On the Rank and Periodic Rank
of Finite Dynamical Systems

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Abstract

A finite dynamical system is a function $f : A^n \to A^n$ where A is a finite alphabet, used to model a network of interacting entities. The main feature of a finite dynamical system is its interaction graph, which indicates which local functions depend on which variables; the interaction graph is a qualitative representation of the interactions amongst entities on the network. The rank of a finite dynamical system is the cardinality of its image; the periodic rank is the number of its periodic points. In this paper, we determine the maximum rank and the maximum periodic rank of a finite dynamical system with a given interaction graph over any non-Boolean alphabet. The rank and the maximum rank are both computable in polynomial time. We also obtain a similar result for Boolean finite dynamical systems (also known as Boolean networks) whose interaction graphs are contained in a given digraph. We then prove that the average rank is relatively close (as the size of the alphabet is large) to the maximum. The results mentioned above only deal with the parallel update schedule. We finally determine the maximum rank over all block-sequential update schedules and the supremum periodic rank over all complete update schedules.

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1   Introduction

Finite Dynamical Systems (FDSs) have been used to represent networks of interacting entities as follows. A network of n entities has a state $x = (x_1, \ldots, x_n) \in [q]^n$, represented by a q-ary variable $x_v \in [q] = \{0, 1, \ldots, q-1\}$ on each entity v, which evolves according to a deterministic function $f = (f_1, \ldots, f_n) : [q]^n \to [q]^n$, where $f_v : [q]^n \to [q]$ represents the update of the local state x_v. FDSs have been used to model gene networks (see [10, 17]), neural networks [2, 9], network coding [14], social interactions [8, 12] and more (see [7]).

The architecture of an FDS $f : [q]^n \to [q]^n$ can be represented via its **interaction graph** $\mathrm{IG}(f)$, which indicates which update functions depend on which variables. More formally, $\mathrm{IG}(f)$ has $\{1, \ldots, n\}$ as vertex set and there is an arc from u to v if $f_v(x)$ depends on x_u. In different contexts, the interaction graph is known–or at least well approximated–, while the actual update functions are not. One main problem of research on FDSs is then to predict their dynamics according to their interaction graphs. However, due to the wide variety of possible local functions, determining properties of an FDS given its interaction graph is in general a difficult problem.

For instance, maximising the number of fixed points of an FDS based on its interaction graph was the subject of a lot of work, e.g. in [1, 2, 6, 13, 14]. The logarithm of the number of fixed points is notably upper bounded by the transversal number of its interaction graph [2, 14]. This upper bound is reached for large classes of graphs (e.g. perfect graphs) but is not tight in general [14]. Moreover, there is a dramatic change whether we assume that the FDS has an interaction graph equal to a certain digraph or only contained in that digraph (this is the distinction between guessing number and strict guessing number in [5]).

In this paper, we are interested in maximising two other very important dynamical parameters of an FDS given its interaction graph. First, the **rank** of an FDS f is the number of images of f. In particular, determining the maximum rank also determines whether there exists a bijective FDS with a given interaction graph. This is equivalent to the existence of so-called reversible dynamics, where the whole history of the system can be traced back in time. Second, because there is only a finite number of states, all the asymptotic points of f are periodic. The number of periodic points of f is referred to as its **periodic rank**. In contrast with the situation for fixed points, we derive a bound on these two quantities which is attained for all interaction graphs and all alphabets. In particular, there exists a bijection with interaction graph contained in D if and only if all the vertices of D can be covered by disjoint cycles. Moreover, we prove that our bound is attained for functions whose interaction graph is equal to a given digraph, and not only contained, for all non-Boolean alphabets. We then show that the average rank is relatively close (as D is fixed and q tends to infinity) to the maximum.

These results can be viewed as the discrete analogue to Poljak's matrix theorem in [11], which proves tat the maximum rank of M^p, where M is a real matrix with given support D and $p \geqslant 1$, is given by the maximum number of pairwise independent p-walks in D (see the sequel for a precise definition). However, our results extend Poljak's result for the discrete case in three ways (but Poljak's result cannot be viewed as a consequence of our results). Firstly, they hold for all functions, not only linear functions. Secondly, they explicitly determine the maximum periodic rank. Thirdly, the average rank of a real matrix cannot be properly defined, hence our result on the average rank of finite dynamical systems is completely novel.

The results mentioned above hold for the so-called parallel update schedule, where all entities update their local state at the same time, and hence x becomes $f(x)$. We then study complete update schedules, where all entities update their local state at least once, and block-sequential schedules where all entities update their local state exactly

once (the parallel schedule being a very particular example of block-sequential schedule). We then prove that the upper bound on the rank in parallel remains valid for any block-sequential schedule but is no longer valid for all complete schedules. We also determine the maximum periodic rank when considering all possible complete schedules. In particular, there exists a function f with interaction graph D and a complete schedule σ such that f^σ is a bijection if and only if all the vertices of D belong to a cycle.

The rest of the paper is organised as follows. Section 2 introduces some useful notation and describes our results on the maximum (periodic) rank in parallel. Section 3 then proves our result on the average rank. Finally, the maximum rank and periodic rank under different update schedules are investigated in Section 4.

2 Maximum (periodic) rank in parallel

2.1 Background and notation

Let $D = (V, E)$ be a digraph on n vertices; let $V = \{1, \ldots, n\}$ be its set of vertices and $E \subseteq V^2$ its set of arcs. The digraph may have loops, but no parallel arcs. The adjacency matrix $M \in \{0, 1\}^{n \times n}$ has entries $m_{u,v} = 1$ if and only if $(u, v) \in E$. We denote the in-neighbourhood of a vertex v in D by

$$N^-(v; D) = \{u \in V : (u, v) \in E\}.$$

When there is no confusion, we shall omit the dependence on D. This is extended to sets of vertices: $N^-(S) = \bigcup_{v \in S} N^-(v)$. The out-neighbourhood is defined similarly. A source is a vertex with empty in-neighbourhood; a sink is a vertex with empty out-neighbourhood. The in-degree of v is the cardinality of its in-neighbourhood and is denoted by d_v.

A **walk** $w = (v_0, \ldots, v_p)$ is a sequence of (not necessarily distinct) vertices such that $(v_s, v_{s+1}) \in E$ for all $0 \leqslant s \leqslant p - 1$. A path is a walk where all vertices are distinct. A cycle is a walk where only the first and last vertices are equal. We refer to p as the length of the walk; a p-walk is a walk of length p. We say that two p-walks $w = (w_0, \ldots, w_p), w' = (w'_0, \ldots, w'_p)$ are **independent** if $w_s \neq w'_s$ for all $0 \leqslant s \leqslant p$. We denote the maximum number of pairwise independent p-walks as $\alpha_p(D)$.

Edmonds gave a formula for $\alpha_1(D)$ in [3], based on the König-Ore formula:

$$\alpha_1(D) = n - \max\{|S| - |N^-(S)| : S \subseteq V\}.$$

This was greatly generalised by Poljak, who showed that $\alpha_p(D)$ could be computed in polynomial time and who gave a formula for $\alpha_p(D)$ for all $p \geqslant 1$ in [11]. Suppose that $C_1, \ldots, C_r$ and $P_1, \ldots, P_s$ are vertex-disjoint cycles and paths. The cycle $C_i = (c_0, \ldots, c_{l-1})$ produces l independent p-walks of the form $W_a = (c_a, c_{a+1}, \ldots, c_{a+p-1})$, where indices are computed mod l and $0 \leqslant a \leqslant l - 1$. The path $P_j = (d_0, \ldots, d_{m-1})$ produces $m - p$ independent p-walks of the form $W_b = (d_b, d_{b+1}, \ldots, d_{b+p-1})$, where $0 \leqslant d \leqslant m - p - 1$. Poljak's theorem asserts that this is the optimal way of producing pairwise independent p-walks. We denote the number of vertices of a cycle C and of a path P as $|C|$ and $|P|$, respectively.

Theorem 1 ([11]). *For every digraph D and a positive integer p,*

$$\alpha_p(D) = \max\left\{\sum_{i=1}^{r}|C_i| + \sum_{j=1}^{s}(|P_j| - p)\right\},$$

where the maximum is taken over all families of pairwise vertex-disjoint cycles and paths $C_1, \ldots, C_r$ and $P_1, \ldots, P_s$.

Corollary 2. *For all $p \geqslant n$,*

$$\alpha_p(D) = \alpha_n(D) = \max\left\{\sum_{i=1}^{r}|C_i|\right\},$$

where the maximum is taken over all families of pairwise vertex-disjoint cycles.

A **finite dynamical system** is a function $f : [q]^n \to [q]^n$, where $[q] = \{0, 1, \ldots, q-1\}$ is a finite alphabet; we denote $f = (f_1, \ldots, f_n)$, where $f_v : [q]^n \to [q]$. The **interaction graph** $\mathrm{IG}(f)$ is the digraph with vertex set $V = \{1, \ldots, n\}$ such that $(u, v) \in E(\mathrm{IG}(f))$ if and only if f_v depends essentially on u, i.e. there exist $x, y \in [q]^n$ which only differ on coordinate u such that $f_v(x) \neq f_v(y)$. The set of all functions over an alphabet of size q and whose interaction graph is (contained in) D is denoted as

$$\mathrm{F}[D, q] := \{f : [q]^n \to [q]^n : \mathrm{IG}(f) = D\},$$
$$\mathrm{F}(D, q) := \{f : [q]^n \to [q]^n : \mathrm{IG}(f) \subseteq D\}.$$

We consider successive iterations of f; we thus denote $f^1(x) = f(x)$ and $f^{k+1}(x) = f(f^k(x))$ for all $k \geqslant 1$. Recall that x is an **image** if there exists y such that $x = f(y)$; x is a **periodic point** of f if there exists $k \in \mathbb{N}$ such that $f^k(x) = x$. We are interested in the following quantities:

1. the **rank** of f is the number of its images: $|\mathrm{Ima}(f)|$;

2. the **periodic rank** of f is the number of its periodic points: $|\mathrm{Per}(f)|$.

It will be useful to scale these two quantities using the logarithm in base q:

$$\mathrm{ima}(f) := \log_q |\mathrm{Ima}(f)|,$$
$$\mathrm{per}(f) := \log_q |\mathrm{Per}(f)|.$$

Moreover, the maximum (periodic) rank over all functions in $\mathrm{F}[D, q]$ is denoted as

$$\mathrm{ima}[D, q] := \max\{\mathrm{ima}(f) : f \in \mathrm{F}[D, q]\},$$
$$\mathrm{per}[D, q] := \max\{\mathrm{per}(f) : f \in \mathrm{F}[D, q]\};$$

and $\mathrm{ima}(D, q)$ and $\mathrm{per}(D, q)$ are defined similarly. We finally note that $\mathrm{per}(f) = \mathrm{ima}(f^p)$ for all $p \geqslant q^n - 1$. Therefore, the main strategy is to maximise the scaled rank of f^p for all p; we thus denote

$$\mathrm{ima}[D, q, p] := \max\{\mathrm{ima}(f^p) : f \in \mathrm{F}[D, q]\},$$
$$\mathrm{ima}(D, q, p) := \max\{\mathrm{ima}(f^p) : f \in \mathrm{F}(D, q)\}.$$

We then have

$$\mathrm{ima}[D, q] = \mathrm{ima}[D, q, 1]$$
$$\mathrm{per}[D, q] = \mathrm{ima}[D, q, q^n],$$

and similarly for $\mathrm{ima}(D, q)$ and $\mathrm{per}(D, q)$.

2.2 Maximum rank and periodic rank

Theorem 3. *For all D, p, and $q \geqslant 3$,*

$$\mathrm{ima}[D, q, p] = \mathrm{ima}(D, q, p) = \alpha_p(D).$$

For all D, p,
$$\mathrm{ima}[D, 2, p] = \alpha_p(D).$$

Corollary 4 (Maximum rank)**.** *For all D and $q \geqslant 3$,*

$$\mathrm{ima}[D, q] = \mathrm{ima}(D, q) = \alpha_1(D).$$

For $q = 2$,
$$\mathrm{ima}(D, 2) = \alpha_1(D).$$

Corollary 5 (Maximum periodic rank)**.** *For all D and $q \geqslant 3$,*

$$\mathrm{per}[D, q] = \mathrm{per}(D, q) = \alpha_n(D).$$

For $q = 2$,
$$\mathrm{per}(D, 2) = \alpha_n(D).$$

The case $q = 2$ is indeed specific, for there exist graphs D such that $\max\{\mathrm{ima}(f^p) : f \in \mathrm{F}[D, 2]\} < \alpha_p(D)$ for all $p \geqslant 1$. We shall investigate this in the next subsection.

We obtain two immediate consequences of Corollary 4. Firstly, we determine which graphs admit so-called reversible dynamics, i.e. for which graphs D we can find a permutation in $\mathrm{F}[D, q]$.

Corollary 6 (Reversible dynamics in parallel)**.** *For any $q \geqslant 3$, there exists $f \in \mathrm{F}[D, q]$ which is a permutation of $[q]^n$ if and only if all the vertices of D can be covered by disjoint cycles.*

Secondly, Robert's seminal theorem indicates that if the interaction graph of f is acyclic, then f^n is constant (i.e. $\mathrm{per}(f) = 0$) [16]. Since $\alpha_n(D) = 0$ if and only if D is acyclic, we obtain the following result.

Corollary 7. *The graph D is acyclic if and only if f^n is constant for all q and all $f \in \mathrm{F}[D, q]$.*

The rest of this subsection is devoted to the proof of Theorem 3. We begin with the upper bound on the scaled rank, which follows a form of max-flow min-cut theorem (or at least, the min-cut uper bound).

We now review the communication model based on terms from logic introduced by Riis and Gadouleau in [15]. Let $\{x_1, \ldots, x_k\}$ be a set of variables and consider a set of function symbols $\{f_1, \ldots, f_l\}$ with respective arities (numbers of arguments) $d_1, \ldots, d_l$. A **term** is defined to be an object obtained from applying function symbols to variables recursively. We say that u is a subterm of t if the term u appears in t. Furthermore, u is a **direct subterm** of t if $t = f_j(v_1, \ldots, u, \ldots, v_{d_j})$, and we denote it by $u \prec t$.

Let $\Gamma = \{t_1, \ldots, t_r\}$ be a set of terms built on variables $x_1, \ldots, x_k$ and function symbols $f_1, \ldots, f_l$ of respective arities $d_1, d_2, \ldots, d_l$. We denote the set of variables that occur in terms in Γ as Γ_{var} and the collection of subterms of one or more terms in Γ as Γ_{sub}. To the term set Γ we associate the acyclic digraph $G_\Gamma = (V_\Gamma = \Gamma_{\mathrm{sub}}, E_\Gamma = \{(u, v) : u \prec v\})$. The set of sources in G_Γ is Γ_{var} and the set of sinks is Γ. The min-cut of Γ is the minimum size of a vertex cut of G_Γ between Γ_{var} and Γ.

An **interpretation** for Γ over $[q]$ is an assignment of the function symbols $\psi = \{\bar{f}_1, \ldots, \bar{f}_l\}$, where $\bar{f}_i : [q]^{d_i} \to [q]$ for all $1 \leqslant i \leqslant l$. We note that $\bar{f}_i$ may not depend essentially on all its d_i variables. Once all the function symbols f_i are assigned functions $\bar{f}_i$, then by composition each term $t_j \in \Gamma$ is assigned a function $\bar{t}_j : [q]^k \to [q]$. We shall abuse notations and also denote the **induced mapping** of the interpretation as $\psi : [q]^k \to [q]^r$, defined as $\psi(a) = \big(\bar{t}_1(a), \ldots, \bar{t}_r(a)\big)$.

Intuitively, if S is a vertex cut of G_Γ between Γ_{var} and Γ, then the terms in Γ "depend on" the terms in S. As such, the scaled rank of any induced mapping ψ cannot be greater than the size of S. This intuition is given formally as follows.

Theorem 8 ([15] with our notation). *Let Γ be a term set with min-cut of ρ and ψ be an interpretation for Γ over $[q]$, then $\mathrm{ima}(\psi) \leqslant \rho$.*

We illustrate the communication model and Theorem 8 by the following example. Consider the term set

$$\Gamma := \{t_1 := f_1(f_2(x_1, x_2, x_3), f_1(x_1, x_2)),$$
$$t_2 := f_3(f_2(x_1, x_2, x_3)),$$
$$t_3 := f_4(f_2(x_1, x_2, x_3), f_1(x_1, x_2))\}.$$

The set of variables is $\Gamma_{\mathrm{var}} = \{x_1, x_2, x_3\}$, while the set of subterms is

$$\Gamma_{\mathrm{sub}} = \{x_1, x_2, x_3, u := f_1(x_1, x_2), v := f_2(x_1, x_2, x_3), t_1, t_2, t_3\}$$

The graph G_Γ is displayed below. We see that $\{u, v\}$ forms a vertex cut of G_Γ between Γ_{var} and Γ: $t_1 = f_1(v, u)$, $t_2 = f_3(v)$ and $t_3 = f_4(u, v)$. In fact, the min-cut is indeed 2.
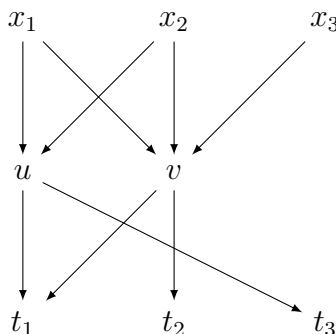
A possible interpretation for Γ over $[2]$ is (all operations mod 2)

$$\bar{f}_1(a_1, a_2) = a_1 + a_2$$
$$\bar{f}_2(a_1, a_2, a_3) = a_1 a_2 a_3$$
$$\bar{f}_3(a_1) = a_1$$
$$\bar{f}_4(a_1, a_2) = 0.$$

The corresponding induced mapping is

$$\psi(a) = (a_1 + a_2 + a_1 a_2 a_3, a_1 a_2 a_3, 0),$$

and its scaled rank is $\log_2 3$, which is indeed no more than 2.

Lemma 9. *For any $p \geqslant 1$ and $\bar{f} \in \mathrm{F}(D, q)$, $\mathrm{ima}(\bar{f}^p) \leqslant \alpha_p(D)$.*

Proof. For all $v \in V$, denoting $N^-(v; D) = \{u_1, \ldots, u_k\}$ sorted in increasing order, we have $\bar{f}_v(x) = \bar{f}_v(x_{u_1}, \ldots, x_{u_k})$. By definition, $\bar{f}^p$ is the induced mapping of an interpretation for $\Gamma^p = \{t_1^p, \ldots, t_n^p\}$, where $\Gamma^0 = \{t_1^0 = x_1, \ldots, t_n^0 = x_n\}$ and for all $1 \leqslant s \leqslant p$,

$$t_v^s = f_v(t_{u_1}^{s-1}, \ldots, t_{u_k}^{s-1}).$$

The graph $G_{\Gamma^p} = (V_{\Gamma^p}, E_{\Gamma^p})$ is then given by

$$V_{\Gamma^p} = \Gamma^0 \cup \cdots \cup \Gamma^p$$
$$E_{\Gamma^p} = \{(t_w^{s-1}, t_v^s) : 1 \leqslant s \leqslant p, w \in N^-(v; D)\}.$$

A flow in G_{Γ^p} is a set of vertex-disjoint paths from Γ^0 to Γ^p. Such a path is of the form $t_W = (t_{w_0}^0, \ldots, t_{w_p}^p)$ where $w_{s-1} \in N^-(w_s; D)$; it naturally induces a walk in D: $W = (w_0, \ldots, w_p)$. Since the paths t_W and $t_{W'}$ are vertex-disjoint, the corresponding walks W and W' are independent. Therefore, the max-flow of G_{Γ^p} is at most $\alpha_p(D)$. By the max-flow min-cut theorem and Theorem 8, $\mathrm{ima}(\bar{f}^p) \leqslant \alpha_p(D)$. $\qquad \square$

Let $W_1, \ldots, W_\alpha$ be $\alpha := \alpha_p(D)$ independent walks of length p, where we denote $W_i = (w_{i,0}, \ldots, w_{i,p})$. According to Theorem 1, those arise from families of disjoint cycles and paths. By construction, if w precedes w' on one walk and w' appears on another walk and has a predecessor there, then w precedes w' in the other walk as well. For all $0 \leqslant s \leqslant p$, we denote $W^s = \{w_{i,s} : 1 \leqslant i \leqslant \alpha\}$, $U^s = V \setminus W^s$ and $U' = V \setminus (W^1 \cup \cdots \cup W^p)$.

We can now construct the finite dynamical systems which attain the upper bound on the scaled rank. The case $q = 2$ and $f \in \mathrm{F}(D, 2)$ is easy. We use a finite dynamical system where $w_{i,s+1}$ simply copies the value $x_{w_{i,s}}$; this will transmit the value $x_{w_{i,0}}$ along the walk W_i.

Lemma 10. *The function $f \in \mathrm{F}(D, 2)$ defined as*

$$f_{w_{i,s+1}}(x) = x_{w_{i,s}} \qquad\qquad 0 \leqslant s \leqslant p - 1, 1 \leqslant i \leqslant \alpha,$$
$$f_u(x) = 0 \qquad\qquad\qquad \text{if } u \in U',$$

satisfies $\mathrm{ima}(f^p) = \alpha_p(D)$.

Proof. Let $X = \{x \in [2]^n : x_{U^0} = (0, \ldots, 0)\}$; we then have $\log_q |X| = |W^0| = \alpha_p(D)$. It is easy to show, by induction on s, that for all $0 \leqslant s \leqslant p$, $|f^s_{W^s}(X)| = |X|$. Thus $\mathrm{ima}(f^p) = \alpha_p(D)$. $\qquad\square$

For $q \geqslant 3$ and $f \in \mathrm{F}[D, q]$, we use a finite dynamical system where $w_{i,s+1}$ wishes to copy the value $x_{w_{i,s}}$ whenever it can. Each other vertex $u \in N^-(w_{i,s+1})$ has a red light (the value 2). If all lights are red, then $w_{i,s+1}$ cannot copy the value $x_{w_{i,s}}$ any more; instead it flips it from 0 to 1 and vice versa.

Lemma 11. *For $q \geqslant 3$, the function $f \in \mathrm{F}[D, q]$ defined as*

$$f_{w_{i,s+1}}(x) = \begin{cases} 1 - x_{w_{i,s}} & \text{if } x_{w_{i,s}} \in \{0, 1\} \text{ and } x_{N^-(w_{i,s+1}) \setminus w_{i,s}} = (2, \ldots, 2), \\ x_{w_{i,s}} & \text{otherwise} \end{cases}$$
$$0 \leqslant s \leqslant p - 1, 1 \leqslant i \leqslant \alpha,$$
$$f_u(x) = \begin{cases} 1 & \text{if } x_{N^-(u)} = (1, \ldots, 1) \\ 0 & \text{otherwise} \end{cases}$$
$$\text{if } u \in U',$$

satisfies $\mathrm{ima}(f^p) = \alpha_p(D)$.

Proof. The proof is similar, albeit more complex, than the one of Lemma 10.

Claim 12. *For all $0 \leqslant s \leqslant p - 1$, if $x_{W^s} \neq y_{W^s}$ and $x_{U^s}, y_{U^s} \in \{0, 1\}^{|U^s|}$, then $f_{W^{s+1}}(x) \neq f_{W^{s+1}}(y)$ and $f_{U^{s+1}}(x), f_{U^{s+1}}(y) \in \{0, 1\}^{|U^{s+1}|}$.*

Proof of Claim 12. We prove the first assertion. First, suppose there exists $w_{i,s} \in W^s$ where $x_{w_{i,s}} \geqslant 2$ and $x_{w_{i,s}} \neq y_{w_{i,s}}$, then

$$f_{w_{i,s+1}}(x) = x_{w_{i,s}} \neq f_{w_{i,s+1}}(y).$$

Second, suppose that for any $w_{i,s} \in W^s$ such that $x_{w_{i,s}} \neq y_{w_{i,s}}$, we have $\{x_{w_{i,s}}, y_{w_{i,s}}\} = \{0, 1\}$. Then

$$f_{w_{i,s+1}}(x) = 1 - x_{w_{i,s}} \Leftrightarrow x_{N^-(w_{i,s+1}) \setminus w_{i,s}} = (2, \ldots, 2)$$
$$\Leftrightarrow (N^-(w_{i,s+1}) \subseteq W^s) \wedge (y_{N^-(w_{i,s+1}) \setminus w_{i,s}} = (2, \ldots, 2))$$
$$\Leftrightarrow f_{w_{i,s+1}}(y) = 1 - y_{w_{i,s}}.$$

For the second assertion, let $v \in U^{s+1}$, then either $v \in U'$ or $v = w_{i,t+1}$ with $0 \leqslant t \neq s$. If $v \in U'$, then $f_v(x) \in \{0, 1\}$ for any x. Suppose that $v = w_{i,t+1}$ such that $f_{w_{i,t+1}}(x) \notin \{0, 1\}$. Then $x_{w_{i,t}} \notin \{0, 1\}$, which implies $w_{i,t} \in W^s$, say $w_{i,t} = w_{j,s}$; but then, $v = w_{j,s+1} \notin U^{s+1}$. ∎

Let $X = \{x \in [q]^n : x_{U^0} = (0, \ldots, 0)\}$; we then have $\log_q |X| = |W^0| = \alpha_p(D)$.

Claim 13. *For all $0 \leqslant s \leqslant p$, $|f_{W^s}^s(X)| = |X|$ and for any $x \in X$, $f_{U^s}^s(x) \in \{0, 1\}^{|U^s|}$.*

Proof of Claim 13. The proof is by induction on s; the statement is clear for $s = 0$. Suppose it holds for up to s. For any distinct $x, y \in X$, we have $f_{W^s}^s(x) \neq f_{W^s}^s(y)$ and $f_{U^s}^s(x), f_{U^s}^s(y) \in \{0, 1\}^{|U^s|}$. By Claim 12, we obtain that $f_{W^{s+1}}^{s+1}(x) \neq f_{W^{s+1}}^{s+1}(y)$ and $f_{U^{s+1}}^{s+1}(x) \in \{0, 1\}^{s+1}$. ∎

□

2.3 Maximum rank in the Boolean case

We first exhibit a class of digraphs for which the upper bound on the rank is not reached in the Boolean case.

Proposition 14. *Let D be a digraph such that $\alpha_1(D) = n$ and $d_v = 2$ for all vertices $v \in V$. Then $\mathrm{ima}(f^p) < \alpha_p(D)$ for all $f \in \mathrm{F}[D, 2]$ and all $p \geqslant 1$.*

Proof. Suppose $f \in \mathrm{F}[D, 2]$ is a permutation of $\{0, 1\}^n$, then all the local functions f_v must be balanced, i.e. $|f_v^{-1}(0)| = |f_v^{-1}(1)|$ for all $v \in V$. Because the in-degree of v is equal to two, say $N^-(v) = \{u_1, u_2\}$, we must have $f_v(x_{u_1}, x_{u_2}) = x_{u_1} + x_{u_2} + c_v$, where $c_v \in \mathrm{GF}(2)$. Therefore, $f(x) = Mx + c$, but since every vertex has even in-degree, the sum of all rows in M (in $\mathrm{GF}(2)$) equals zero and M is singular. □

For instance, if D is the undirected cycle on n vertices, or the directed cycle on n vertices with a loop on each vertex, then for all $p \geqslant 1$, $\alpha_p(D) = n$ but $\mathrm{ima}(f^p) < n$ for all $f \in \mathrm{F}[D, 2]$.

It is unknown whether there exist other such examples. On the other hand, we can easily exhibit a class of digraphs which do reach the bound. For instance, let $D = \mathring{K}_n$ be the clique with a loop on each vertex (alternatively, $E = V^2$). Then the following $f \in \mathrm{F}[\mathring{K}_n, 2]$ is a permutation:

$$f_v(x) = \begin{cases} x_v & \text{if } x \notin \{(0, \ldots, 0), (1, \ldots, 1)\} \\ x_v + 1 & \text{otherwise}; \end{cases}$$

indeed f is the transposition of $(0, \ldots, 0)$ and $(1, \ldots, 1)$. Less obviously, the clique also admits a permutation of $\{0, 1\}^n$.

Proposition 15. *For any $n \neq 3$, $\mathrm{ima}[K_n, 2] = n$.*

Proof. Firstly, let n be even. Then we claim that $f(x) = Mx$ is a permutation, or equivalently that $\det(M) = 1$. For $\det(M) = d(n) \mod 2$, where $d(n)$ is the number of derangements (fixed point-free permutations) of $[n]$. Enumerating the permutations of $[n]$ according to their number p of fixed points, we have

$$n! = d(n) + \sum_{p=1}^{n-1} \binom{n}{p} d(n-p) + 1.$$

Since $n!$ and $\binom{n}{1}, \ldots, \binom{n}{n-1}$ are all even, it follows that $d(n)$ is odd, thus $\det(M) = 1$.

Secondly, let $n \geqslant 5$ be odd. We prove the result by induction on n odd. Let us settle the case where $n = 5$. We construct $f \in \mathrm{F}[K_5, 2]$ as follows:

$$(f_1, f_2, f_3)(x) = \begin{cases} (x_3, x_1, x_2) & \text{if } x_4 = x_5 \\ (x_2, x_3, x_1) & \text{otherwise,} \end{cases}$$

$$(f_4, f_5)(x) = \begin{cases} (x_5, x_4) & \text{if } (x_1, x_2, x_3) = (0, 0, 0) \\ (x_5 + 1, x_4 + 1) & \text{otherwise.} \end{cases}$$

It is easy to check that f is a permutation of $[2]^5$.

The inductive case is similar. Suppose that $g \in \mathrm{F}[K_n, 2]$ is a permutation, then construct $f \in \mathrm{F}[K_{n+2}, 2]$ as follows:

$$(f_1, \ldots, f_n)(x) = \begin{cases} g(x_1, \ldots, x_n) & \text{if } x_{n+1} = x_{n+2} \\ g(x_1, \ldots, x_n) + (1, \ldots, 1) & \text{otherwise,} \end{cases}$$

$$(f_{n+1}, f_{n+2})(x) = \begin{cases} (x_{n+2}, x_{n+1}) & \text{if } (x_1, \ldots, x_n) = (0, \ldots, 0) \\ (x_{n+2} + 1, x_{n+1} + 1) & \text{otherwise.} \end{cases}$$

Again, it is easy to check that f is a permutation of $[2]^n$. $\qquad\square$

Problem 16. Find a good lower bound on the maximum rank or maximum periodic rank in $\mathrm{F}[D, 2]$.

3 Average rank

Theorem 17. *The average scaled rank in $\mathrm{F}[D, q]$ tends to $\alpha_1(D)$:*

$$\lim_{q \to \infty} \frac{1}{|F[D, q]|} \sum_{f \in F[D, q]} \mathrm{ima}(f) = \alpha_1(D).$$

Proof. The case $\alpha_1(D) = 0$ is trivial, thus let $a := \alpha_1(D) \geqslant 1$ and $(u_1, v_1), \ldots, (u_a, v_a)$ be a collection of pairwise independent arcs. Let q be large enough and f be chosen uniformly at random amongst $\mathrm{F}[D, q]$. Let $h^0 = (x_{u_1}, \ldots, x_{u_a}) : [q]^n \to [q]^a$ and for any $1 \leqslant i \leqslant a$, let

$$h^i = (f_{v_1}, \ldots, f_{v_i}, x_{u_{i+1}}, \ldots, x_{u_a}) : [q]^n \to [q]^a.$$

Let c_i be defined as $c_0 = 1$ and $c_i = \frac{c_{i-1}^2}{8}$ for $1 \leqslant i \leqslant a$.

Since $|\mathrm{Ima}(f)| \geqslant |\mathrm{Ima}(h^a)|$, all we need is to prove the following claim: with high probability, $|\mathrm{Ima}(h^i)| \geqslant c_i q^a$.

The proof is by induction on i. The claim clearly holds for $i = 0$; suppose it holds for i. Let $g = (f_{v_1}, \ldots, f_{v_i}, x_{u_{i+2}}, \ldots, x_{u_a}) : [q]^n \to [q]^{a-1}$ and consider the set Z of images of g which appear frequently in the image of h^i:

$$Z := \left\{ z \in \mathrm{Ima}(g) : |(z, x_{i+1}) \in \mathrm{Ima}(h^i)| \geqslant \frac{1}{2} c_i q \right\}.$$

Then

$$|Z| \geqslant \frac{1}{2} c_i q^{a-1},$$

for otherwise, we would have

$$|\mathrm{Ima}(h^i)| < q|Z| + \left(\frac{1}{2} c_i q \right) q^{a-1} \leqslant c_i q^a.$$

Now let N be the in-neighbourhood of v_{i+1}; note that $u_{i+1} \in N$. Therefore, for each $z \in Z$, there exist at least $\frac{1}{2} c_i q$ values of x_N such that $z = g(x_N, y_{V \setminus N})$ for some $y_{V \setminus N}$; denote this set of values as X. On X, $f_{v_{i+1}}(x_N)$ is chosen uniformly at random.

Claim 18. *With probability exponentially small, $|f_{v_{i+1}}(X)| \leqslant \frac{1}{2}|X|$.*

Proof. For any $Y \subseteq [q]$ with $|Y| \leqslant \frac{1}{2}|X|$, the number of functions $\phi : X \to [q]$ whose image is contained in Y is $|Y|^{|X|} \leqslant (|X|/2)^{|X|}$. We obtain

$$
\begin{aligned}
P\left(|f_{v_{i+1}}(X)| \leqslant \frac{1}{2}|X| \right) &\leqslant \binom{q}{|X|/2} \left(\frac{|X|}{2q} \right)^{|X|} \\
&\leqslant \left(\frac{2eq}{|X|} \right)^{|X|/2} \left(\frac{|X|}{2q} \right)^{|X|} \\
&= \left(\frac{e|X|}{2q} \right)^{|X|/2} \\
&\leqslant \left(\frac{ec_i}{4} \right)^{c_i q/4}. \qquad \square
\end{aligned}
$$

Therefore, with high probability, $|f_{v_{i+1}}(X)| > \frac{1}{2}|X|$ for all $z \in Z$, and hence

$$|\mathrm{Ima}(h^{i+1})| \geqslant |Z| \frac{1}{4} c_i q \geqslant c_{i+1} q^a. \qquad \square$$

We make two remarks about Theorem 17.

Firstly, the theorem only gives an approximation of the average rank. Obtaining more detailed information seems difficult, because the average rank can vary widely with the digraph D. For instance, let us compare the complete graph with n loops $\mathring{K}_n$ to the empty graph with n loops $\mathring{L}_n$; both graphs have $\alpha_1(D) = n$. It is well known that the average rank of a function $[r] \to [r]$ tends to ϵr, where $\epsilon = 1 - e^{-1}$. Then the average rank in $\mathrm{F}[\mathring{K}_n, q]$ tends to ϵq^n, while in $\mathrm{F}[\mathring{L}_n, q]$ it tends to $\epsilon^n q^n$.

Secondly, there is no analogue of the theorem for the periodic rank. Again, let us use $\mathring{K}_n$. The average periodic rank of a function $[r] \to [r]$ tends to $\delta\sqrt{r}$, where $\delta = \sqrt{\pi/2}$ [4]. Then, the average periodic rank in $\mathrm{F}[\mathring{K}_n, q]$ tends to $\delta q^{n/2} = o(q^{\alpha_n(\mathring{K}_n)})$.

4   Maximum (periodic) rank under different update schedules

An update schedule, or simply schedule, corresponds to the way the different entities of the underlying network represented by f update their local state. More formally, a **schedule** for $f \in \mathrm{F}[D, q]$ is any $\sigma = (\sigma_1, \dots, \sigma_t)$ where $\sigma_i \subseteq V$. We denote the application of f using the schedule σ as f^σ: for any $S \subseteq V$, we let $f^{(S)}$ where

$$f_v^{(S)} = \begin{cases} f_v(x) & \text{if } v \in S, \\ x_v & \text{otherwise,} \end{cases}$$

and

$$f^\sigma = f^{\sigma_t} \circ \cdots \circ f^{\sigma_1}.$$

We now review three important classes of schedules.

1. σ is **complete** if every entity updates its local state at least once, i.e. if $\bigcup_{i=1}^{t} \sigma_i = V$.

2. σ is **block-sequential** if every entity updates its local state exactly once, i.e. if $\bigcup_{i=1}^{t} \sigma_i = V$ and $\sigma_i \cap \sigma_j = \varnothing$ for all $i \neq j$.

3. σ is **parallel** if all entities update their state once and at the same time, i.e. if $\sigma = (V)$. Clearly, $f^{(V)} = f$.

We first prove that the $\alpha_1(D)$ upper bound on the scaled rank remains valid for block-sequential schedules.

Theorem 19. *If σ is a block-sequential schedule and $f \in \mathrm{F}[D, q]$, then $\mathrm{ima}(f^\sigma) \leqslant \alpha_1(D)$.*

Proof. We use a proof technique similar to that of Theorem 9. Let $\sigma = (\sigma_1, \dots, \sigma_t)$ be a block-sequential schedule. Construct the term set Γ built on $x_1, \dots, x_n$ and the $n+1$ function symbols $f_1, \dots, f_n, g$, where f_i is d_i-ary and g is unary, uniquely defined as such.

1. The subterm graph $G_\Gamma = (V_\Gamma, E_\Gamma)$ is as follows: $V_\Gamma = V^0 \cup \cdots \cup V^t$ consists of $t+1$ copies of V, and $(u^{i-1}, v^i) \in E_\Gamma$ if either $(u, v) \in E$ and $v \in \sigma_i$ or $u = v$ and $v \notin \sigma_i$.

2. On v^i, Γ uses the function symbol f_v if $v^i \in \sigma_i$ and the function symbol g if $v^i \notin \sigma_i$.

Then it is clear that for any $\bar{f} \in \mathrm{F}(D, q)$, $\bar{f}^{\sigma}$ can be viewed as an interpretation of Γ, where g is interpreted as the identity. Therefore, $\mathrm{ima}(\bar{f}^{\sigma})$ is no more than the min-cut of Γ.

All that is left is to show that G_Γ has at most $\alpha_1(D)$ disjoint paths from V^0 to V^t. Let $P_1, \ldots, P_m$ be a family of disjoint paths starting, without loss, at vertices $1, \ldots, m$ and let $v_1, \ldots, v_m$ be the "first updated vertices" on the respective paths. Formally, let $P_i = (w_0^0, \ldots, w_t^t)$, where $w_0^0 = i$, let $a = \min\{b : w_b^b \in \sigma_b\}$ (such a always exists since σ is complete) and $v_i = w_a$. We then have $(w_0, w_1, \ldots, w_{a-1}, w_a) = (i, i, \ldots, i, v_i)$..

Then for $i \neq j$, we have: (i, v_i) and (j, v_j) are arcs in D, $i \neq j$, and $v_i \neq v_j$ (clear if v_i and v_j are in different parts of σ, otherwise if $v_i, v_j \in \sigma_a$ then because the paths are disjoint we have $v_i^a \neq v_j^a$). In other words, $(1, v_1), \ldots, (m, v_m)$ are independent arcs in D, thus $m \leqslant \alpha_1(D)$. $\qquad\square$

In particular, we can refine Corollary 6 on the presence of reversible dynamics.

Corollary 20. *For any $q \geqslant 3$, the following are equivalent:*

1. $\mathrm{F}[D, q]$ *contains a permutation of* $[q]^n$,

2. *there exist* $f \in \mathrm{F}[D, q]$ *and a block-sequential schedule* σ *such that* f^{σ} *is a permutation of* $[q]^n$,

3. *all the vertices of D can be covered by disjoint cycles.*

Problem 21. Is there an analogue of Theorem 19 for the periodic rank?

However, the maximum rank when considering any complete schedule is not bounded by $\alpha_1(D)$. In fact, the periodic rank can be much larger, as seen below. For any D and q, we denote
$$\overline{\mathrm{per}}[D, q] = \max\{\mathrm{per}(f^{\sigma}) : f \in \mathrm{F}[D, q], \sigma \text{ complete}\},$$
and $\overline{\mathrm{per}}(D, q)$ is defined similarly.

Recall that a strong component of a digraph is **trivial** if it has no cycle, or equivalently if it is a single loopless vertex. Clearly, a vertex v belongs to a cycle of D if and only if $\{v\}$ is not a trivial strong component of D. We denote the trivial strong components of D as $T_1, \ldots, T_t$ and their number as $T(D)$. We shall show that $\overline{\mathrm{per}}(D, q) \leqslant n - T(D)$. On the other hand, we will also prove that this bound is actually an equality.

Proposition 22. *For all D and $q \geqslant 2$,*

$$\overline{\mathrm{per}}(D, q) = n - T(D).$$

Proof. Let $f \in \mathrm{F}[D, q]$ and σ be a complete schedule. Then (u, v) is an arc of $\mathrm{IG}(f^{\sigma})$ only if there is a path from u to v in D. Consequently, if $\{v\}$ is a trivial strong component of D, then $\{v\}$ is a trivial strong component of $\mathrm{IG}(f^{\sigma})$. By Corollary 5, we have $\mathrm{per}(f^{\sigma}) \leqslant n - T(D)$.

Conversely, let us remove all the arcs connecting strong components of D and all the chords of any cycle in D. We obtain a new graph D' which is the disjoint union of strong chordless graphs; the trivial components $T_1, \ldots, T_t$ of D' are exactly those of D. Let $C_1, \ldots, C_k$ be a collection of cycles of D' which cover all the vertices that do not belong to a trivial component and $\sigma = (T_1, \ldots, T_t, C_1, \ldots, C_k)$. Let $f \in \mathrm{F}[D', q]$ such that

$$f_v(x) = \sum_{u \in N^-(v)} x_u \mod q,$$

where an empty sum is equal to zero and the neighbourhood is according to D'. It is easy to check that $f_v^{(C_i)}$ is a permutation for all $1 \leqslant i \leqslant k$ and hence that $\{x \in [q]^n : x_{T_1} = \ldots x_{T_t} = 0\}$ is a set of $q^{n-T(D)}$ periodic points of f^σ. $\qquad \square$

Next, by a similar argument we prove that $\overline{\mathrm{per}}(D, q)$ actually approaches $n - T(D)$.

Theorem 23. *For all D,*
$$\sup_{q \geqslant 2} \{\overline{\mathrm{per}}[D, q]\} = n - T(D).$$

Proof. Let $C_1, \ldots, C_k$ be a collection of cycles which cover all vertices belonging to a cycle, W denote the set of remaining vertices and let $\sigma = (W, C_1, \ldots, C_k)$. Let $q - 1 = 2^m$ be large enough ($m \geqslant 2^{n^2+1}$) and let α be a primitive element of $\mathrm{GF}(q-1)$. Denote the arcs in D as $e_1, \ldots, e_l$. Let $A \in \mathrm{GF}(q-1)^{n \times n}$ such that $a_{u,v} = \alpha^{2^i}$ if $(u, v) = e_i$ and $a_{u,v} = 0$ if $(u, v) \notin E$ and let $g(x) = Ax$. Now $f \in \mathrm{F}[D, q]$ is given as follows: view $[q] = \mathrm{GF}(q-1) \cup \{q-1\}$ and

$$f_w(x) = \begin{cases} 0 & \text{if } x_u \in \mathrm{GF}(q-1) \text{ for all } u \in N^-(w), \\ q-1 & \text{otherwise}, \end{cases} \quad \forall w \in W$$

$$f_v(x) = \begin{cases} g_v(x) & \text{if } x_u \in \mathrm{GF}(q-1) \text{ for all } u \in N^-(v), \\ q-1 & \text{otherwise}, \end{cases} \quad \forall v \notin W.$$

Then f acts like g on the set of states $X = \{x \in \mathrm{GF}(q-1)^n : x_W = (0, \ldots, 0)\}$; in particular, we have $f(X) \subseteq X$. We can then remove W and consider $h \in \mathrm{F}[D \setminus W, q-1]$ such that $h_v(x_{V \setminus W}) = g_v(x_{V \setminus W}, 0_W)$ for all $v \notin W$ instead. All we need to prove is that $h^{(C_1, \ldots, C_k)}$ is a permutation of $\mathrm{GF}(q-1)^{n-T(D)}$.

Denote the square submatrix of A induced by the vertices of C_j as A_j. Then we remark that $\det(A_j) \neq 0$ for any $1 \leqslant j \leqslant k$. Indeed, let $K_1, \ldots, K_l$ denote all the hamiltonian cycles in the subgraph induced by the vertices of C_j (and without loss, $K_1 = C_j$). For any $1 \leqslant a \leqslant l$, let $S(a) = \sum_{e_i \in K_l} 2^i$. We note that $S(1), \ldots, S(l)$ are all distinct, hence $\alpha^{S(1)}, \ldots, \alpha^{S(l)}$ are all linearly independent (when viewed as vectors over $\mathrm{GF}(2)$) and

$$\det(A_j) = \sum_{a=1}^{l} \alpha^{S(a)} \neq 0.$$

Now $h^{(C_j)}(x) = A'_j x$, where

$$A'_j = \left(\begin{array}{c|c} A_j & B_j \\ \hline 0 & I \end{array} \right),$$

where $(A_j | B_j)$ are the rows of A corresponding to C_j and I is the identity matrix of order $n - T(D) - |C_j|$. Since A_j is nonsingular, so is A'_j. Hence $h^{(C_j)}$ is a permutation of $\mathrm{GF}(q-1)^{n-T(D)}$, and by composition, so is $h^{(C_1,\dots,C_k)}$. $\qquad \square$

If W is empty, then we can simplify the proof of Theorem 23 and work with $\mathrm{GF}(q)^n$ instead of $\mathrm{GF}(q-1)^{n-T(D)}$ (this time $q = 2^p$), hence we obtain a permutation. This yields the following corollary on the presence of reversible dynamics.

Corollary 24. *There exist q, σ and $f \in \mathrm{F}[D, q]$ such that f^σ is a permutation of $[q]^n$ if and only if all the vertices of D belong to a cycle.*

The theorem brings the following natural question.

Problem 25. Is there an analogue of Theorem 23 for the rank?

Acknowledgements

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