}^n$ is an end point of the snake and l_0^n is on the snake), and each of these vertices has at least two neighbours on the snake. (If not, then the snake could have been extended from $\mathbf{0}^n$ and thus would not be maximal.) Thus, if all the vertices of the snake are infected, then in one percolation step, each of the vertices, $l_i^n, 1 \leq i < n$, gets infected. Thus, each vertex in the set $U^n = \{l_i^n \mid 0 \leq i < n\}$ is infected. By Proposition 7 in [4], U^n is a minimal percolating set in Q_n for $n \geq 2$. Thus, every maximal n-snake is a percolating set. □

4. Minimal percolating sets and snakes

Lemma 4.1. *Suppose $P = v_0, v_1, \ldots, v_l$ is an n-snake. Then, $G' = (Q_n \backslash \hat{P})$ is connected.*

Proof. Let $d_1, d_2, \ldots, d_l \in \mathbf{[n]}$ such that for each i, $1 \le i \le l$, $v_{i-1} \overset{d_i}{\longleftrightarrow} v_i$. Let $N_P(v_i)$ be defined as:

$$N_P(v_i) = \{u \mid u \notin P \text{ and } Ham(u, v_i) = 1 \text{ and } (\forall j \in \mathbf{[i]}) Ham(u, v_j) > 1\}.$$

It suffices to show that for each vertex u at distance 1 from P, there is a path in G' from v_0 to u, i.e., for each $i \in \mathbf{[l]}$, for each vertex u in $N_P(v_i)$, there is a path in G' from v_0 to u. (To show that there is a path in G' from v_l to u, we can reverse the labeling of vertices on P and apply the argument below.) We will use mathematical induction on i.

Base Case : $i = 0$. Every vertex in $N_P(v_0)$ is a neighbour of v_0, and thus the claim is trivially true.

Induction Hypothesis : For some $k \in \mathbf{[n]}$, for all k', $0 \le k' \le k$, for each vertex u in $N_P(v_{k'})$, there is a path in G' from v_0 to u.

To show that : For each vertex u in $N_P(v_{k+1})$, there is a path in G' from v_0 to u.

Let u' be the vertex such that $u \overset{d_{k+1}}{\longleftrightarrow} u'$. Clearly, then, u' is a neighbour of v_k, and $u' \notin P$ by the definition of N_P. (If $u' \in P$, then, since P is an induced path, $u' = v_{k-1}$, a neighbour of u, contradicting $u \in N_P(v_{k+1})$.) Thus, for some $k' \le k$, $u' \in N_P(v'_k)$. Then, by the induction hypothesis there is a path in G' from v_0 to u' and thus, there is a path in G' from v_0 to u.

□

As a corollary of the above result we have

Corollary 1. *Suppose $P = v_0, v_1, \ldots, v_l$ is an n-snake. Then for each vertex $w \in V_n \backslash P$, there exist n-snakes, P_1 and P_2, in $Q_n \backslash \hat{P}$ such that P_1 has end points v_0 and w, and P_2 has end points v_l and w.*

Lemma 4.2. *Every set $A \subseteq V_n$ that is isomorphic to U^n is contained in an n-snake, and both the end points of the snake are in A.*

Proof. For each $i \ne j \in \mathbf{[n]}$, let l^n_{ij} denote the n-bit label that has ones in bit positions i and j and zeroes everywhere else. Then, consider the path defined by the sequence of vertices

$$l^n_0, l^n_{01}, l^n_1, l^n_{12}, \ldots, l^n_{(n-2)}, l^n_{(n-2)(n-1)}, l^n_{(n-1)}$$

It can easily be verified that this path is an n-snake. Moreover, U^n is contained in this path and both the end points of the path are in U^n. □

Lemma 4.3. *Let $A \subseteq V_n$ be a minimal percolating set in Q_n such that $A = B \cup C$ where $\langle B \rangle = Q_{n-1}$ and $C = \{u\}$ such that $u \notin \langle B \rangle$. Suppose P is a snake in $\langle B \rangle$ such that P contains each vertex in B, and both the end points of P are in B. Then, there is a snake P' in Q_n that contains each vertex in A, and both the end points of P' are in A.*

Proof. Suppose $P = v_0, v_1, \ldots, v_k$. We consider the two cases: u is at distance 1 in Q_n from P, and u is at distance greater than 1 in Q_n from P.

Case 1 Suppose u is at distance 1 in Q_n from P. Since $u \notin \langle B \rangle$, u is a neighbour of at most one vertex in P.

If u is a neighbour of one of the two end points, say v_0, of P, then P' is simply P extended by the edge (v_0, u). Clearly, P' is a snake in Q_n that contains each vertex of A, and both the end points of P' are in A.

Suppose u is a neighbour of an internal vertex v_i in P, and $v_i \overset{d}{\longleftrightarrow} u$. There are two cases to consider: $v_i \in B$ and $v_i \notin B$.

$v_i \in B$ Then, by the minimality of A, $v_{i-1} \notin A$ and $v_{i+1} \notin A$. Since $v_{i-1} \notin A$, it is not an end point of P. Then, consider the vertices u_1 and u_2 such that $v_{i-1} \overset{d}{\longleftrightarrow} u_1$ and $v_{i-2} \overset{d}{\longleftrightarrow} u_2$. (Note that v_{i-2} exists since v_{i-1} is not an end point of P.) u_1 and u_2 are not in $\langle B \rangle$, u_1 is a neighbour of u and u_2 is a neighbour of u_1. Let P' be the path P with the edges (v_{i-2}, v_{i-1}) and (v_{i-1}, v_i) replaced by the path $v_{i-2}, u_2, u_1, u, v_i$. Then, P' is a snake in Q_n that contains each vertex of A, and both the end points of P' are in A.

$v_i \notin B$ Consider the vertices u_1 and u_2 such that $v_{i-1} \overset{d}{\longleftrightarrow} u_1$ and $v_{i+1} \overset{d}{\longleftrightarrow} u_2$. u_1 and u_2 are not in $\langle B \rangle$, u_1 is a neighbour of u and u_2 is a neighbour of u, and u_1 and u_2 are not neighbours (since they are neighbours, along the same direction d, of two vertices at distance 2 in P, and P is a snake). Let P' be the path P with the path v_{i-1}, v_i, v_{i+1} replaced by the path $v_{i-1}, u_1, u, u_2, v_{i+1}$. Then, P' is a snake in Q_n that contains each vertex of A, and both the end points of P' are in A.

Case 2 Suppose u is at distance greater than 1 in Q_n from P. Since $\langle B \rangle = Q_{n-1}$, there is one bit position that has the same value for the labels on all the vertices in $\langle B \rangle$. Without loss of generality, let bit position 0 for the labels on each vertex in $\langle B \rangle$ be 0. Let u' be the vertex such that $u \overset{0}{\longleftrightarrow} u'$. Since $u \notin \langle B \rangle$, $u' \in \langle B \rangle$, and $u' \notin P$. Then, by Corollary 1 there is a snake $(v_l =)w'_0, w'_1, \ldots w'_m(= u')$ in $\langle B \rangle \backslash \hat{P}$. For each $i, 0 \leq i \leq m$, let w_i be the vertex such that $w_i \overset{0}{\longleftrightarrow} w'_i$. Then, $P' = v_0, \ldots, v_l, w_0, w_1, \ldots, w_m(= u)$ is a snake in Q_n that contains each vertex of A, and both the end points of P' are in A.

□

Lemma 4.4. *Let $A \subseteq V_n$ be a minimal percolating set in Q_n such that $A = B \cup C$ where $\langle B \rangle = Q_{n-2}$ and $C = \{u\}$ such that $u \notin \langle B \rangle$, and u is at distance 2 in Q_n from $\langle B \rangle$. Suppose P is a snake in $\langle B \rangle$ such that P contains each vertex in B, and both the end points of P are in B. Then, there is a snake P' in Q_n that contains each vertex in A, and both the end points of P' are in A.*

Proof. Without loss of generality, let $\langle B \rangle = * * \cdots * * 00$. Then, u is in the subcube $* * \cdots * * 11$. Let v_0 and v_l be the end points of P. Consider the vertices u_1 and u_2 such that $v_l \overset{0}{\longleftrightarrow} u_1$ and $u_1 \overset{1}{\longleftrightarrow} u_2$. Clearly, u_1 is in the subcube $* * \cdots * * 01$, and u_2 is in the subcube $* * \cdots * * 11$. Moreover, since P is a snake, u_1 is at distance at least 2 from all the vertices in P, except v_l, and u_2 is at distance at least 2 in Q_n from each vertex in P. Let P_u be a snake in the subcube $* * \cdots * * 11$ from u_2 to u. Clearly, each vertex of P_u is at distance at least 2 from P. Now let P' be the path P extended by the edge (v_l, u_1), followed by the edge (u_1, u_2) and then followed by P_u. It can be easily verified that P' is a snake in Q_n, and both the end points of P' are in A. □

In what follows, we will use some additional notation: For a set $C \subseteq$ **[n]**, $Q_n|_C$ denotes the subcube $b_{n-1} \ldots b_0$ of Q_n where for each $i \notin C$, b_i is an asterisk, and for each $i \in C$, $b_i \in \{0, 1\}$.

Lemma 4.5. *For $n \geq 6$, suppose $C, D, E \subseteq$ **[n]** such that $|C| = 2$, $|D| = s \geq 2$, $|E| = t \geq 2$, and C, D and E are mutually exclusive. Let $F =$ **[n]**$\backslash(C \cup D \cup E)$. Let $P = v_0, \ldots, v_l$ be a snake in the $(n - (s + 2))$-dimensional subcube $Q_n|_{C \cup D}$, characterised by the bits c_i and d_i for $i \in C$ and $i \in D$, respectively. Then, for any vertex u in the subcube $Q_n|_{C \cup D \cup F}$, characterised by the bits c_i, $\overline{d_i}$, and $(v_l)_i$, for $i \in C$, $i \in D$ and $i \in F$, respectively, P can be extended to an $(n - 2)$-dimensional snake in the subcube $Q_n|_C$, characterised by the bits c_i for $i \in C$, with end points v_0 and u.*

(An example may help clarify the statement of the lemma. Let $n = 8$, $C = \{0, 1\}$, $D = \{2, 3\}$ and $E = \{4, 5, 6\}$. Thus, $s = 2$, $t = 3$ and $F = \{7\}$. Let $Q_n|_{C \cup D}$ be the subcube $* * * * 1001$. Suppose P is a snake in this subcube with end points $v_0 = 00001001$ and $v_l = 10111001$. Then, for any vertex u in the subcube $1 * * * 0101$, say the vertex 11010101, P can be extended to an $(n-2)$-snake in the subcube $* * * * * * 01$ such that the end points of this snake are $v_0 = 00001001$ and $u = 11010101$.)

Proof. Without loss of generality, let $C = \{0, 1\}$, $D = \{2, \ldots, s+1\}$ and $E = \{s+2, \ldots, s+t+1\}$. Then, $F = \{s+t+2, \ldots, n-1\}$. Let $P = v_0, \ldots, v_l$ be a snake in the subcube given by

$$(*)_{n-(s+t+2)} \;\; (*)_t \;\; b_{s+1} \cdots b_2 \;\; b_1 b_0,$$

and let u be a vertex in the subcube given by

$$(v_l)_{n-1} \cdots (v_l)_{(s+t+2)} \;\; (*)_t \;\; \overline{b_{s+1}} \cdots \overline{b_2} \;\; b_1 b_0.$$

Now consider the following

$$\begin{array}{rcl} v_l & = & (v_l)_{n-1} \cdots (v_l)_{(s+t+2)} \;\; (v_l)_{(s+t+1)} \cdots (v_l)_{(s+2)} \;\; b_{s+1} \cdots b_2 \;\; b_1 b_0 \\ & & \qquad\qquad\qquad\qquad \downarrow H_1 \\ w & = & (v_l)_{n-1} \cdots (v_l)_{(s+t+2)} \;\; (v_l)_{(s+t+1)} \cdots (v_l)_{(s+2)} \;\; \overline{b_{s+1}} \cdots \overline{b_2} \;\; b_1 b_0 \\ & & \qquad\qquad\qquad\qquad \downarrow H_2 \\ u & = & (v_l)_{n-1} \cdots (v_l)_{(s+t+2)} \;\; (u)_{(s+t+1)} \cdots (u)_{(s+2)} \;\; \overline{b_{s+1}} \cdots \overline{b_2} \;\; b_1 b_0 \end{array}$$

where H_1 is a shortest path between v_l and w, and H_2 is a shortest path between w and u. Since P is a snake in the subcube S, each vertex $v_i, i < l$ differs from v_l in at least one bit position a_i where $a_i \notin \{0, \ldots, (s+1)\}$. Each vertex of H_1, except the vertex v_l, differs from v_l in at least one bit position $j \in \{0, \ldots, (s+1)\}$. Since $s \geq 2$, the length of H_1 is at least 2, and so each vertex of H_2, differs from each vertex of P in at least two bit positions. Moreover, each vertex h of H_1, except w, differs from w in at least one bit position $j_h \notin \{(s+2), \ldots, (s+t+1)\}$, and each vertex g of H_2 differs from w in at least one bit position $j_g \in \{(s+2), \ldots, (s+t+1)\}$. Thus, P concatenated with H_1 concatenated with H_2 is a snake that has end points v_0 and u, and is contained in the $(n-2)$-dimensional subcube given by

$$(*)_{(n-(s+t+2))} \;\; (*)_t \;\; (*)_s \;\; b_1 b_0.$$

□

The following lemma follows from the proof of Proposition 9 in [4]. Our proof is essentially the proof from [4]; for completeness we provide the relevant parts of the proof here.

Lemma 4.6. *Let $A \subseteq V_n$ be a minimal percolating set in Q_n. Then, there exists an execution path $\bigcup_{u \in A}\{\{u\}\} = \boldsymbol{A}_0, \ldots, \boldsymbol{A}_k = \{V_n\}$, where $\boldsymbol{A}_{k-1}$ consists of exactly two subcubes S_1 and S_2 such that $dim(S_1) \geq dim(S_2)$ and exactly one of the following is true:*

C1 *: $dim(S_1) = n-1$, $S_2 = \{v\}$, and $v \notin S_1$.*

C2 *: $dim(S_1) = n-2$ and $S_2 = \{v\}$ at distance 2 from S_1.*

C3 *: $dim(S_1) \leq n-4$ and $dim(S_2) \leq n-4$, and S_1 and S_2 are at distance 2 from each other.*

Proof. Since A percolates in Q_n, for any execution path of the percolation process $\mathbf{A}_k = V_n$, and so $\mathbf{A}_{k-1}$ must consist of exactly two subcubes, say S_1 and S_2, which together infect Q_n. Amongst all execution paths with $dim(S_1) \geq dim(S_2)$, choose one where $dim(S_1)$ is the largest. By minimality of A, $dim(S_1) \leq n-1$. We consider the cases depending on $dim(S_1)$.

Case 1 $dim(S_1) = n - 1$. Then, by the minimality of A, there must be a single vertex v in $A \cap (Q_n \backslash S_1)$ such that A percolates in Q_n. Thus, $S_2 = \{v\}$ in this case.

Case 2 $dim(S_1) = n - 2$. By the choice of the execution path that has $dim(S_1)$ the largest possible, there cannot be a vertex v in $A \cap S_2$ such that the distance of v from S_1 is at most 1, since otherwise S_1 could be extended to a subcube of dimension $n - 1$. Thus, by the minimality of A, there must be a single vertex v in $A \cap (Q_n \backslash S_1)$ such that the distance of v from S_1 is 2 and A percolates in Q_n.

Case 3 $dim(S_1) = n - 3$. There cannot be a vertex of $A \cap S_2$ within distance 2 of S_1, as this contradicts the maximality of $dim(S_1)$ in our choice of execution path. Hence, $A \cap S_2$ is contained in a subcube of Q_n at distance 3 from S_1, as the set of vertices which are at distance 3 from S_1 is a subcube of dimension $(n - 3)$. Thus S_1 and S_2 are at distance (in Q_n) 3 from each other, contradicting the fact that A percolates. Hence, this case cannot occur.

Case 4 $dim(S_1) \leq n-4$. Then, by the maximality of $dim(S_1)$ in the choice of execution path, $dim(S_2) \leq n - 4$. Moreover, since A percolates in Q_n, S_1 and S_2 must be at distance 2 from each other.

□

Theorem 4.7. *Every minimal percolating set $A \subseteq V_n$ is contained in an n-snake.*

Proof. We will use mathematical induction on the dimension n to show that every minimal percolating set $A \subseteq V_n$ is contained in an n-snake, and both the end points of the snake are in A.

Base cases $n \leq 3$: We will consider each of the three cases, $n = 1$, $n = 2$ and $n = 3$, separately.

For $n = 1$, it is easy to see that the only minimal percolating set is V_1, and that is contained in the unique 1-snake, and both the end points of the snake are in V_1.

For $n = 2$, the only (up to isomorphism) minimal percolating set in Q_2 is U^2, and by Lemma 4.2, this minimal percolating set is contained in a 2-snake, and both the end points of the snake are in U^2.

For $n = 3$, there are two (up to isomorphism) minimal percolating sets: U^3 and the set $A = \{000, 001, 111\}$. Lemma 4.2 asserts the existence of a 3-snake containing U^3 and the 3-snake $000, 001, 011, 111$ contains A. Moreover, in each case, both the end points of the snake are in the minimal percolating set.

Induction Hypothesis : For some $m \geq 3$, for all $m' \leq m$, every minimal percolating set $A \subseteq V_{m'}$ in $Q_{m'}$ is contained in an m'-snake, and both the end points of the snake are in A.

To show that : Every minimal percolating set $A \subseteq V_{m+1}$ in Q_{m+1} is contained in an $(m + 1)$-snake, and both the end points of the snake are in A.

By Lemma 4.6, there exists an execution path $\bigcup_{u \in A} \{u\} = \mathbf{A}_0, \ldots, \mathbf{A}_k = V_{m+1}$, where $\mathbf{A}_{k-1}$ consists of exactly two subcubes S_1 and S_2 such that $dim(S_1) \geq dim(S_2)$, satisfying one of the three mutually exclusive cases listed in the lemma. We show that in each case, A is contained in an $(m + 1)$-snake. (C1, C2 and C3 refer to the three cases listed in the statement of Lemma 4.6.)

C1 In this case, by the induction hypothesis there is an m-snake in S_1 that contains each vertex in $S_1 \cap A$, and both the end points of the snake are in $S_1 \cap A$. Lemma 4.3 applies and asserts that A is contained in an $(m + 1)$-snake, and both the end points of this snake are in A.

C2 In this case, by the induction hypothesis there is an $(m - 1)$-snake in S_1 that contains each vertex in $S_1 \cap A$, and both the end points of the snake are in $S_1 \cap A$. Lemma 4.4 applies and asserts that A is contained in an $(m + 1)$-snake, and both the end points of this snake are in A.

C3 In this case, there exist integers s and t such that

$$\begin{aligned} dim(S_1) &= ((m+1)-s) \leq ((m+1)-4) \text{ and} \\ dim(S_2) &= ((m+1)-t) \leq ((m+1)-4). \end{aligned}$$

Then, $s \geq 4$ and $t \geq 4$. Let $D', E' \subseteq \mathbf{[(m+1)]}$ such that S_1 is the subcube $Q_n|_{D'}$, characterised by p_i for each $i \in D'$, and S_2 is the subcube $Q_n|_{E'}$, characterised by r_i for each $i \in E'$. Since S_1 and S_2 are at distance 2 from each other, $|D' \cap E'| = 2$ and $p_i \neq r_i$ for $i \in (D' \cap E')$. Let $C = D' \cap E'$, $D = D' \backslash C$, $E = E' \backslash C$ and $F = \mathbf{[(m+1)]} \backslash (C \cup D \cup E)$. Clearly, then $|C| = 2$, $|D| = s \geq 2$, $|E| = t \geq 2$, and $|F| = (m+1) - (s+t+2)$. Without loss of generality, let $C = \{0,1\}$, $D = \{2, \ldots, s+1\}$, and $E = \{s+2, \ldots, s+t+1\}$, and let $p_0 = p_1 = 0$ and $r_0 = r_1 = 1$, i.e.,

$$\begin{aligned} S_1 &= (*)_{(m+1)-(s+t+2)} \quad (*)t \quad p_{s+1} \cdots p_2 \;\; 00, \text{ and} \\ S_2 &= (*)_{(m+1)-(s+t+2)} \quad r_{s+t+1} \cdots r_{s+2} \quad (*)_s \;\; 11. \end{aligned}$$

By the induction hypothesis, there is an $(m+1)-(s+2)$-snake, P_1 in S_1 that contains each vertex in $S_1 \cap A$, and both the end points, say v_0 and v_a, of P_1 are in $S_1 \cap A$, and there is an $(m+1)-(t+2)$-snake, P_2 in S_2 that contains each vertex in $S_2 \cap A$, and both the end points, say w_0 and w_b, of P_2 are in $S_2 \cap A$.
By Lemma 4.5 P_1 can be extended to a snake P_1^* with end points v_0 and the vertex u_1 given by

$$u_1 = (v_a)_m \ldots (v_a)_{(s+t+2)} \;\; \overline{r_{s+t+1}} \cdots \overline{r_{s+2}} \;\; \overline{p_{s+1}} \cdots \overline{p_2} \;\; 00.$$

Similarly, by Lemma 4.5 P_2 can be extended to a snake P_2^* with end points w_0 and the vertex u_2 given by

$$u_2 = (w_b)_m \ldots (w_b)_{(s+t+2)} \;\; \overline{r_{s+t+1}} \cdots \overline{r_{s+2}} \;\; \overline{p_{s+1}} \cdots \overline{p_2} \;\; 11.$$

Now consider

$$\begin{aligned} u_1 &= (v_a)_m \ldots (v_a)_{(s+t+2)} \;\; \overline{r_{s+t+1}} \cdots \overline{r_{s+2}} \;\; \overline{p_{s+1}} \cdots \overline{p_2} \;\; 00 \\ & \qquad\qquad\qquad\qquad \downarrow \\ u_x &= (v_a)_m \ldots (v_a)_{(s+t+2)} \;\; \overline{r_{s+t+1}} \cdots \overline{r_{s+2}} \;\; \overline{p_{s+1}} \cdots \overline{p_2} \;\; 01 \\ & \qquad\qquad\qquad\qquad \Big\downarrow P_3 \\ u_y &= (w_b)_m \ldots (w_b)_{(s+t+2)} \;\; \overline{r_{s+t+1}} \cdots \overline{r_{s+2}} \;\; \overline{p_{s+1}} \cdots \overline{p_2} \;\; 01 \\ & \qquad\qquad\qquad\qquad \downarrow \\ u_2 &= (w_b)_m \ldots (w_b)_{(s+t+2)} \;\; \overline{r_{s+t+1}} \cdots \overline{r_{s+2}} \;\; \overline{p_{s+1}} \cdots \overline{p_2} \;\; 11 \end{aligned}$$

where P_3 is a shortest path in the subcube

$$(*)_{(m+1)-(s+t+2)} \;\; \overline{r_{s+t+1}} \cdots \overline{r_{s+2}} \;\; \overline{p_{s+1}} \cdots \overline{p_2} \;\; 01.$$

Each vertex of this subcube differs from P_1 in at least $s \geq 2$ bit positions, and differs from P_2 in at least $t \geq 2$ bit positions. By the reasoning of Lemma 4.5, P_3 differs from P_1^* and P_2^* in at least two bit positions. Thus, the concatenation of P_1^* with the edge (u_1, u_x) followed by P_3 is a snake. Similarly, the concatenation of P_2^* with the edge (u_2, u_y) is a snake. Moreover, these two snakes concatenated together is a snake with end points v_0 and w_0, both of which are in A.

$\square$

5. Conclusions and open questions

As noted earlier, our interest in maximal snakes derives from properties of maximal snakes in lower dimensions that are useful heuristics in generating long maximal snakes in higher dimensions. The heuristics essentially seed the exhaustive search with an initial segment of the snake. Our hope is that minimal percolating sets can prove to be better seeds and will speed up the exhaustive search somewhat. Our intuition comes from the observation that 1) minimal pecolating set vertices are sprinkled throughout the hypercube, and 2) at each step of the proofs above where we use a shortest path or any snake between two vertices, we could use a suitable *longest* path instead.

We would also like to explore the possibility of stronger results that may characterize longest maximal snakes in terms of minimal percolating sets. For example, we would like to consider questions such as

1. Is there a difference in the set of minimal percolating sets contained in a maximal, but not longest, snake, and the set of minimal percolating sets contained in a longest snake?
2. In some dimensions, notably 4 and 6 of the known ones, there is a unique (up to isomorphism) longest snake. Is there a stronger relationship between the longest snake and minimal percolating sets in these dimensions?

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