Isomorphic Boolean networks and dense interaction graphs

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May 26, 2021

Abstract

A Boolean network (BN) with n components is a discrete dynamical system described by the successive iterations of a function $f : \{0,1\}^n \to \{0,1\}^n$. In most applications, the main parameter is the interaction graph of f: the digraph with vertex set $\{1,\dots,n\}$ that contains an arc from j to i if f_i depends on input j. What can be said on the set $\mathcal{G}(f)$ of the interaction graphs of the BNs h isomorphic to f, that is, such that $h\circ\pi = \pi\circ f$ for some permutation π of $\{0,1\}^n$? It seems that this simple question has never been studied. Here, we report some basic facts. First, if $n \geq 5$ and f is neither the identity or constant, then $\mathcal{G}(f)$ is of size at least two and contains the complete digraph on n vertices, with n^2 arcs. Second, for any $n \geq 1$, there are n-component BNs f such that every digraph in $\mathcal{G}(f)$ has at least $n^2/9$ arcs.

1 Introduction

A *Boolean network* (network for short) with n components is a finite dynamical system defined by the successive iterations of a function

$$f : \{0,1\}^n \to \{0,1\}^n, \quad x = (x_1,\dots,x_n) \mapsto f(x) = (f_1(x),\dots,f_n(x)).$$

Boolean networks have many applications; in particular, they are omnipresent in the modeling of neural and gene networks (see [4] for a review).

The "network" terminology comes from the fact that the *interaction graph* $G(f)$ of f is often considered as the main parameter of f: the vertex set is $[n] = \{1,\dots,n\}$ and there is an arc from j to i if f_i depends on input j, that is, if there are $x, y \in \{0,1\}^n$ which only differ in $x_j \neq y_j$ such that $f_i(x) \neq f_i(y)$. For instance, in the context of gene networks, the interaction graph is often well approximated while the actual dynamics is not. One is thus faced with the following question: *what can be said on the dynamics*

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This work is supported by the Young Researcher project ANR- 18-CE40-0002-01 "FANs" and project STIC AmSud CoDANet 19-STIC-03 (Campus France 43478PD).

described by f from $G(f)$ only. There are many results in this direction (see [1] for a review). In most cases, the studied dynamical properties are invariant by isomorphism: number of fixed or periodic points, number and size of limit cycles, transient length and so on. However, the interaction graph is *not* invariant by isomorphism: even if f and h are isomorphic, their interaction graphs can be very different (by Theorem 1 below, $G(f)$ can have n^2 arcs while $G(h)$ has a single arc). Surprisingly, this variation seems to have never been studied, and we report here some basic facts.

Given a network f, let $\mathcal{G}(f)$ be the set of interaction graphs $G(h)$ such that h is a network isomorphic to f, that is, such that $h \circ \pi = \pi \circ f$ for some permutation π of $\{0,1\}^n$. Hence, we propose to study $\mathcal{G}(f)$. For instance, if f is constant, we write this $f = \text{cst}$, then $\mathcal{G}(f)$ contains a single digraph, the digraph on $[n]$ without arcs, and if f is the identity, we write this $f = \text{id}$, then $\mathcal{G}(f)$ also contains a single digraph, the digraph on $[n]$ with n loops (cycles of length one) and no other arcs.

Our first result shows that, excepted few exceptions (including the two above examples), $\mathcal{G}(f)$ always contains the complete digraph on $[n]$, with n^2 arcs, denoted K_n.

Theorem 1. *$K_n \in \mathcal{G}(f)$ for all networks $f \neq \text{cst}, \text{id}$ with $n \geq 5$ components.*

Our second result shows that, for $n \geq 5$, there are no networks f such that $\mathcal{G}(f)$ only contains the complete digraph.

Theorem 2. *$\mathcal{G}(f) \neq \{K_n\}$ for all networks f with $n \geq 5$ components.*

From these theorems we deduce the following property, which might seem innocente but that doesn't seem to have a one-line proof: *If f is a network with $n \geq 5$ components, then $|\mathcal{G}(f)| = 1$ if and only if $f = \text{id}$ or $f = \text{cst}$.*

Even if, for $n \geq 5$, $\mathcal{G}(f)$ cannot only contain the complete digraph, using a well-known isoperimetric inequality in hypercubes, we show that, at least, $\mathcal{G}(f)$ can only contain digraphs with many arcs.

Theorem 3. *For every $n \geq 1$, there is a network f with n components such that every digraph in $\mathcal{G}(f)$ has at least $n^2/9$ arcs.*

Concerning short term perspectives, we checked by computer that the first theorem holds for $n = 3$ (for $n = 2$ it fails; see the appendix) and that the second holds for $n = 2, 3$. For $n = 4$ this is much time-consuming and we didn't do it, hoping to find instead dedicated arguments, since those given for $n \geq 5$ do not work. A more involved perspective, related to the third theorem, is to prove that, for any $\epsilon > 0$ and n large enough, any digraph in $\mathcal{G}(f)$ has at least $(1-\epsilon)n^2$ arcs for some f. We also want to study networks f such that $\mathcal{G}(f)$ is very large and ask: do we have, for any $\epsilon > 0$ and n large enough, $|\mathcal{G}(f)|/2^{n^2} > 1 - \epsilon$ for some f?

The three theorems above are proved the in following three sections. Before going on, we give some basic definitions. An element x of $\{0,1\}^n$ is a *configuration*, and elements in $[n]$ are *components*. We set $\mathbf{1}(x) = \{i \in [n] \mid x_i = 1\}$ and $\mathbf{0}(x) = [n] \setminus \mathbf{1}(x)$. The *weight* of x is $w(x) = |\mathbf{1}(x)|$. We denote by e_i the configuration such that $\mathbf{1}(e_i) = \{i\}$. For $x, y \in \{0,1\}^n$, the sum $x + y$ is applied component-wise modulo two. Hence x and $x + e_i$ only differ in component i. We denote by $\mathbf{1}$ (resp. $\mathbf{0}$) the configuration of weight n (resp. 0). Thus x and $x + \mathbf{1}$ differ in every component. Given $A \subseteq \{0,1\}^n$, we set $A + x = \{a + x \mid a \in A\}$. Let f be a n-component network. A *fixed point* is a configuration x such that $f(x) = x$. Let $\Gamma(f)$ be the digraph with vertex set $\{0,1\}^n$ and an arc from x to $f(x)$ for every $x \in \{0,1\}^n$. A *limit cycle* of f is a cycle of $\Gamma(f)$. Hence fixed points correspond to limit cycles of length one. An *independent set* of f is an independent set of $\Gamma(f)$, equivalently, it is a set $A \subseteq \{0,1\}^n$ such that $f(A) \cap A = \emptyset$.

2 Proof of Theorem 1

We proceed by showing that, for $n \geq 5$ and $f \neq \text{cst}, \text{id}$, we have $K_n \in \mathcal{G}(f)$ if at least one of the following three conditions holds: f has at least $2n$ fixed points; or f has at least n limit cycles of length ≥ 3; or f has an independent set of size $\geq 2n$. We then prove that, because $n \geq 5$, at least one of the three conditions holds, and Theorem 1 follows.

Lemma 1. *Let f be a network with n components, which is not the identity. If f has at least $2n$ fixed points then $K_n \in \mathcal{G}(f)$.*

Proof. Since $f \neq \text{id}$ we have $f(c) \neq c$ for some c, and since f has at least $2n$ fixed points, it has $2n - 1$ fixed points distinct from $f(c)$, say $a^0, a^1, \dots, a^n, b^3, \dots, b^n$. Let π be any permutation of $\{0,1\}^n$ such that $\pi(a^0) = \mathbf{0}$, $\pi(a^i) = e_i$ for $1 \leq i \leq n$, $\pi(b^i) = e_1 + e_2 + e_i$ for $3 \leq i \leq n$, $\pi(c) = e_1 + e_2$ and $\pi(f(c)) = e_1 + e_2 + \mathbf{1}$. Let $h = \pi \circ f \circ \pi^{-1}$. We will prove that $G(h) = K_n$. For $i \in [n]$, we have $h(\mathbf{0}) = \pi(f(a^0)) = \pi(a^0) = \mathbf{0}$ and $h(e_i) = \pi(f(a^i)) = \pi(a^i) = e_i$, hence $h(\mathbf{0})$ and $h(e_i)$ differ in component i, and we deduce that $G(h)$ has an arc from i to itself. It remains to prove that $G(h)$ has an arc from i to j for distinct $i, j \in [n]$. We have $h(e_1 + e_2) = \pi(f(c)) = e_1 + e_2 + \mathbf{1}$. Hence $h(e_2) = e_2$ and $h(e_1 + e_2)$ differ in every component $j \neq 1$, and thus $G(h)$ has an arc from 1 to every $j \neq 1$. We prove similarly that $G(h)$ has an arc from 2 to every $j \neq 2$. For $3 \leq i \leq n$, we have $h(e_1 + e_2 + e_i) = \pi(f(b^i)) = \pi(b^i) = e_1 + e_2 + e_i$, so $h(e_1 + e_2 + e_i)$ and $h(e_1 + e_2)$ differ in every component $j \neq i$, and we deduce that $G(h)$ has an arc from i to every $j \neq i$. □

Lemma 2. *Let f be a network with n components. If f has at least n limit cycles of length ≥ 3, then $K_n \in \mathcal{G}(f)$.*

Proof. Suppose that f has n limit cycles of length ≥ 3; this implies $n \geq 4$. Let $a^1, \dots, a^n$ be configurations inside distinct limit cycles of f of length

≥ 3. For $i \in [n]$ let $b^i = f(a^i)$ and $c^i = f(b^i)$. Then $a^1, \ldots, a^n$, $b^1, \ldots, b^n$, $c^1, \ldots, c^n$ are all distinct. For $i \in [n]$, let $x^i = e_{i-1} + e_i$, $y^i = e_{i-1}$ and $z^i = e_{i-1} + \mathbf{1}$, where e_0 means e_n. Since $n \geq 4$, the configurations $x^1, \ldots, x^n$, $y^1, \ldots, y^n$, $z^1, \ldots, z^n$ are all distinct. Hence there is a permutation π of $\{0,1\}^n$ such that, for $i \in [n]$, $\pi(a^i) = x^i$, $\pi(b^i) = y^i$ and $\pi(c^i) = z^i$. Let $h = \pi \circ f \circ \pi^{-1}$. For $i \in [n]$ we have $h(e_{i-1} + e_i) = h(x^i) = \pi(f(a^i)) = \pi(b^i) = y^i = e_{i-1}$ and $h(e_{i-1}) = h(y^i) = \pi(f(b^i)) = \pi(c^i) = z^i = e_{i-1} + \mathbf{1}$. Hence $h(e_{i-1} + e_i)$ and $h(e_{i-1})$ differ in every component, and since $e_{i-1} + e_i$ and e_{i-1} only differ in component i, we deduce that $G(h)$ has an arc from i to every $j \in [n]$. Thus $G(h) = K_n$. □

Lemma 3. *Let f be a non-constant network with $n \geq 5$ components. If f has an independent set of size $\geq 2n$, then $K_n \in \mathcal{G}(f)$.*

Proof. Let A be an independent set of f. We first prove:

(1) *If $|A| \geq n + k$ and $|f(A)| = 2k$ for some $1 \leq k \leq n$, then $K_n \in \mathcal{G}(f)$.*

Suppose these condition holds. One easily check that there is an independent set A with $|A| = n + k$ and $|f(A)| = 2k$ for some $1 \leq k \leq n$. Let us write $f(A) = \{a^1, \ldots, a^{2k}\}$, and let $A_p = f^{-1}(a^p) \cap A$ for $p \in [2k]$. Let $X_1, \ldots, X_{2k}$ be disjoint subsets of $\{0,1\}^n$ of size $|A_1|, \ldots, |A_{2k}|$ such that, for all $i \in [n]$, there is $p \in [k]$ and $x \in X_{2p-1}$ with $x + e_i \in X_{2p}$; that these sets exist is the "technical" part of the proof, given by Lemma 8 in appendix.

Let $X = X_1 \cup \cdots \cup X_{2k}$, let Y be the set of $y \in \{0,1\}^n$ with $y_1 = 0$, and let Y' be the set of $y \in Y$ such that $y, y + \mathbf{1} \notin X$. Since $n \geq 5$ and $n \geq k$:

$$|Y'| \geq |Y| - |X| = 2^{n-1} - (n + k) \geq 2^{n-1} - 2n \geq n \geq k.$$

Thus there are k distinct configurations in $y^1, \ldots, y^k \in Y'$ and by construction, $Y'' = \{y^1, \ldots, y^k\}$ and $Y'' + \mathbf{1}$ are disjoint and disjoint from X.

Hence there is a permutation π of $\{0,1\}^n$ such that, for all $p \in [k]$, $\pi(a^{2p-1}) = y^p$, $\pi(a^{2p}) = y^p + \mathbf{1}$, $\pi(A_{2p-1}) = X_{2p-1}$ and $\pi(A_{2p}) = X_{2p}$. Let $h = \pi \circ f \circ \pi^{-1}$. By construction, for every $i \in [n]$ there is $p \in [k]$ and $x \in X_{2p-1}$ with $x + e_i \in X_{2p}$. Since $\pi^{-1}(x) \in A_{2p-1}$ and $\pi^{-1}(x + e_i) \in A_{2p}$, we have $h(x) \in \pi(f(A_{2p-1})) = \{\pi(a^{2p-1})\} = \{y^p\}$ and $h(x + e_i) \in \pi(f(A_{2p})) = \{\pi(a^{2p})\} = \{y^p + \mathbf{1}\}$. Thus $h(x)$ and $h(x + e_i)$ differ in every component, and we deduce that $G(h) = K_n$. This proves (1).

We next prove another condition on A to obtain the complete digraph.

(2) *If $|A| > n$ and $|f(A)| = 1$, then $K_n \in \mathcal{G}(f)$.*

Let $a \in \{0,1\}^n$ such that $f(A) = \{a\}$. Since $f \neq \text{cst}$, there is $b \in \{0,1\}^n$ with $f(b) \neq a$, and thus $b \notin A$. We consider three cases.

Suppose first that $f(a) \neq a$. Since $|A| > n$, there are n configurations $a^1, \ldots, a^n$ in A distinct from $f(a)$. Then $a^1, \ldots, a^n, a, f(a)$ are all distinct, so there is a permutation π with $\pi(a) = \mathbf{0}$, $\pi(f(a)) = \mathbf{1}$ and $\pi(a^i) = e_i$ for $1 \leq i \leq n$. Let $h = \pi \circ f \circ \pi^{-1}$. For $i \in [n]$, we have $h(e_i) = \pi(f(a^i)) = \pi(a) = \mathbf{0}$ and $h(\mathbf{0}) = \pi(f(a)) = \mathbf{1}$, so $h(e_i)$ and $h(\mathbf{0})$ differ in every component, and thus $G(h) = K_n$.

Suppose now that $f(a) = a$ and $f(b) = b$. Let $a^1, \dots, a^n \in A$, all distinct. Then $a^1, \dots, a^n, a, b$ are all distinct since $b = f(b) \neq a$. So there is a permutation π with $\pi(a) = \mathbf{1}$, $\pi(b) = \mathbf{0}$ and $\pi(a^i) = e_i$ for $i \in [n]$. Let $h = \pi \circ f \circ \pi^{-1}$. For all $i \in [n]$, we have $h(e_i) = \pi(f(a^i)) = \pi(a) = \mathbf{1}$ and $h(\mathbf{0}) = \pi(f(b)) = \pi(b) = \mathbf{0}$, so $h(e_i)$ and $h(\mathbf{0})$ differ in every component, and thus $G(h) = K_n$.

Suppose finally that $f(a) = a$ and $f(b) \neq b$. Since $|A| > n$, there is $A' \subseteq A \setminus \{f(b)\}$ of size n. Then $A' \cup \{b\}$ is an independent set of size $n+1$ and $|f(A' \cup \{b\})| = |\{a, f(b)\}| = 2$ so $K_n \in \mathcal{G}(f)$ by (1). This proves (2).

We can now conclude the proof. Suppose that $|A| \geq 2n$. Then we can choose A so that $|A| = 2n$. Suppose, for a contradiction, that $K_n \notin \mathcal{G}(f)$. If $|f(A)|$ is even then $K_n \in \mathcal{G}(f)$ by (1) and if $|f(A)| = 1$ then $K_n \in \mathcal{G}(f)$ by (2). Thus $|f(A)| = 2k + 1$ for some $1 \leq k < n$. Let us write $f(A) = \{a^1, \dots, a^{2k+1}\}$, and let $A_p = f^{-1}(a^p) \cap A$ for $1 \leq p \leq 2k + 1$. Suppose, without loss, that $|A_1| \leq |A_2| \leq \dots \leq |A_{2k+1}|$. Then $A' = A \setminus A_1$ is an independent set with $|f(A')| = 2k$. Setting $m = n + k - 1$, if $|A'| > m$, then $K_n \in \mathcal{G}(f)$ by (2). So $2k|A_2| \leq |A'| \leq m$, thus $|A_1| \leq |A_2| \leq m/2k$. We deduce that $2n = |A| = |A_1| + |A'| \leq m/2k + m$. However, one easily checks that $2n > m/2k + m$ when $1 \leq k < n$, a contradiction. Thus $K_n \in \mathcal{G}(f)$ $\square$

We are ready to prove Theorem 1. Let $f \neq \text{cst}, \text{id}$ with $n \geq 5$ components. Suppose, for a contradiction, that $K_n \notin \mathcal{G}(f)$. Let F be the set of fixed points of f, and let L be a smallest subset of $\{0, 1\}^n$ intersecting every limit cycle of f of length ≥ 3. Let Γ' be obtained from $\Gamma(f)$ by deleting the vertices in $F \cup L$; then Γ' has only cycles of length two, thus it is bipartite. Since $K_n \notin \mathcal{G}(f)$, by Lemmas 1 and 2, we have $|F| < 2n$ and $|L| < n$, thus Γ' has at least $N = 2^n - 3n + 2$ vertices. Since Γ' is bipartite, it has an independent set A of size $\geq N/2$. Then A is an independent set of f and since $K_n \notin \mathcal{G}(f)$, we deduce from Lemma 3 that $|A| < 2n$. Thus $2n > N/2$, that is, $7n > 2^n + 3$, which is false since $n \geq 5$. Thus $K_n \in \mathcal{G}(f)$.

3 Proof of Theorem 2

We first give a necessary and sufficient condition for the presence of a digraph in $\mathcal{G}(f)$ that misses some arc with distinct ends. It has been obtained with Kévin Perrot, whom we thank, and its proof is in appendix. Given an n-component network f, and $1 \leq k \leq 2^{n-1}$, a *k-nice set* of f is a set $A \subseteq \{0, 1\}^n$ of size $2k$ with $|f^{-1}(A)|$ and $|f^{-1}(A) \cap A|$ even.

Lemma 4. *Let f be an n-component network and distinct $i, j \in [n]$. Some digraph in $\mathcal{G}(f)$ has no arc from j to i if and only if f has a (2^{n-2})-nice set.*

Hence, to prove Theorem 2, it is sufficient to prove that, for $n \geq 5$, f has always a (2^{n-2})-nice set. To use induction, it is more convenient to prove something stronger: if $n \geq 4$ and $8 \leq k \leq 2^{n-1}$ then f has always a k-nice set. In particular, if $n \geq 5$ then $2^{n-2} \geq 8$ thus f has a (2^{n-2})-nice set and we are done. So it remains to prove:

Lemma 5. *Let f be a network with $n \geq 4$ components and $8 \leq k \leq 2^{n-1}$. Then f has a k-nice set.*

Proof. We proceed by induction on k, decreasing from 2^{n-1} to 8. For the base case, observe that $\{0,1\}^n$ is a (2^{n-1})-nice set of f. Suppose that $8 < k \leq 2^{n-1}$, and suppose that f has a k-nice set A. We will prove that f has a $(k-1)$-nice set included in A, thus completing the induction step. For that, we will define an equivalence relation on A, with at most 8 equivalence classes, and show that, since $A \geq 18$, there always are two equivalent elements $x, y \in A$ such that $A \setminus \{x, y\}$ is a $(k-1)$-nice set of f. This relation is defined through 3 binary properties on the elements of A, defined below.

Let $\alpha, \beta, \gamma : A \to \{0, 1\}$ be defined by: for all $x \in A$,

1. $\alpha(x) = 1$ if and only if $f(x) \in A$,
2. $\beta(x) = 1$ if and only if $|f^{-1}(x)|$ is even,
3. $\gamma(x) = 1$ if and only if $|(f^{-1}(x) \cap A) \setminus \{x\}|$ is even.

We say that $x, y \in A$ are *equivalent* if $\alpha(x) = \alpha(y)$ and $\beta(x) = \beta(y)$ and $\gamma(x) = \gamma(y)$. We say that $x, y \in A$ are *independent* if $f(x) \neq y$ and $f(y) \neq x$. It is straightforward (and annoying) to check that if $x, y \in A$ are equivalent and independent, then $A \setminus \{x, y\}$ is a $(k-1)$-nice of f.

Suppose now that f has no $(k-1)$-nice set. By the above property, there is no equivalence class containing two independent elements. Let $A_0 = \alpha^{-1}(0)$ and $A_1 = \alpha^{-1}(1)$. Each of A_0, A_1 contains at most 4 equivalence classes. If $x, y \in A_0$, then $f(x), f(y) \notin A$, and thus x and y are independent. We deduce that each of the classes contained in A_0 is of size < 2, and thus $|A_0| \leq 4$. Also, one easily checks that any class of size ≥ 4 contains two independent elements. Hence each of the classes contained in A_1 is of size < 4, and thus $|A_1| \leq 12$. But then $|A| = |A_1| + |A_2| \leq 16$, a contradiction. Thus f has a $(k-1)$-nice set. □

4 Proof of Theorem 3

If $1 \leq n \leq 9$ and f is the identity on $\{0,1\}^n$, then $\mathcal{G}(f)$ contains a unique digraph, which has $n = n^2/n \geq n^2/9$ vertices. This proves the theorem for $n \leq 9$. We treat the other cases with an explicit construction.

Given $A \subseteq \{0,1\}^n$ with $\mathbf{0} \in A$, we denote by f^A the n-component network such that $f^A(A) = \{\mathbf{0}\}$ and $f^A(b) = b$ for all $b \notin A$. We will prove, in the next lemma, that if the size of A is carefully chosen, then, independently on the structure of A, $G(f^A)$ has at least $n^2/9$ arcs. It is then easy to prove that this lower bound holds for every digraph in $\mathcal{G}(f^A)$.

Lemma 6. *Let $n \geq 9$ and $A \subseteq \{0,1\}^n$ of size $\lceil 2^{n/4} \rceil$ with $\mathbf{0} \in A$. Then $G(f^A)$ has at least $n^2/9$ arcs.*

The key tool is the following lemma, which can be easily deduced from the well-known Harper's isoperimetric inequality in the hypercube (see the appendix). Let Q_n be the hypercube graph, with vertex set $\{0,1\}^n$ and an edge between x and y if and only if x and y differ in exactly one component.

Lemma 7. *Let $A \subseteq \{0,1\}^n$ be non-empty, and let d be the average degree of the subgraph of Q_n induced by A. Then $|A| \geq 2^d$.*

Proof of Lemma 6. Let $f = f^A$ and let m be the number of arcs in $G(f)$. Suppose, for a contradiction that $m < n^2/9$. Let I be the set of $i \in [n]$ with $a_i = 1$ for some $a \in A$. Note that $|I| \geq n/4$. Indeed, let B be the set of $b \in \{0,1\}^n$ such that $b_i = 0$ for all $i \notin I$. Then $A \subseteq B$, and $|B| = 2^{|I|}$, thus $|I| = \log_2 |B| \geq \log_2 |A| \geq n/4$. From that observation, we can say something stronger:

(1) $|I| > n/2$.

Let $i \in I$ and $j \notin I$. Let $a \in A$ such that $a_i = 1$. Since $j \notin I$, $a + e_j \notin A$, thus $f(a) = \mathbf{0}$ and $f(a + e_j) = a + e_i$, and $f_i(a + e_j) = a_i = 1$ since $j \neq i$. Hence $G(f)$ has an arc from j to i. We deduce that $|I| \cdot (n - |I|) \leq m < n^2/9$, so $n/4 \cdot (n - |I|) < n^2/9$. Thus $|I| > 5n/9 > n/2$. This proves (1).

We deduce that some $a \in A$ has a large weight.

(2) *There is $a \in A$ with $w(a) > 3n/4$.*

Suppose that $w(a) \leq 3n/4$ for all $a \in A$. Let $i \in I$. Let $a \in A$ with $a_i = 1$, and $w(a)$ maximal for that property. Then, for all $j \in \mathbf{0}(a)$, we have $a + e_j \notin A$. Hence $f(a) = \mathbf{0}$ and $f(a + e_j) = a + e_j$ so $f_i(a + e_j) = a_i = 1$ since $i \neq j$. Thus $G(f)$ has an arc from j to i. We deduce that the in-degree of i in $G(f)$ is at least $|\mathbf{0}(a)| = n - w(a) \geq n/4$. Hence $m \geq |I| \cdot n/4$ and since $|I| > n/2$ by (1) we obtain $m > n^2/8 > n^2/9$, a contradiction. This proves (2).

Let A' be the set of $a \in A$ with $w(a) \geq n/3 - 1$, which is not empty by (2). For $a \in A$, let $J(a)$ be the set of $j \in [n]$ such that $a + e_j \in A$, and let $J'(a)$ be the set of $j \in [n]$ such that $a + e_j \in A'$. Let H be the subgraphs of Q_n induced by A'. If $a \in A'$, then $d(a) = |J'(a)|$ is the degree of a in H. We will prove in (3) and (4) below that each vertex in H has large degree.

(3) *If $a \in A'$ and $w(a) \geq n/3$ then $d(a) > n/3$.*

Indeed, since $w(a) \geq n/3$, for $j \in J(a)$ we have $w(a+e_j) \geq n/3 - 1$ thus $j \in J'(a)$. Hence $J(a) = J'(a)$ so $d(a) = |J(a)|$. For all $i \notin J(a)$ we have $f(a) = \mathbf{0}$ and $f(a+e_i) = a+e_i$, thus $G(f)$ has an arc from i to each component in $\mathbf{1}(a+e_i)$. Thus the out-degree of i in $G(f)$ has at least $w(a+e_i) \geq n/3 - 1$. We deduce that $(n - |J(a)|) \cdot (n/3 - 1) \leq m < n^2/9$, so $d(a) = |J(a)| > 2n/3 - 3$ and since $n \geq 9$ we obtain $d(a) > n/3$. This proves (3).

(4) *If $a \in A'$ and $w(a) < n/3$ then $d(a) > n/3$.*

Let $K = \mathbf{0}(a) \setminus J'(a)$ and $i \in K$. We have $w(a+e_i) = w(a) + 1 \geq n/3$, thus if $a + e_i \in A$ then $a + e_i \in A'$; but then $i \in J'(a)$, a contradiction. Thus $a+e_i \notin A$, so $f(a) = \mathbf{0}$ and $f(a+e_i) = a+e_i$. We deduce that the out-degree of i in $G(f)$ is at least $w(a+e_i) \geq n/3$. Thus $|K| \cdot n/3 \leq m < n^2/9$ so $|K| < n/3$. Since $w(a) < n/3$ we have $|\mathbf{0}(a)| > 2n/3$. So $|K| \geq 2n/3 - |J'(a)|$ and thus $d(a) = |J'(a)| > n/3$. This proves (4).

We are now in position to finish the proof. Let d be the average degree of H. By (3) and (4), we have $d > n/3$. Using Lemma 7 we obtain $2^{n/3} < 2^d \leq |A'| \leq |A| = \lceil 2^{n/4} \rceil$, which is false because $n \geq 9$. □

We are now in position to conclude. Let $n \geq 9$ and $A \subseteq \{0,1\}^n$ of size $\lceil 2^{n/4} \rceil$ with $\mathbf{0} \in A$, and let $f = f^A$. Let π be any permutation of $\{0,1\}^n$ and $h = \pi \circ f \circ \pi^{-1}$. We will prove that $G(h)$ has at least $n^2/9$ arcs. Let h' be the n-component network defined by $h'(x) = h(x + \pi(\mathbf{0})) + \pi(\mathbf{0})$ for all $x \in \{0,1\}^n$. We have $G(h) = G(h')$. Let $A' = \pi(A) + \pi(\mathbf{0})$. We have $\mathbf{0} \in A'$ and one easily check that $h' = f^{A'}$. Since $|A'| = |A| = \lceil 2^{n/4} \rceil$, by Lemma 6, $G(h') = G(h)$ has at least $n^2/9$ arcs.

References

[1] Maximilien Gadouleau. On the influence of the interaction graph on a finite dynamical system. *Natural Computing*, 19(1):15–28, 2020.

[2] Lawrence Hueston Harper. Optimal assignments of numbers to vertices. *Journal of the Society for Industrial and Applied Mathematics*, 12(1):131–135, 1964.

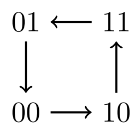
[3] Jeff Kahn and Jinyoung Park. An isoperimetric inequality for the hamming cube and some consequences. *Proceedings of the American Mathematical Society*, 148(10):4213–4224, 2020.

[4] Nicolas Le Novère. Quantitative and logic modelling of molecular and gene networks. *Nature Reviews Genetics*, 16:146–158, 2015.

A Examples

Consider the 6 following networks with two components, denoted from f^1 to f^6 (each is given under three forms: a table, a graph, and formulas).

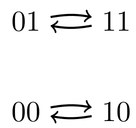
x	$f^1(x)$
00	10
01	00
10	11
11	01



$f^1_1(x) = x_2 + 1$

$f^1_2(x) = x_1$

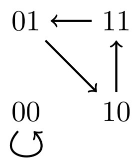
x	$f^2(x)$
00	10
01	11
10	00
11	01



$f^2_1(x) = x_1 + 1$

$f^2_2(x) = x_2$

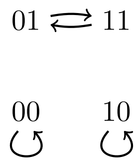
x	$f^3(x)$
00	00
01	10
10	11
11	01



$f^3_1(x) = x_1 + x_2$

$f^3_2(x) = x_1$

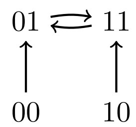
x	$f^4(x)$
00	00
01	11
10	10
11	01



$f^4_1(x) = x_1 + x_2$

$f^4_2(x) = x_2$

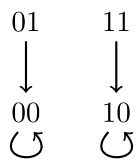
x	$f^5(x)$
00	01
01	11
10	11
11	01



$f^5_1(x) = x_1 + x_2$

$f^5_2(x) = 1$

x	$f^6(x)$
00	00
01	00
10	10
11	10

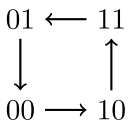


$f^6_1(x) = x_1$

$f^6_2(x) = 0$

One can check that, given a network $f \neq \text{cst}, \text{id}$ with 2 components: $K_2 \notin \mathcal{G}(f)$ *if and only if f is isomorphic to one of the networks given above.* Thus these 6 networks are the counter examples of Theorem 1 for $n = 2$. For instance, there are 6 networks isomorphic to f^1, denoted from h^1 to h^6 (with $h^1 = f^1$, given below with their interactions graphs. We deduce that $\mathcal{G}(f^1)$ contains three digraphs, each distinct from K_2.

x	$h^1(x)$
00	10
01	00
10	11
11	01

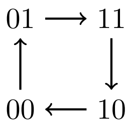


$h^1_1(x) = x_2 + 1$

$h^1_2(x) = x_1$

$G(h^1)$

x	$h^2(x)$
00	01
01	11
10	00
11	01

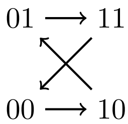


$h^2_1(x) = x_2$

$h^2_2(x) = x_1 + 1$

$G(h^2)$

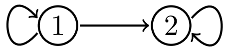
x	$h^3(x)$
00	10
01	11
10	01
11	00



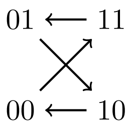
$h^3_1(x) = x_1 + 1$

$h^3_2(x) = x_1 + x_2$

$G(h^3)$



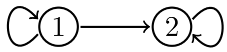
x	$h^4(x)$
00	11
01	10
10	00
11	01



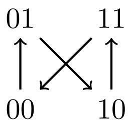
$h^4_1(x) = x_1 + 1$

$h^4_2(x) = x_1 + x_2 + 1$

$G(h^4)$



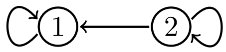
x	$h^5(x)$
00	01
01	10
10	11
11	00



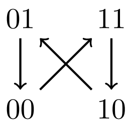
$h^5_1(x) = x_1 + x_2$

$h^5_2(x) = x_2 + 1$

$G(h^5)$



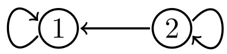
x	$h^6(x)$
00	11
01	00
10	01
11	10



$h^6_1(x) = x_1 + x_2 + 1$

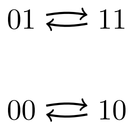
$h^6_2(x) = x_2 + 1$

$G(h^6)$



A corollary of Theorems 1 and 2, stated in the introduction, is that, for any network f with $n \geq 5$ components, we have $|\mathcal{G}(f)| = 1$ if and only if $f = \text{id}$ or $f = \text{cst}$. This is also true for $n = 3$ (checked by computer) and open for $n = 4$. But for $n = 2$, f^2 is a counter example, the only one with two components. Indeed, there are 3 networks isomorphic to f^2, denoted from g^1 to g^3 (with $g^1 = f^2$), given below, and they have the same interaction graph, with a loop on each vertex, as for the identity.

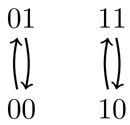
x	$g^1(x)$
00	10
01	11
10	00
11	01



$g^1_1(x) = x_1 + 1$
$g^1_2(x) = x_2$

$G(g^1)$

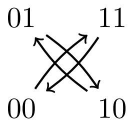
x	$g^2(x)$
00	01
01	00
10	11
11	10



$g^2_1(x) = x_1$
$g^2_2(x) = x_2 + 1$

$G(g^2)$

x	$g^3(x)$
00	11
01	10
10	01
11	00



$g^3_1(x) = x_1 + 1$
$g^3_2(x) = x_2 + 1$

$G(g^3)$

B Lemma for the proof of Theorem 1

Lemma 8. *Let $1 \leq k \leq n$ and let $s_1, \dots, s_{2k}$ be positive integers with sum equal to $n+k$. If $n \geq 5$, then there are disjoint subsets $X_1, \dots, X_{2k} \subseteq \{0,1\}^n$ of size $s_1, \dots, s_{2k}$ such that, for every $i \in [n]$, there is $p \in [k]$ and $x \in X_{2p-1}$ with $x + e_i \in X_{2p}$.*

Proof. Let $I_1, \dots, I_{2k}$ be a partition of $[n]$ (with some members possibly empty) such that, for $1 \leq \ell \leq 2k$, the size of I_ℓ is $s_\ell - 1$ if ℓ is odd, and s_ℓ otherwise; it exists since the sum of the s_ℓ is $n + k$. For $1 \leq p \leq k$, select a configuration $x^{2p-1} \in \{0,1\}^n$, a component $j_{2p} \in I_{2p}$, and let

$$\begin{aligned} X_{2p-1} &= \{x^{2p-1}\} \cup \{x^{2p-1} + e_{j_{2p}} + e_i \mid i \in I_{2p-1}\}, \\ X_{2p} &= \{x^{2p-1} + e_i \mid i \in I_{2p}\}. \end{aligned}$$

Clearly, $|X_{2p-1}| = |I_{2p-1}| + 1 = s_{2p-1}$ and $|X_{2p}| = |I_{2p}| = s_{2p}$. Let $i \in [n]$. Then $i \in I_\ell$ for some $1 \leq \ell \leq 2k$. If $\ell = 2p - 1$ then, setting $x = x^{2p-1} + e_{j_{2p}} + e_i$, we have $x \in X_{2p-1}$ and $x + e_i = x^{2p-1} + e_{j_{2p}} \in X_{2p}$. If $\ell = 2p$ then, setting $x = x^{2p-1}$, we have $x \in X_{2p-1}$ and $x + e_i \in X_{2p}$. Thus we only have to prove that we can choose the configurations x^{2p-1} so that the sets $X_1, \dots, X_{2k}$ are pairwise disjoint. This is obvious if $k = 1$ (and it works for any choice of x^1). If $k = 2$, then, since $n \geq 5$, one easily check that $X_1, \dots, X_{2k}$ are disjoint by taking $x^1 = \mathbf{0}$ and $x^3 = \mathbf{1}$. Suppose now that $k \geq 3$ and choose $x^{2p-1} = e_{j_{2p-2}}$ for all $p \in [k]$, where j_0 means j_{2k}. Then each X_{2p-1} contains configurations of weight 1 or 3 and each X_{2p} contains configurations of weight 2. Hence, given $1 \leq p < q \leq k$, we have to prove that $X_{2p-1} \cap X_{2q-1} = \emptyset$ and $X_{2p} \cap X_{2q} = \emptyset$. Suppose that $x \in X_{2p-1} \cap X_{2q-1}$. If $w(x) = 1$ then we deduce that $x = e_{j_{2p-2}} = e_{j_{2q-2}}$ which is false since $p \neq q$. If $w(x) = 3$ then $x_i = 1$ for some $i \in I_{2p-1}$ while $y_i = 0$ for all $y \in X_{2q-1}$, a contradiction. Thus $X_{2p-1} \cap X_{2q-1} = \emptyset$. Suppose now that $x \in X_{2p} \cap X_{2q}$. Then $x = e_{j_{2p-2}} + e_{i_{2p}} = e_{j_{2q-2}} + e_{i_{2q}}$ for some $i_{2p} \in I_{2p}$ and $i_{2q} \in I_{2q}$. Thus $i_{2p} = j_{2q-2}$ and $i_{2q} = j_{2p-2}$. Hence $j_{2q-2} \in I_{2p}$, and since $p < q$ this implies $q = p + 1$. Also, $j_{2p-1} \in I_{2q}$ and since $p < q$ this implies $p = 1$ and $q = k$, but then $q \neq p + 1$ since $k \geq 3$. Thus indeed $X_{2p} \cap X_{2q} = \emptyset$. Hence the sets $X_1, \dots, X_{2k}$ are indeed pairwise disjoint. □

C Lemma for the proof of Theorem 2

We prove Lemma 4, restated below. We first give some definitions. Given $X \subseteq \{0,1\}^n$ and $i \in [n]$, we say that X is *closed* by e_i if $X = X + e_i$. One easily check that if $X, Y \subseteq \{0,1\}^n$ are closed by e_i, then so is $X \cap Y$. Also, if $|X|$ is closed by e_i then $|X|$ is even. Indeed, let X_0 be the set of of $x \in X$ with $x_i = 0$ and $X_1 = X \setminus X_0$. We have $X_0 + e_i \subseteq X_1$, thus $|X_0| \leq |X_1|$ and similarly, $X_1 + e_i \subseteq X_0$ thus $|X_1| \leq |X_0|$. Hence $|X_0| = |X_1|$ so $|X|$ is even.

Lemma 4. *Let f be a n-component network and distinct $i, j \in [n]$. Some digraph in $\mathcal{G}(f)$ has no arc from j to i if and only if f has a (2^{n-2})-nice set.*

Proof. Let $h = \pi \circ f \circ \pi^{-1}$ for some permutation π of $\{0,1\}^n$, and suppose that $G(h)$ has no arc from j to i. Let X be the set of $x \in \{0,1\}^n$ with $x_i = 0$, of size 2^{n-1}, and let $X^- = h^{-1}(X)$. If $x \in X^-$, that is, $h_i(x) = 0$, then $h_i(x + e_j) = 0$ since otherwise $G(h)$ has an arc from j to i. Thus $x + e_j \in X^-$. Hence X^- is closed by e_j thus $|X^-|$ is even. Since $j \neq i$, X is also closed by e_j, so $X^- \cap X$ is closed by e_j and thus $|X^- \cap X|$ is even. Let $A = \pi^{-1}(X)$. Then one easily check that $f^{-1}(A) = \pi^{-1}(X^-)$ and that $f^{-1}(A) \cap A = \pi^{-1}(X^- \cap X)$. So $|f^{-1}(A)|$ and $|f^{-1}(A) \cap A|$ are even, and thus A is a (2^{n-2})-nice set of f.

Conversely, suppose that f has a (2^{n-2})-nice set A, thus of size 2^{n-1}. Let $A^- = f^{-1}(A)$. Then $|A|$, $|A^-|$ and $|A^- \cap A|$ are even, so $|A \setminus A^-|$ and $|A^- \setminus A|$ are also even. Hence there is a a balanced partition (A_1, A_2) of $A \cap A^-$, a balanced partition (A_3, A_4) of $A \setminus A^-$, and a balanced partition (A_3^-, A_4^-) of $A^- \setminus A$. Then (A_1, A_2, A_3, A_4) is a partition of A and (A_1, A_2, A_3^-, A_4^-) is a partition of A^-, and $A_1, A_2, A_3, A_4, A_3^-, A_4^-$ are disjoint.

For $k = 0, 1$, let Y_k be the set of $x \in \{0,1\}^n$ with $x_i = k$ and $x_j = 0$. Since $|A| = 2^{n-1}$ we have $|A_1| + |A_3| = 2^{n-2}$ thus there is a partition (X_1, X_3) of Y_0 with $|X_1| = |A_1|$ and $|X_3| = |A_3|$. Since $|A_3^-| = |A^- \setminus A|/2 \leq (2^n - |A|)/2 = 2^{n-2}$ there is $X_3^- \subseteq Y_1$ of size $|A_3^-|$. Let $X_2 = X_1 + e_j$, $X_4 = X_3 + e_j$ and $X_4^- = X_3^- + e_j$. Then $X_1, X_2, X_3, X_4, X_3^-, X_4^-$ are disjoint and of size $|A_1|, |A_2|, |A_3|, |A_4|, |A_3^-|, |A_4^-|$. Hence there is a permutation π of $\{0,1\}^n$ that sends $A_1, A_2, A_3, A_4, A_3^-, A_4^-$ on $X_1, X_2, X_3, X_4, X_3^-, X_4^-$, respectively.

Let $h = \pi \circ f \circ \pi^{-1}$. Let $X = X_1 \cup X_2 \cup X_3 \cup X_4$ and $X^- = X_1 \cup X_2 \cup X_3^- \cup X_4^-$. One easily check that: X is the set of $x \in \{0,1\}^n$ with $x_i = 0$; X^- is closed by e_j; and $X^- = h^{-1}(X)$. We will prove that $G(h)$ has no arc from j to i. Suppose, for a contradiction, that there is $x \in \{0,1\}^n$ with $h_i(x) \neq h_i(x + e_j)$. Without loss, we can assume that $h_i(x) = 0$, that is, $h(x) \in X$. So $x \in X^-$, hence $x + e_j \in X^-$, thus $h(x + e_j) \in X$, that is, $h_i(x + e_j) = 0$, a contradiction. Thus $G(h)$ has no arc from j to i. □

D Lemma for the proof of Theorem 3

For $X \subseteq \{0,1\}^n$, let $\partial(X)$ be the number of edges in Q_n with exactly one end in X; equivalently, it is the number of pairs (x, i) with $x \in X$ and $i \in [n]$ such that $x + e_i \notin X$. We can regard $|X|$ as the volume of X and $\delta(X)$ as its perimeter and ask: what is the minimum perimeter for a given volume? The answer is Harp's isoperimetric inequality, from 1964 [2]. We denote by L_k the first k configurations in $\{0,1\}^n$ according to the lexicographic order (e.g. for $n = 4$ we have $L_5 = \{0000, 1000, 0100, 1100, 0010\}$).

Theorem 4 ([2])**.** *If $n \geq 1$ and $X \subseteq \{0,1\}^n$ then $\partial(X) \geq \partial(L_{|X|})$.*

In practice, the following approximation is often used; see [3] for instance.

Corollary 1. *If $n \geq 1$ and $X \subseteq \{0,1\}^n$ is non-empty, then*

$$\partial(X) \geq |X|(n - \log_2 |X|).$$

From this inequality, we deduce Lemma 7, that we restate.

Lemma 7. *Let $A \subseteq \{0,1\}^n$ be non-empty, and let d be the average degree of the subgraph of Q_n induced by A. Then $|A| \geq 2^d$.*

Proof. For $a \in A$, let $d(a)$ be the degree of a in the subgraph of Q_n induced by A, and let d be the average degree, that is, $d = \sum_{a \in A} d(a)/|A|$. Since, for each $a \in A$, there are exactly $n - d(a)$ components $i \in [n]$ such that $a + e_i \notin A$, we have, using Corollary 1,

$$\partial(A) = \sum_{a \in A} n - d(a) = |A|n - |A|d = |A|(n - d) \geq |A|(n - \log_2 |A|),$$

thus $d \leq \log_2 |A|$ as desired. □