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Dynamics of neural networks over undirected graphs

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ABSTRACT

In this paper we study the dynamical behavior of neural networks such that their interconnections are the incidence matrix of an undirected finite graph $G = (V, E)$ (i.e., the weights belong to $\{0, 1\}$). The network may be updated synchronously (every node is updated at the same time), sequentially (nodes are updated one by one in a prescribed order) or in a block-sequential way (a mixture of the previous schemes). We characterize completely the attractors (fixed points or cycles). More precisely, we establish the convergence to fixed points related to a parameter $\alpha(G)$, taking into account the number of loops, edges, vertices as well as the minimum number of edges to remove from E in order to obtain a maximum bipartite graph. Roughly, $\alpha(G') < 0$ for any G' subgraph of G implies the convergence to fixed points. Otherwise, cycles appear. Actually, for very simple networks (majority functions updated in a block-sequential scheme such that each block is of minimum cardinality two) we exhibit cycles with non-polynomial periods.

1. Introduction

Symmetric neural networks were first studied in the context of the majority functions and generalizations in Goles and Olivos (1980) as well as the application to associative memories in Hopfield (1982). The network's dynamics on undirected graphs have been widely studied to model situations in physics, biology, sociology, as we will review later on. This model has been included as an important case of neural networks for associative memories (Hopfield networks), percolation problems, infection, segregation, and other social problems, therefore, there exists now a vast community interested both in theoretical results as well as applications of symmetric neural networks.

The principal updating modes considered in these networks are the parallel, the asynchronous, and the sequential one. For the parallel updating scheme it was proved that any symmetric neural network converges only to fixed points or two cycles (Goles & Olivos, 1980). The fixed point convergence for symmetric networks, with non negative loops, updated sequentially was proved in Goles (1982). The unique general result about arbitrary block-sequential updates was established in Goles-Chacc, Fogelman-Soulie, and Pellegrin (1985). Convergence results and generalizations can be seen in Goles and Martínez (1990), where the class of Heaviside functions is extended to the positive or cyclically-monotone functions. A general approach of an energy operator for this kind of networks can be seen in Goles (2003) and Goles and Martínez (1990). Further, in Cosnard and Goles (1997) a characterization of networks which admits an energy operator is done (roughly speaking energy operators are associated to quasi-symmetric matrices). The first studies related to different updating schemes appeared in the context of Boolean networks for the parallel and sequential updating schemes (Robert, 1986). More recently, such studies have been developed in Aracena, Goles, Moreira, and Salinas (2009) and Montalva (2011) where equivalent dynamics classes were established for different block-sequential updating schemes over Boolean networks. In Noual (2012) some theoretical results as well as biological considerations related with different updating schemes were developed. More recently, networks driven by Heaviside local functions have been used in statistical physics and social dynamics, like voter models (Castellano, Fortunato, & Loretto, 2009) and the Schelling's segregation dynamics (Goles-Domic, Goles, & Rica, 2011). In biology, applications have been developed in the framework of regulatory networks. In this context, a general overview about the application of Boolean networks can be seen in Bornholdt (2008). More concerned with this paper, Heaviside functions have been used to model the yeast cell cycle (Davidich & Bornholdt, 2008; Li, Long, Lu, Ouyang, & Tang, 2004). From these works we characterized the network's dynamics under every deterministic updating scheme (Goles, Montalva,

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& Ruz, 2013). In a similar way, the complete deterministic dynamic for the mammalian cell cycle network has been analyzed in Ruz, Goles, Montalva, and Fogel (2014). Further, for the specific threshold class of disjunctive networks, the dynamical behavior was characterized for arbitrary directed graphs (non necessarily symmetric) and defined complexity classes related with the obtained attractors (fixed points or cycles) (Goles & Noual, 2012). The relationship between the positive and negative circuits of the connection graph and the fixed points of discrete neural networks is studied in Aracena, Demongeot, and Goles (2004), obtaining necessary and sufficient conditions for the existence of fixed points in discrete neural networks. Recently, it has been studied and characterized some decision problems related with whether or not an arbitrary vertex of a network may change its state (from 0 to 1) for the majority networks (a particular case of a Heaviside function) under different updates (Goles & Montealegre-Barba, in press-a; Goles, Montealegre-Barba, & Todinca, 2013). In relation to applications using Hopfield networks, Maetschke and Ragan (2014) constructed Hopfield networks from cancer expression data and then used them to show that the resulting attractors correspond to cancer subtypes. The effect of removing the links of fully connected Hopfield networks and then analyzing the convergence to a designated attractor is presented in Anafi and Bates (2010). The results from that study were used to speculate about human diseases and how they may represent biological networks that converge to an abnormal attractor. In the context of machine learning, it has been shown that restricted Boltzmann machines, typically for classification and feature detection, are thermodynamically equivalent to a Hopfield network (Barra, Bernacchia, Santucci, & Contucci, 2012). A Hopfield neural network in Pajares, Guijarro, and Ribeiro (2010) is used to combine simple classifiers for classifying natural textures in images.

In this work we focus on networks such that their interconnections correspond to the incidence matrix of a finite undirected graph $G = (V, E)$, i.e., the matrix's entries, w_{ij}, are 0's or 1's according to whether the edge $(j, i) \in E$. In this context, we characterize completely, for any updating scheme, the attractors of such networks.

The paper is organized as follows. Section 2 gives some definitions as well as theorems that will be useful throughout the paper. In Section 3 we introduce a parameter depending on the graph structure, $\alpha(G)$, such that the parallel updating scheme converges to fixed points if and only if $\alpha(G') < 0$ for any subgraph G' of G. Otherwise, cycles appear. In particular we prove that it is enough to have in the graph two connected vertices without loops in order to find a subgraph G' such that $\alpha(G') \geq 0$ or, equivalently to have a two-cycle. Further, we characterize completely the attractor's behavior for some classes of graphs like, forest, trees, bipartite and complete graphs with or without loops. We extend the previous result to any updating scheme over the network by considering for the analysis the subgraphs associated to each partition of the updating scheme. In this context we get as corollaries some convergence results for block-sequential updating schemes, taking into account the cardinality of each block. Roughly, by assuming $diag(G) = \vec{1}$, we conclude that for partitions of size 3 the dynamics converge to fixed points. We also obtain a slightly similar convergence result by considering also partitions of size 4 and 5, where some specific subgraphs are forbidden.

In Section 4 we proved that there exist very simple block-sequential schemes (every partition composed of two connected vertices without loops) under majority local functions such that cycles with non-polynomial periods appear. The same construction allows to establish a similar non-polynomial behavior for the transient time. Comments on the range of the energy operator and how it relates to directed graphs as well as an example that illustrates the theorems developed in this paper are presented in Section 5. Finally, in Section 6, we present the general conclusions as well as some comments related to the complexity of the computation of the parameter $\alpha(G)$.

2. Background

Let us consider an integer $n \times n$ symmetric matrix $W = (w_{ij})$, $x \in \{0, 1\}^n$, a threshold vector $\Theta \in \mathbb{Z}$ and the set of n Heaviside functions:

$$f_i(x_1, \dots, x_n) = \mathbf{H}\left(\sum_{j=1}^{n} w_{ij}x_j - \theta_i\right) \quad i \in \{1, \dots, n\} \tag{1}$$

where

$$\mathbf{H}(u) = \begin{cases} 1 & \text{if } u \geq 0 \\ 0 & \text{if } u < 0. \end{cases}$$

Since the entries are integers, it is always possible to determine equivalent functions with thresholds $\theta_i = p_i + 1/2$, $p_i \in \mathbb{Z}$, such that $|\sum w_{ij}x_j - \theta_i| \geq 1/2$, $\forall x \in \{0, 1\}^n$, $\forall i = 1 \dots n$. We associate a dynamic to the previous functions by considering a partition $\{\{I_1\}, \dots, \{I_p\}\}$ of the set $V = \{1, \dots, n\}$ such that the nodes of the network are updated one by one following the partition's order. So, when I_l is updated; we consider the new values of the previous nodes belonging to $\cup_{j \leq l-1} I_j$ and the old values for the nodes in $\cup_{j \geq l} I_j$. We call this procedure the block-sequential update. As two important particular updates we have the parallel (or synchronous) update, when $I_1 = \{1, \dots, n\}$ is the unique block, i.e., every node is updated at the same time. When the nodes are iterated one by one in a prescribed order given by a partition $\{\{\sigma_i\}\}_{i=1}^{n}$, where $\sigma = (\sigma_1 \dots \sigma_n)$ is a permutation of the set of nodes, we have the sequential update. Since a partition can be constructed for every subset of V, there is an exponential number of updates.

We define a neural network as a triple $N = (W, \Theta, \tau)$ where W is an integer symmetric matrix, Θ the threshold vector and τ the updating scheme. It was proved in Goles (1982) and Goles and Olivos (1980) that the parallel update on symmetric neural networks always converges to bounded limit cycles, more precisely, fixed points or cycles with period 2. It was established also a related convergence result for the sequential updating scheme (Goles, 1982). The most general result about block-sequential updates and fixed point behavior is Theorem 2.1. We will sketch its proof in order to introduce an energy functional that will be useful in the paper.

Theorem 2.1 (Goles-Chacc et al., 1985). *Let us consider the block-sequential updating scheme $\tau = \{\{I_1\}, \dots, \{I_p\}\}$ and the symmetric neural network $N = (W, \Theta, \tau)$. Let $W(I_k)$ be the sub-matrix associated to the block I_k of the partition. Then, if for every $k \in \{1, \dots, p\}$, $W(I_k)$ is non-negative definite, then the network admits only fixed points.*

Proof. Let us introduce the following operator:

$$E(x) = -\frac{1}{2}\sum_{i=1}^{n} x_i \sum_{j=1}^{n} w_{ij}x_j + \sum_{i=1}^{n} \theta_i x_i. \tag{2}$$

Let us consider that we update the kth block from the configurations $x = (x_1, \dots, x_n)$, hence $x'_i = x_i$ $\forall i \notin I_k$ and $x'_i = \mathbf{H}(\sum_{j=1}^{n} w_{ij}x_j - \theta_i)$ $\forall i \in I_k$. Since W is symmetric:

$$\Delta E = E(x') - E(x) = -\sum_{i \in I_k}(x'_i - x_i)\left(\sum_{j=1}^{n} w_{ij}x_j - \theta_i\right) - \frac{1}{2}\sum_{i \in I_k}(x'_i - x_i)\sum_{j \in I_k} w_{ij}(x'_j - x_j) \tag{3}$$

therefore,

$$\Delta E = \sum_{i \in I_k} \delta_i - \frac{1}{2} y^t W(I_k) y \tag{4}$$

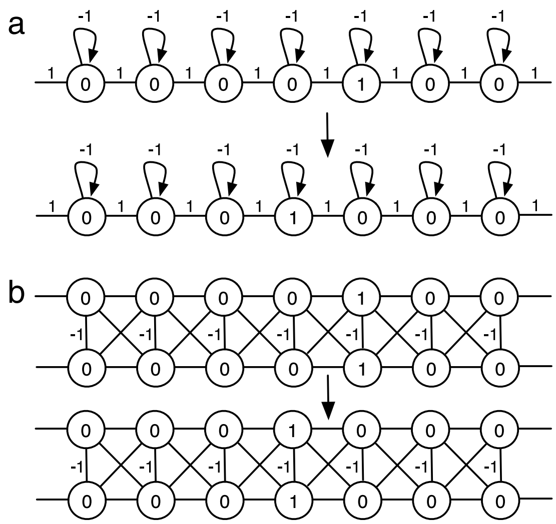

Fig. 1. (a) n-periodic dynamics for the sequential update $\{\{1\}, \ldots, \{n\}\}$. (b) n-periodic dynamics for a block sequential update $\{\{1_u, 1_d\}, \ldots, \{i_u, i_d\}, \ldots, \{n_u, n_d\}\}$ where i_u codes the upper sites and i_d the down sites.

where $y = (x' - x) \in \{-1, 0, 1\}$ and $\delta_i = -(x'_i - x_i)(\sum_{j=1}^{n} w_{ij}x_j - \theta_i)$. Suppose that $x'_i \neq x_i$ then $\delta_i \leq 0$. Furthermore, $\theta_i = p_i + 1/2 \Longrightarrow \delta_i \leq -1/2$. So, $x' \neq x$ implies $\sum_{i \in I_k} \delta_i < 0$. Since $W(I_k)$ is non-negative definite then $y^t W(I_k) y \geq 0$, $\forall y \in \{-1, 0, 1\}^n$. So $\Delta E < 0$, which implies directly that the network converges to fixed points. □

As a corollary we have:

Corollary 2.1. (a) *If we consider the parallel update $P = \{\{1, \ldots, n\}\}$, then if matrix W is non negative-definite the neural network $N = (W, \Theta, P)$ admits only fixed points (two-cycles disappear).* (b) *If we consider $diag(W) \geq \vec{0}$ and a sequential updating scheme, $s = \{\{\sigma_i\}\}_{i=1}^{n}$ then the neural network $N = (W, \Theta, s)$ has only fixed points.*

Proof. (a) For the parallel update there exists only one block $I_1 = \{1, \ldots, n\}$, so $W(I_1) = W$ and the result is direct from Theorem 2.1. (b) In this case $W(I_i) = (w_{\sigma_i \sigma_i})$, so $w_{\sigma_i \sigma_i} \geq 0 \iff W(I_i)$ non-negative definite; $y_{\sigma_i} w_{\sigma_i \sigma_i} y_{\sigma_i} \geq 0$. □

Remark 2.1. When matrix W admits blocks such that some $W(I_k)$ are not longer non-negative definite, non bounded cycles may appear.

Let us consider, for $n \geqslant 3$, the network with thresholds $\theta_i = \frac{1}{2}$ and the matrix W:

$$w_{ij} = \begin{cases} 1 & \text{if } |i - j| = 1 \\ 1 & \text{if } (i = n \text{ and } j = 1) \text{ or } (i = 1 \text{ and } j = n) \\ -1 & \text{if } i = j \\ 0 & \text{otherwise.} \end{cases}$$

By taking the sequential update $\{\{1\}, \ldots, \{n\}\}$, the vector $x = (0, 1, 0, \ldots, 0)$ belongs to a cycle of period n (see Fig. 1(a)). Clearly, $diag(W) = -\vec{1} < \vec{0}$, so the hypothesis of the previous corollary is not longer true. Furthermore, it happens also for other block sequential partitions. Consider for instance the network given in Fig. 1(b), updated under the block-sequential partition $\{\{1_u, 1_d\}, \ldots, \{i_u, i_d\}, \ldots, \{n_u, n_d\}\}$. Hence the configuration:

$$\begin{pmatrix} x_{1u} & x_{2u} & \cdots & x_{nu} \\ x_{1d} & x_{2d} & \cdots & x_{nd} \end{pmatrix} = \begin{pmatrix} 0 & 1 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \end{pmatrix}$$

belongs to a cycle of period n. In this case the associated matrix to each partition is:

$$W(\{k_u, k_d\}) = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

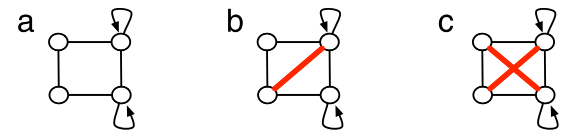

Fig. 2. (a) Bipartite graph, $p = 0$ and $d = 2$ (b) $p = 1$ and $d = 2$ (c) $p = 2$ and $d = 2$. In red the edges to be removed to obtain a maximum bipartite graph. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

which is no longer non-negative-definite. It is important to remark that in both previous examples the matrices have some negative entries. But we will see that the non-bounded periodic behavior remains even when the matrix entries belong to the set $\{0, 1\}$, i.e., when the connections correspond to the incidence matrix of an undirected graph, situation that we will study with further details in this paper.

3. Convergence to fixed points for undirected graphs

In this section we will study the convergence for neural networks defined by the incidence matrix of graphs (0's and 1's entries). Since we have to study each block (so, its incidence matrix) of the partition, we will first establish conditions and results for only one block, i.e., the network updated synchronously. After that, we will apply the results obtained for one block to every partition in the whole block-sequential updating scheme. In fact, given a incidence matrix W of an undirected graph G, as we saw in the previous section, there are large families such that W is no longer non-negative definite. However, W could not be non-negative definite but in spite of that, the functional $\Delta E = \sum_{i \in I_k} \delta_i - \frac{1}{2} y^t W(I_k) y$ continues to be negative (E always decreases) which implies only fixed points for the synchronous update. For instance, let us consider the network: $f_1(x_1, x_2) = \mathbf{H}(x_1 + x_2 - \theta_1)$; $f_2(x_1, x_2) = \mathbf{H}(x_1 - \theta_2)$; $\theta_i \in \mathbb{Q}$, for $i = 1, 2$. Its incidence matrix, $W = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}$, is not non-negative definite. In fact, $(1, -1) \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = -1 < 0$. But, as we will see, for any thresholds, the synchronous update converges to fixed points. Below we will study this kind of situations in a general framework.

Let $G = (V, E)$ be an undirected graph, $|V| = n$ and $|E| = m$, with $0 \leq d \leq n$ loops. We denote $V_i = \{j \in V / (i, j) \in E\}$ the neighborhood of vertex $i \in V$. As we saw in the previous section (Corollary 2.1(b)) non-negative loops are enough for the convergence of the sequential updating scheme. In this section we considered at each vertex the possibility to have a loop, i.e., $w_{aa} = 1 \Leftrightarrow (a, a) \in E$, (0, otherwise). Let us consider the quantity

$$\alpha(G) = -n - d + 2m - 4p, \tag{5}$$

where d is the number of loops (circuits of length 1) and p is the minimum number of edges to remove in G, without considering loops, in order to obtain a maximum bipartite graph (see Fig. 2). We will say that G' is a subgraph of G, (we denote $G' \subseteq G$) if and only if $V' \subsetneq V$ and $E' \subsetneq E$ the set of edges in E associated to the subset of vertices V'. That is to say, every subgraph we will consider is constructed by removing vertices as well as the edges connected to these vertices. In this context the main result of this section is the following:

Theorem 3.1. *Let us consider an undirected graph $G = (V, E)$, $W = W(G)$ its incidence matrix and a neural network updated in parallel, $N = (W, \Theta, \{1, \ldots, n\})$, then: if $\alpha(G') < 0$, $\forall G' \subseteq G$, then the network admits only fixed points for any threshold vector. Otherwise, if there exists $G' \subseteq G$ such that $\alpha(G') \geq 0$, then there exist threshold vectors such that cycles with period 2 appear.*

To prove the previous theorem we will first develop some tools and lemmas. Then, we will give some corollaries which establish the classes of graphs such that cycles appear.

Let us consider the transition from x to x' for the parallel updating scheme and that each vertex changes its value (i.e., $x_i' \neq x_i$ or $y_i = (x_i' - x_i) \in \{-1, 1\}$ for any $i \in V$). Also, let us consider the energy difference established in (4):

$$\Delta E = \sum_{i=1}^{n} \delta_i - \frac{1}{2} y^t W y \tag{6}$$

where

$$\delta_i = -(x_i' - x_i) \left(\sum_{j=1}^{n} w_{ij} x_j - \theta_i \right).$$

Recall that the w_{ij} are integers, therefore, it is always possible to determine equivalent functions with thresholds $\theta_i = p_i + 1/2,\ p_i \in \mathbb{Z}$, such that $|\sum w_{ij} x_j - \theta_i| \geq 1/2,\ \forall x \in \{0, 1\}^n,\ \forall i = 1 \ldots n$. Also, we know that $x_i' \neq x_i \Longrightarrow \delta_i \leq -1/2$. Since every node changes its value, by considering the number of loops, d, in G we have:

$$\Delta E \leq -\frac{n}{2} - \frac{1}{2} \left\{ d + y^t (W^* y) \right\} \tag{7}$$

where $diag(W^*) = \vec{0}$. In order to analyze if ΔE decreases, we have to study the quadratic form

$$\varphi(y) = -\frac{1}{2} y^t W^* y; \quad y \in \{-1, 1\}^n. \tag{8}$$

From where we can obtain

$$\max_{z \in \{-1,1\}^n} \varphi(z) = m - 2p. \tag{9}$$

The proof of (9) appears in Appendix A. So, from (9), if $x_i' \neq x_i$, $\forall i \in V$:

$$\Delta E \leq -\frac{n}{2} - \frac{d}{2} + \varphi(y) \leq -\frac{n}{2} - \frac{d}{2} + m - 2p. \tag{10}$$

From (10) we conclude: If $x_i' \neq x_i,\ \forall i \in V$, then:

$$-\frac{n}{2} - \frac{d}{2} + m - 2p < 0 \Longrightarrow \Delta E < 0$$

which is equivalent to: $\alpha(G) < 0 \Longrightarrow \Delta E < 0$. The previous analysis considered that each vertex changes its value. The same approach may be used for the general case. Suppose that from the transition from x to x' some vertices remain constant at state 0 or 1, which is equivalent to consider some $y_i = 0$. In this situation we consider the subgraph G', where $V' = V \setminus \{i \in V / y_i = 0\}$. Clearly, over this subgraph, every node changes its value, and the previous analysis holds over G'. From that we may formulate the following proposition:

Proposition 3.1. *If $\alpha(G') < 0,\ \forall G' \subseteq G$ then the neural network $N = (W = W(G), \Theta, \{1, \ldots, n\})$ admits only fixed points.*

Proof. Let us consider x' the configuration obtained from the parallel update over x. Let $X = \{i / x_i = x_i'\}$ be the set of nodes of constant states. Suppose $x \neq x'$, then $X \subsetneq V$. Let the subgraph $G' = (V \setminus X, E')$. Clearly in G' every vertex changes its value, then by applying previous analysis over G': $\Delta E \leq \frac{\alpha(G')}{2}$ so from the hypothesis we conclude that $\Delta E < 0$, then the network converges to fixed points. □

Remark 3.1. In general $\alpha(G) < 0 \not\Longrightarrow \alpha(G') < 0$ for every $G' \subseteq G$.

For instance, let us consider the graph in Fig. 3. We have for $G,\ d = 3,\ p = 2,\ n = 6,\ m = 8$. So $\alpha(G) = -1 < 0$. Suppose we remove vertices $\{2, 5, 6\}$. We obtain the subgraph G' from Fig. 3, such that, $\alpha(G') = 1 > 0$. Since we are working on undirected graphs (matrix W being symmetric), we know that the parallel update converges to fixed points or two-cycles (Goles & Olivos, 1980; Goles-Chacc et al., 1985). Let us see, for incidence matrices $W(G)$, if we may construct *total* two-cycles, i.e., those such that every vertex changes its value. Let us consider a set $X = \{v_1, \ldots, v_p\} \subsetneq E$ which

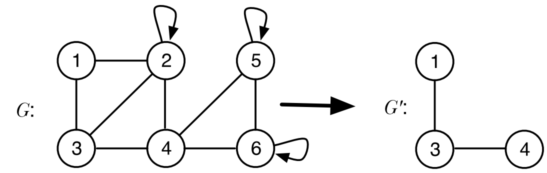

Fig. 3. Graphs G and G' obtained by considering $y_2 = y_5 = y_6 = 0$.

realizes the minimum number of edges to remove to obtain a maximum bipartite graph. So, for each vertex $i \in V$, we have two kinds of vertices, O_i: vertices such that their incident edges to vertex i belong to X, and P_i: vertices such that their incident edges belong to $E \setminus X$. So $V_i = O_i \bigcup P_i$. Of course, for some vertices, the set O_i may be empty. Let configurations x and x' be such that they are different for each vertex and are constructed such that for every edge $(i, j) \in E \setminus X,\ y_i \neq y_j$ (i.e., $x_i \neq x_j$ and $x_i' \neq x_j'$). Moreover, for the edges belonging to X, their vertices have the same value. Now, let us see the possibility to construct a *total* two cycle. For that, it is enough to analyze the existence of thresholds for the Heaviside function realizing the cycle in every vertex. We have two cases to consider:

Case a: (*Vertices with loops*): Clearly, if the vertex $i \in V$ belongs to an edge $v = (i, \beta) \in X$, then $x_i = x_\beta$. So if we have for the parallel updating: $x \leftrightarrow x'$, such that $x_i \neq x_i',\ \forall i \in V : |P_i| - \theta_i \geq 0$ and $|O_i| + 1 - \theta_i < 0$. So, $|P_i| \geq \theta_i$ and $|O_i| + 2 \leq \theta_i$, then

$$|P_i| \geq |O_i| + 2 \quad \forall i \in V, \text{ with loops.} \tag{11}$$

Case b: (*Vertices without loops*). Similarly, we have:

$$|P_i| \geq |O_i| + 1 \quad \forall i \in V, \text{ without loops.} \tag{12}$$

If such conditions hold for some realization $X = \{v_1, \ldots, v_p\}$ then the parallel updating admits previous *total* two-cycle.

Remark 3.2. By adding conditions (11) and (12) over the graph, we obtain:

$$\sum_{i \in V} |P_i| \geq \sum_{i \in V} |O_i| + |V| + d$$

therefore,

$$2(m - p) \geq 2p + n + d$$
$$\Rightarrow \alpha(G) = -n - d + 2m - 4p \geq 0.$$

So, a necessary condition to obtain a *total* two-cycle is $\alpha(G) \geq 0$. But it is not sufficient. In Fig. 4 we exhibit a graph such that every realization of the set X does not satisfy conditions (11) and (12), so it does not admit a *total* two-cycle. Let us consider the graph in Fig. 4(a). Clearly, $\alpha(G) = 8 > 0$ and $p = 1$. It is easy to see that, for any set X which realizes a maximum bipartite graph, conditions (11) and (12) do not hold (see Fig. 4(b)). For instance, consider $X = \{v_2 = (2, 3)\}$. We have $O_2 = \{3\}$ and $P_2 = \{1\}$, so condition (11) does not hold, so there is not a *total* two-cycle. But, by considering an OR for vertex 1, the majority rule for the rest of the vertices, and by setting vertex 2 at value zero, we obtain the following two-cycle $x = (x_1, \ldots, x_9) = (0, 0, 1, 0, 1, 0, 1, 0, 1) \leftrightarrow (1, 0, 0, 1, 0, 1, 0, 1, 0)$ (Fig. 4(c)) which is equivalent to consider the subgraph $G' = (V \setminus \{2\}, E \setminus \{(1, 2), (2, 3)\})$ (see Fig. 4(d)).

The other interesting case to consider in order to analyze the possibility to have *total* two-cycles is $p = 0$, i.e., bipartite graphs. In this context, conditions (11) and (12) can be interpreted as follows:

Lemma 3.1. *Given a bipartite graph without isolated vertices or vertices with a loop with only one neighbor, then it admits a total two-cycle.*

Proof. Since G is bipartite, for any $i \in V,\ O_i = \emptyset$. So, conditions (11) and (12) are the following: $|V_i| \geq 2$ for vertices with loops and $|V_i| \geq 1$, otherwise. □

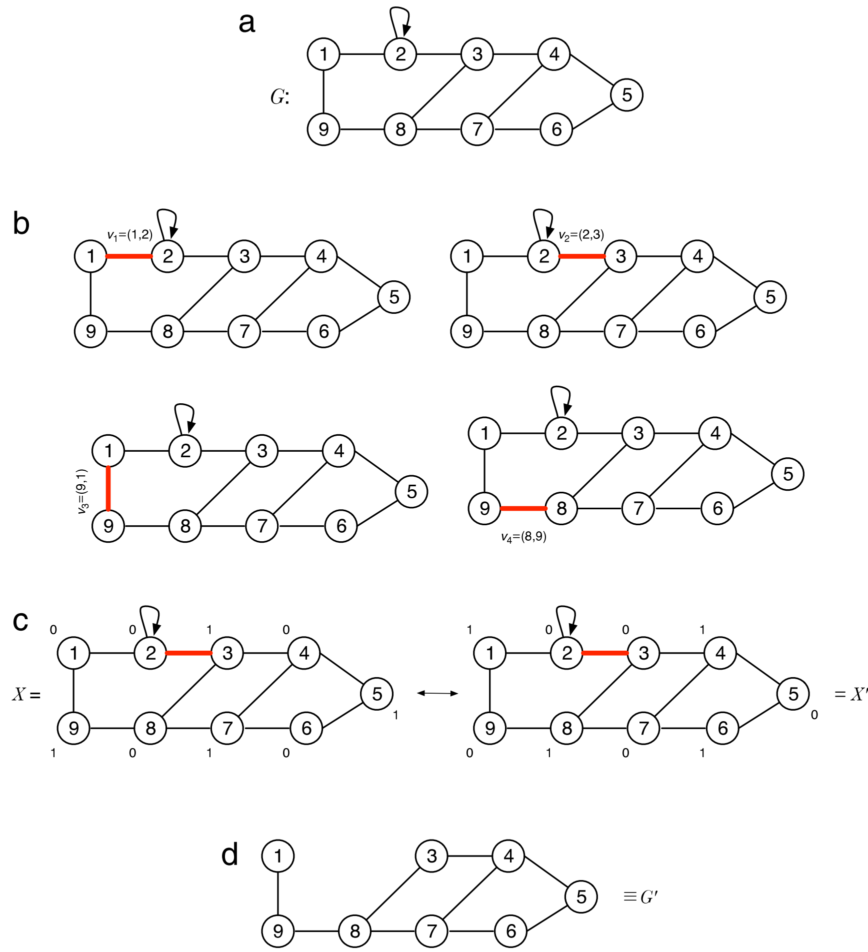

Fig. 4. (a) A graph with $p = 1$ and $\alpha(G) = 8 > 0$. (b) The four realization of a bipartite graph by dropping the set $\{v_1\}$ or $\{v_2\}$ or $\{v_3\}$ or $\{v_4\}$. (c) The two-cycle for the parallel update for $X = \{v_2\}$, such that the second vertex remains constant ($x_2 = 0$) and the Heaviside function for vertex 1 is an OR and the Heaviside function for the rest of the vertices is the majority. (d) $G' \subseteq G$ when $x_2 = 0$ (constant).

Also related to the existence of two-cycles is the appearance of positive loops, which seems important in order to "freeze" the dynamics of the network (convergence to fixed points). Actually, it is enough to have two connected vertices without loops in order to obtain two-cycles:

Proposition 3.2. *For any undirected graph $G = (V, E)$ such that it admits at least two connected vertices without loops then there exists $G' \subseteq G$ such that $\alpha(G') \geq 0$ as well as a threshold vector Θ such that the neural network $N = (W(G), \Theta, \{1, \ldots, n\})$ (i.e., updated in parallel) admits two-cycles.*

Proof. Let us consider two connected vertices $a, b \in V$ and a minimum path $P = (V(P) = \{a = v_1, \ldots, v_q = b\}, E(P) = \{(v_1, v_2), \ldots, (v_{q-1}, v_q)\})$, clearly, $P \subseteq G$ and $\alpha(P) = -q - d(P) + 2(q-1)$, where $d(P)$ is the number of loops in P, since vertices a and b do not have loops, $d(P) \leq q-2$ then $\alpha(P) \geq 0$, which proves the first assertion. Taking the same subgraph P, let us consider the neural network such that for any vertex $i \in V(P)$:

$$f_a(x) = \mathbf{H}\left(x_{v_2} + \sum_{j \in V \setminus V(P)} w_{aj} x_j - \frac{1}{2}\right)$$

$$f_{v_i}(x) = \mathbf{H}\left(x_{v_{i-1}} + \sum_{j \in V \setminus V(P)} w_{v_i j} x_j + w_{v_i v_i} x_{v_i} + x_{v_{i+1}} - \frac{3}{2}\right) \quad \text{for } i \in \{2, \ldots, q-1\}$$

$$f_b(x) = \mathbf{H}\left(x_{v_{q-1}} + \sum_{j \in V \setminus V(P)} w_{bj} x_j - \frac{1}{2}\right).$$

For vertices in $V \setminus V(P)$ we take high enough thresholds in order for these vertices to remain constant at value 0. So we have the two cycle $(x_{v_1}, \ldots, x_{v_q}, x_{V \setminus V(P)}) = (1, 0, 1, 0, \ldots, \vec{0}) \longleftrightarrow (0, 1, 0, 1, \ldots, \vec{0})$. $\square$

Remark 3.3. It is direct from the previous proposition that for a connected component of size q of a given graph, the number of loops $d \leq q - 2$ implies two cycles.

Proposition 3.3. *Suppose $\alpha(G) \geq 0$ such that one of the conditions (11), (12) do not hold, then there exists $G' \subseteq G$, such that $\alpha(G') \geq 0$.*

Proof. Let us consider first $n \leq 4$. In this case, the number of connected graphs (without loops) for two vertices is one, for three vertices is two, and for four vertices is six. If we consider loops, then for each of these graphs there are 2^n ways to place the loops (from no vertices with loops up to all the vertices with loops). If we analyze these graphs, and only select the ones such that $\alpha(G) \geq 0$ and properties (11), (12) do not hold, then, the remaining graphs that satisfy the previous conditions are shown in Fig. 5. Additionally, for each graph in Fig. 5, there exists $G' \subseteq G$, such that $\alpha(G') \geq 0$ and that satisfies properties (11), (12). Therefore, the theorem is true for $n \leq 4$.

Suppose now $n > 4$ and condition (11) does not hold, so there exists $c \in V$ such that $(c, c) \in E$ such that:

$$|P_c| < |O_c| + 2 \iff |P_c| \leq |O_c| + 1. \quad (13)$$

Let us consider first $O_c = \emptyset$, i.e., vertex c is not connected to the set X. In this case we have $|V_c| = |P_c| \leq 1$. So, by considering G', the

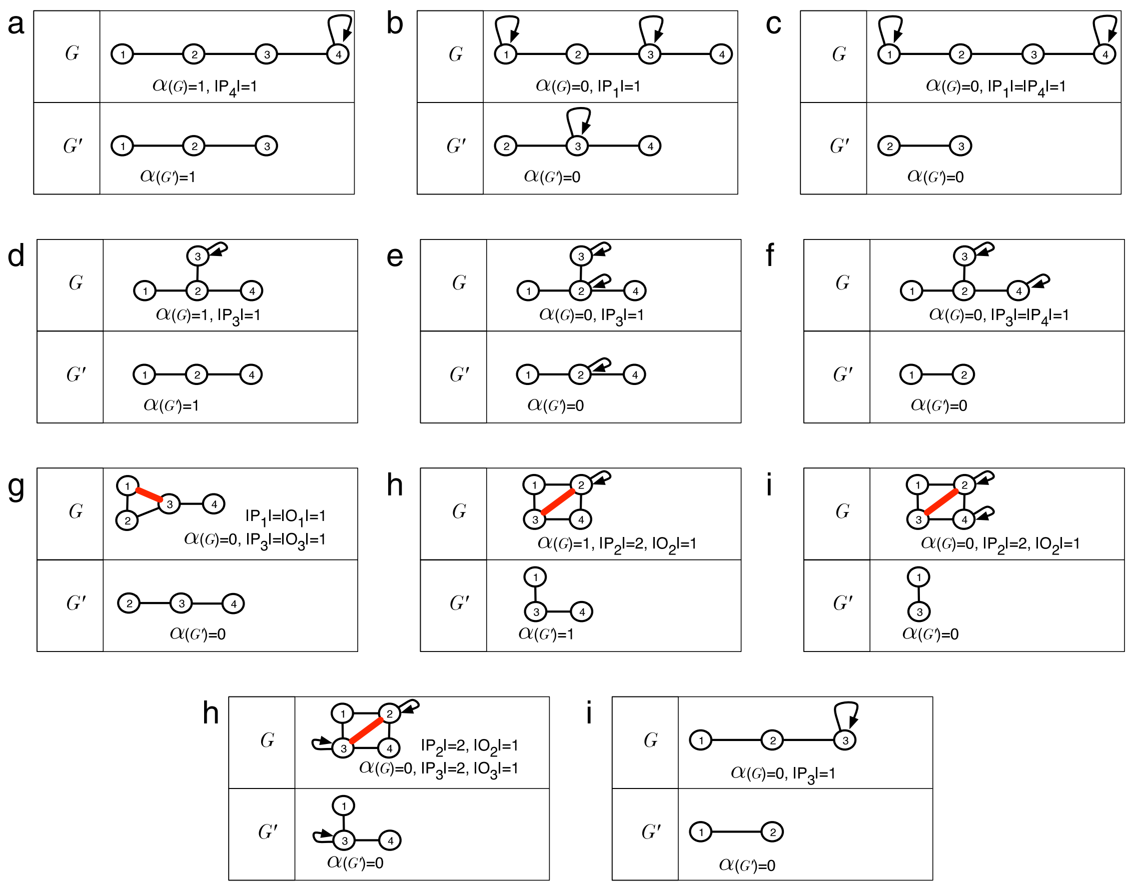

Fig. 5. Every connected graph with $|V| \leq 4$ such that $\alpha(G) \geq 0$ and conditions (11) and (12) do not hold. The graph G' is a subgraph such that $\alpha(G') \geq 0$ and conditions (11) and (12) are satisfied. The thicker edges (red) are the edges that can be removed to obtain a maximum bipartite graph. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

subgraph of G obtained by removing vertex c, we have

$$\alpha(G') = -(n-1) - (d-1) + 2(m - |V_c|) - 4p \geq \alpha(G) \geq 0$$

which proves the property. Let us suppose now that $O_c \neq \emptyset$. As in the previous case let us consider the subgraph G' by removing vertex c. We have two cases to consider: $|V_c| = 2q$ (even) or $|V_c| = 2q+1$ (odd). For $|V_c| = 2q$, from (13) we have $|P_c| \leq q$ hence $|O_c| = |V_c| - |P_c| \geq q = \lfloor \frac{|V_c|}{2} \rfloor$. Suppose now $|V_c| = 2q+1$ so (from (13)) $|P_c| \leq q+1$ hence $|O_c| \geq |V_c| - q - 1 = q = \lfloor \frac{|V_c|}{2} \rfloor$. Therefore, in both cases $|O_c| \geq \lfloor \frac{|V_c|}{2} \rfloor$. Now let us compute α:

$$\alpha(G') = -(n-1) - (d-1) + 2(m - |V_c|) - 4p'$$

but

$$p' \leq p - |O_c|$$

hence

$$\alpha(G') \geq -n - d + 2 + 2m - 2|V_c| - 4p + 4\left\lfloor \frac{|V_c|}{2} \right\rfloor \geq -n - d + 2m - 4p - 2(2q+1) + 4q + 2 = \alpha(G) \geq 0.$$

Assume now condition (12) does not hold: $c \in V$ such that $(c, c) \notin E$ and $|P_c| < |O_c| + 1 \Leftrightarrow |P_c| \leq |O_c|$. If $O_c = \emptyset$ then $|V_c| = |P_c| = 0$, i.e., the vertex c is isolated then by removing it we obtain $\alpha(G') = \alpha(G) + 1 \geq 0$. Let us consider $O_c \neq \emptyset$. Similar to the previous analysis, we have for $|V| = 2q$, that $|P_c| \leq q$ then $|O_c| \geq q$. For $|V_c| = 2q+1$, then $|P_c| \leq q$ hence $|O_c| \geq q+1$, so:

$$\alpha(G') = -(n-1) - d + 2(m - |V_c|) - 4p'$$

where

$$p' \leq p - |O_c|$$

hence

$$\alpha(G') \geq -n - d + 2m + 1 - 2|V_c| - 4p + 4|O_c| \geq -n - d + 2m - 4p + 1 = \alpha(G) + 1 \geq 0. \quad \square$$

Now we have the tools in order to prove Theorem 3.1:

Proof. If $\alpha(G') < 0$, $\forall G' \subseteq G$, the result is direct from (9). Suppose now there exists $G' \subseteq G$ such that $\alpha(G') \geq 0$. From previous analysis we have two possibilities: The graph G' satisfies conditions (11) and (12). In this situation there exists a threshold vector such that the parallel update admits a *total* two-cycle. Otherwise, i.e., some of the conditions are no longer true, from the previous proposition we construct a new graph G'' by removing vertices which do not satisfy the conditions, such that $\alpha(G'') \geq 0$. By iterating this procedure we will finally obtain a graph $G^* = (V^*, E^*)$ with at most four vertices with $\alpha(G^*) \geq 0$. For every one of these graphs we obtain easily *total* two-cycles (see Figs. 5 and 6) which can be extended to the original graph G by setting every vertex in $V \setminus V^*$ constant at value 0 (i.e., a Heaviside function with a threshold big enough). $\square$

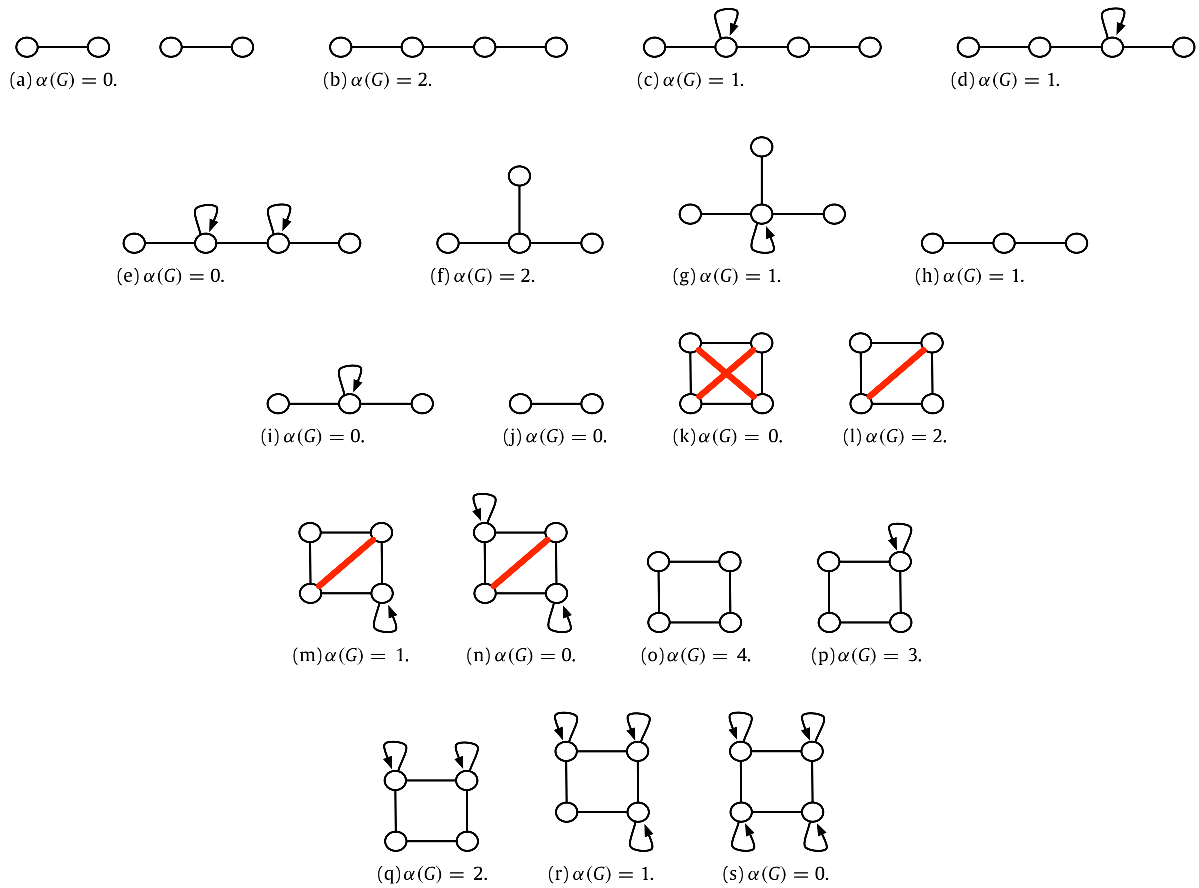

Fig. 6. The family of graphs with $2 \leq |V| \leq 4$, $\alpha(G) \geq 0$, such that they admit total two-cycles. The thicker edges (red) are the edges that can be removed to obtain a maximum bipartite graph. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Remark 3.4. It is interesting to see the application of the main theorem to two classes of graphs, the skinny ones (forest or trees) and the fat ones (complete graphs):

For bipartite graphs ($p = 0$), $\alpha(G) = -n-d+2m$. If we consider that every node has a loop, i.e., $d = n$, so $\alpha(G) = -2n + 2m$. Then $\alpha(G) < 0$ is equivalent to $n > m$. Furthermore, if the initial graph is a forest (no circuits) with loops and $n > m$, any subgraph G' has the same property so it verifies $\alpha(G') < 0$. If we consider now complete graphs, K_n, such that every vertex has a loop, it is not difficult to compute the maximum of the quadratic expression of $\varphi(z)$ given in (9). Actually, it is reached for balanced configurations (i.e., same number of $+1$'s and -1's for n even, a minimum difference of one, for n odd). In this context, following (9), we have: $m - 2p = \max_{z \in \{-1,1\}^n} \varphi(z) = \left\lfloor \frac{n}{2} \right\rfloor$. From where we obtain:

$$p = \begin{cases} 2q(q-1) & \text{for } K_{2q} \\ 2q^2 & \text{for } K_{2q+1} \end{cases}$$

then $\alpha(K_n) < 0$. Since any subgraph (by deleting vertices) of K_n is also a complete graph, $\alpha(G') < 0$ for any $G' \subseteq K_n$. The previous remarks can be summarized as follows:

Lemma 3.2. (a) *The parallel updating scheme over a forest with loops (in particular a tree) converges to fixed points.* (b) *The parallel updating scheme on complete graphs with loops admits only fixed points.*

3.1. Main theorem for block-sequential updates

Now we announce the general result concerning arbitrary block-sequential updates, i.e., arbitrary partitions. Let us consider a block sequential updating scheme $\tau = \{\{I_1\}, \ldots, \{I_p\}\}$. Let $G(I_k)$ be the subgraph associated to the set I_k, as well as $W(I_k)$ its incidence matrix:

Theorem 3.2. *Let us consider the neural network $N = (W(G), \Theta, \tau)$, then: if for any $k \in \{1, \ldots, p\}$ and $G' \subseteq G(k)$, $\alpha(G') < 0$, then N admits only fixed points for any threshold vector. Otherwise, if there exist $k \in \{1, \ldots, p\}$ and a subgraph $G' \subseteq G(k)$ such that $\alpha(G') \geq 0$, then there exist threshold vectors such that N admits cycles with period at least 2.*

Proof. Since the update is block by block, the first part is direct from the first part of the main theorem (each block is updated in parallel). For the second part, the proof is roughly the same as that the second part of the main theorem, but in this case we have to fix the external thresholds. Actually, if the graph $G' \subset G(k)$, such that $\alpha(G') \geq 0$ so inside the graph $G(k) = (V(I_k), E(I_k))$ we determine a two cycle for its parallel update like in the parallel case explicited in the previous theorem. For vertices belonging to the other blocks, i.e., $v \in V \setminus V(I_k)$, we put $x_v = 0$ as well as a threshold large enough to maintain constant this value whatever happens inside the kth block. In fact, it suffices to consider θ_v big enough. From that, we may exhibit a two cycle inside the kth partition while the remaining vertices are at state 0. □

The previous theorem implies the following result, which has been proven previously by Mortveit (2012) using another approach.

Corollary 3.1. *Let us consider a neural network $N = (W(G), \Theta, \tau = \{\{I_1\}, \ldots, \{I_p\}\})$, such that $diag(W(G)) = \vec{1}$ (i.e., each vertex has a loop) then, $|I_k| \leq 3$, for $k \in \{1, \ldots, p\}$, implies that the network*

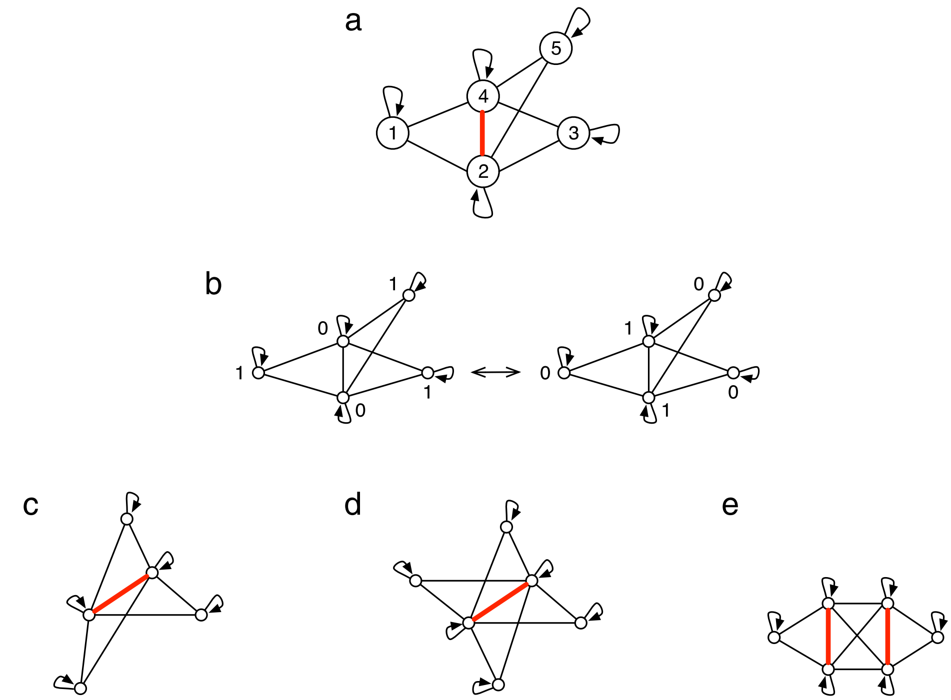

Fig. 7. (a) A graph with $p = 1$. $X = \{(2, 4)\}$ a realization of an edge to be eliminated (colored) to obtain a maximum bipartite graph. Further, $|O_2| = |O_4| = 1 < |P_2| = |P_4| = 3$ and $|P_1| = |P_3| = |P_5| = 2$. So, G with X verifies conditions (11) and (12). (b) A total two-cycle over G. Graphs which admit total-two cycles without the existence of a four-circuit without a cord (c) $n = 5,\ p = 1$ (d) $n = 6,\ p = 1$ (e) $n = 6,\ p = 2$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

converges to fixed points for any threshold vector Θ. Otherwise (i.e., at least a partition has cardinality four or more) there exist a graph and a threshold vector such that cycles appear.

Proof. See Appendix B.

Remark 3.5. It is important to point out that the previous corollary can be refined. In fact, for partition of cardinality ≥ 4, there are a huge but finite number of graphs. By computing α it is possible to characterize whether or not the associated graph admits cycles.

In Fig. B.11 (Appendix B) we exhibit the family of connected graphs with loops ($diag(W) = \vec{1}$) with $n \leq 4$, and in Fig. D.12 (Appendix D) with $n = 5$. From that, we may announce a more general convergence result.

Corollary 3.2. *Let us consider a neural network $N = (W(G), \Theta, \tau = \{\{I_1\}, \ldots, \{I_p\}\})$, such that $diag(W(G)) = \vec{1}$ (i.e., each vertex has a loop). Suppose $|I_k| \leq 5$, for $k \in \{1, \ldots, p\}$, such that any partition containing a four-circuit without cords or the graph of size 5 given in Fig. 7(c) is forbidden, then the network converges to fixed points for any threshold vector Θ. Elsewhere, there exists a threshold vector such that cycles appear.*

Proof. For partitions of size 1, 2 or 3 it is the same proof of the previous corollary. For partitions of size 4, the only graphs which admit a two cycle are those which contains a four-circuit without cords (see Figs. 6(s) and B.11). In this situation, to define a two cycle is enough to fix every vertex at 0 outside the four-circuit (by taking thresholds high enough) and over the circuit taking Heaviside functions with threshold 1/2. In this context $(0, 1, 0, 1, \vec{0}) \leftrightarrow (1, 0, 1, 0, \vec{0})$ is a two-cycle. For a partition I of size 5, if $G(I)$ does not contain a four circuit without cords or it is not equal to the graph given in Fig. 7(c), then, as we see in Fig. D.12, $\alpha(G') < 0$ for any $G' \subseteq G(I)$. With that we proved the convergence to fixed point. Otherwise, if $G(I)$ contains a four-circuit without cords one may exhibit total two cycles (see Fig. 6(o)-(s)), moreover, if $G(I)$ is equal to the graph of Fig. 7(c) then one may exhibit the *total* two-cycle of Fig. 7(b). □

Remark 3.6. It is important to point out that naturally one may conjecture that there exists $\alpha(G') \geq 0$, $G' \subseteq G$ if and only if G' contains an even circuit without odd cords (i.e., cords such that they generate inside the circuit two odd circuits).

From one side it is trivial, if there exists such circuit C, then directly $\alpha(C) \geq 0$. From the other side, it is no longer true. Actually, it is related to the possibility to have *total* two-cycles. Let us consider, for instance, some of the graphs of Fig. 7. It is easy to see that for all of them $\alpha(G) \geq 0$ and conditions (11), (12) are satisfied. Furthermore, none of them nor their subgraphs admits four-circuit without a cord. So, for partitions such that their cardinality is bigger than four, it is not enough to avoid even circuits without odd cords. We exhibit for $n \in \{5, 6\}$ in Fig. 7(c)–(e), every graph to be excluded (excluding every circuit without odd cords) in order to have the fixed point behavior.

4. Non-polynomial cycles associated to block-sequential updating

Contrary to the usual intuition (supported by simulations), in these networks the limit cycles, if they exist, have small periods for any updating scheme, in fact, there are even conjectures that the periods have length at most two (Mortveit, 2012). We will show evidence that supports the opposite, i.e., large cycles can appear. In this section we will prove that when the conditions on the partitions and the associated graph, presented in the previous section, do not hold, very large cycles appear. We will only consider incidence matrices $W = W(G)$ of a graph $G = (V, E)$, i.e., entries 0's or 1's. In what follows we show that by constructing a very simple majority network (a particular case of the Heaviside function) with an updating scheme that considers only partitions of cardinality two, it is possible to generate attractors with non-polynomial periods. Further, directly from the same construction we will prove that block-sequential updates admit also non-polynomial transients.

Let us consider the graph $G = (V, E)$, $V = \{1, 1', 2, 2', \ldots, n, n'\}$ and the set of edges shown in Fig. 8(a). We call the previous

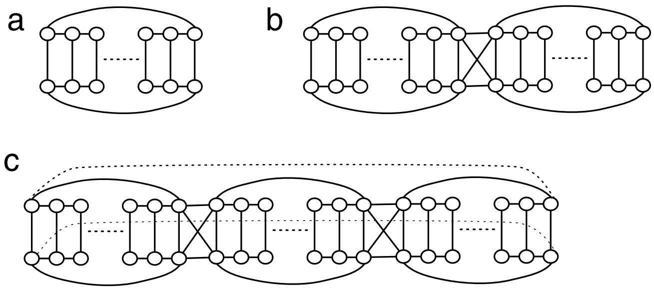

Fig. 8. (a) A staircase model. (b) Two staircases connected by a joint. (c) Several staircases connected by joints.

graph a *staircase*. We consider over each node the majority function:

$$f_1(x_n, x_{1'}, x_2) = \mathbf{H}\left(x_n + x_{1'} + x_2 - \frac{3}{2}\right)$$

$$f_{1'}(x_{n'}, x_1, x_{2'}) = \mathbf{H}\left(x_{n'} + x_1 + x_{2'} - \frac{3}{2}\right)$$

$$f_i(x_{i-1}, x_{i'}, x_{i+1}) = \mathbf{H}\left(x_{i-1} + x_{i'} + x_{i+1} - \frac{3}{2}\right)$$

$$f_{i'}(x_{(i-1)'}, x_i, x_{(i+1)'}) = \mathbf{H}\left(x_{(i-1)'} + x_i + x_{(i+1)'} - \frac{3}{2}\right)$$

$$f_n(x_{n-1}, x_{n'}, x_1) = \mathbf{H}\left(x_{n-1} + x_{n'} + x_1 - \frac{3}{2}\right)$$

$$f_{n'}(x_{(n-1)'}, x_n, x_{1'}) = \mathbf{H}\left(x_{(n-1)'} + x_n + x_{1'} - \frac{3}{2}\right)$$

for $2 \le i \le n-1$. We also denote a configuration as follows.

$$X = \begin{pmatrix} x_1, \dots, x_i, \dots, x_n \\ x_{1'}, \dots, x_{i'}, \dots, x_{n'} \end{pmatrix}.$$

In the previous context, let us consider the block-sequential partition

$$\tau = \left\{ \begin{Bmatrix} 1 \\ 1' \end{Bmatrix}, \begin{Bmatrix} n \\ n' \end{Bmatrix}, \begin{Bmatrix} n-1 \\ n'-1 \end{Bmatrix}, \dots, \begin{Bmatrix} 2 \\ 2' \end{Bmatrix} \right\}$$

and the initial configuration

$$X(0) = \begin{pmatrix} 0, 0, \dots, 0, 1 \\ 1, 1, \dots, 1, 0 \end{pmatrix}.$$

The new configurations by applying the partition τ one time, two times, and three times are as follows:

$$X(1) = \begin{pmatrix} 1, 1, 0, \dots, 0 \\ 0, 0, 1, \dots, 1 \end{pmatrix}$$

$$X(2) = \begin{pmatrix} 0, 0, 1, 0, \dots, 0 \\ 1, 1, 0, 1, \dots, 1 \end{pmatrix}$$

$$X(3) = \begin{pmatrix} 0, 0, 0, 1, 0, \dots, 0 \\ 1, 1, 1, 0, 1, \dots, 1 \end{pmatrix}.$$

It is direct that, after applying $n-1$ times the partition:

$$X(n-1) = \begin{pmatrix} 0, 0, 0, \dots, 0, 1 \\ 1, 1, 1, \dots, 1, 0 \end{pmatrix} = X(0).$$

So, we have a cycle of period $T = n-1$. Therefore, the previous majority network updated as above admits a non-bounded cycle of period $T = n-1$. Further, we have:

Theorem 4.1. *There exists a neural network $N = (W, \Theta, \mu)$ which admits cycles with non polynomial period.*

Proof. Let us consider a connected graph composed of a connected union of staircases, each one with a prime limit cycle. Given a prime number p by taking a "staircase" with length $p+1$ (i.e., $2(p+1)$ vertices) and the previous block partition, one may exhibit a cycle with period p. From that, suppose we have staircases of size $2(p_1+1), 2(p_2+1), \dots, 2(p_l+1)$, where $2 \le p_1 \le p_2 \le \cdots \le p_l$ are the first l consecutive prime numbers. Given two consecutive primes and its staircases, say p_k, p_{k+1} we generate a linked (connected graph) staircase by connecting two staircases as follows: for vertices a and a' in the first stair and b and b' in the other and creating the following edges between them: $(a, b), (a, b'), (a', b), (a', b')$. The structure of connecting two staircases is shown in Fig. 8(b). Remark that, given our initial configuration in staircases, the local configuration

$$\begin{pmatrix} X_i \\ X_{i'} \end{pmatrix} \in \left\{ \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \end{pmatrix} \right\}$$

never appears, then the contribution of the two external edges of a joint to the staircase's dynamics is always neutral (a 0 and a 1), so there are no changes to the inner staircase dynamics. Let us consider the set of l first majority functions staircases (associated to prime cycles p_l)

$$G = \bigcup_{k=1}^{l} G_k$$

connected by joints as in Fig. 8(c). Then, the staircase configuration:

$$X^k(0) = \begin{pmatrix} 0 & \cdots & 0 & 1 \\ 1 & \cdots & 1 & 0 \end{pmatrix} \quad 1 \le k \le l$$

and the partition:

$$\tau = \left\{ \tau^1, \dots, \tau^l \right\}$$

where τ^k is the partition associated to the kth staircase. Since every staircase is in a different prime cycle, then the global period of G is at least:

$$T \ge \prod_{i=1}^{l} p_i.$$

From that, by following a technique first used in Kiwi, Ndoundam, Tchuente, and Goles (1994), it is easy to see that the period is bounded by an exponential value. Let $l = \pi(m)$ where $\pi(m)$ denotes the number of primes not exceeding m. This yields

$$|V(G)| = 2\sum_{i=1}^{l}(p_i + 1) \le 2\pi(m)(m+1). \tag{14}$$

Also we may write $\prod_{i=1}^{l} p_i = e^{\theta(m)}$, where $\theta(m) = \sum_{i=1}^{\pi(m)} \log p_i$, then

$$T \ge \prod_{i=1}^{l} p_i = e^{\theta(m)}. \tag{15}$$

Using the Prime Number Theorem (Hardy, Wright, Heath-Brown, & Silverman, 2008) that states that $\pi(m) = \Theta(m/\log m)$, also from Hardy et al. (2008), $\theta(m) = \Theta(\pi(m)\log m)$, which together with (14) and (15) implies that

$$T \ge e^{\Omega(\sqrt{|V(G)|\log|V(G)|})}. \quad \square$$

Remark 4.1. We see that for every partition on the previous network, the local incidence matrix is

$$W(\{i, i'\}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

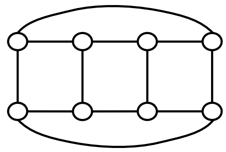

Fig. 9. Staircase model with the majority function over each node.

Obviously, it is not semi non-negative definite on the set $\{-1, 1\}$.

It is not difficult to prove, by using roughly the same construction of Theorem 4.1 that:

Corollary 4.1. *There exists a neural network* $N = (W, \Theta, \mu)$ *which admits non-polynomial transients.*

Proof. See Appendix C.

From the previous result we know that for incidence matrices of undirected connected graph, very simple local threshold functions and two size partitions admit cycles with non-polynomial periods and transients.

5. Illustrative example of different updating schemes, energy, and convergence

We present an example where the relation of the energy operator with our theorems and $\alpha(G)$ is illustrated. Let us consider the staircase of Fig. 9, with the majority function over each node as described in the previous section, and the initial configuration

$$X(0) = \begin{pmatrix} 0, 0, 0, 1 \\ 1, 1, 1, 0 \end{pmatrix}.$$

This initial configuration evaluated in (2) gives $E(X(0)) = 4$. Let us consider first the parallel update, in that case we have $\alpha(G) = 16 > 0$, then by Theorem 3.1 we have that cycles of period 2 appear. In fact,

$$X(1) = \begin{pmatrix} 1, 0, 1, 0 \\ 0, 1, 0, 1 \end{pmatrix}$$

$$X(2) = \begin{pmatrix} 0, 1, 0, 1 \\ 1, 0, 1, 0 \end{pmatrix}$$

and $X(3) = X(1)$. Also we have that $E(X(1)) = E(X(2)) = 6$, which is an increase from $E(X(0))$, therefore, there is no convergence to fixed points.

Let us consider now the following partition, $I_1 = \{1, 1'\}$, $I_2 = \{4, 4'\}$, $I_3 = \{3, 3'\}$, and $I_4 = \{2, 2'\}$ and the block sequential update

$$\tau = \left\{ \begin{Bmatrix} 1 \\ 1' \end{Bmatrix}, \begin{Bmatrix} 4 \\ 4' \end{Bmatrix}, \begin{Bmatrix} 3 \\ 3' \end{Bmatrix}, \begin{Bmatrix} 2 \\ 2' \end{Bmatrix} \right\}.$$

For the subgraphs $G_{I_1} = (\{1, 1'\}, (1, 1'))$, $G_{I_2} = (\{4, 4'\}, (4, 4'))$, $G_{I_3} = (\{3, 3'\}, (3, 3'))$, and $G_{I_4} = (\{2, 2'\}, (2, 2'))$, we have that $\alpha(G_{I_i}) = 0$ for $i = 1, 2, 3, 4$, then by Theorem 3.2, we have that cycles appear. In fact,

$$X(1) = \begin{pmatrix} 1, 1, 0, 0 \\ 0, 0, 1, 1 \end{pmatrix}$$

$$X(2) = \begin{pmatrix} 0, 0, 1, 0 \\ 1, 1, 0, 1 \end{pmatrix}$$

and $X(3) = X(0)$, i.e., a cycle of period 3. The energy for all the configurations within the cycle equals 4, thus, no energy decrease, therefore, no convergence to fixed points.

Finally, let us consider the sequential update. In this case each partition is a singleton, therefore, $G_{I_i} = (\{i\})$ for $i = 1, \ldots, 4, 1', \ldots, 4'$ and $\alpha(G_{I_i}) = -1 < 0\ \forall i$, then by Theorem 3.2, it must converge to a fixed point. In fact, let us consider the sequential update $\tau = \{\{1\}, \{2\}, \{3\}, \{4\}, \{4'\}, \{3'\}, \{2'\}, \{1'\}\}$, we have that

$$X(1) = \begin{pmatrix} 1, 1, 1, 1 \\ 1, 1, 1, 1 \end{pmatrix}$$

and $X(2) = X(1)$, i.e., a fixed point. Using the energy operator we have that $E(X(1)) = 0$, which is an energy decrease from $E(X(0))$, therefore we have convergence to a fixed point. An energy plot which summarizes the three cases analyzed (parallel (P), block sequential (BS), and sequential (S)) is shown in Fig. 10(a). Also, Fig. 10(b)–(d), shows a histogram of the energy value where each of the $2^8 = 256$ initial configurations converges to, for the three cases respectively.

6. Discussions and conclusions

In this paper we have studied the relationship between attractors (cycles or fixed points) of neural networks defined over an undirected finite graph (i.e., the entries of the interconnection matrix are 0's and 1's) and some characteristics of the graph like loops and circuits. From our study it can be deduced that the number of nodes, edges, loops and odd circuits are the relevant parameters in order to characterize the attractors. For the parallel dynamics we know from Goles and Olivos (1980) that the network converges to fixed points or two-cycles. An interesting question is, when does the network reach one of them?, this is captured by the parameter $\alpha(G)$: If it is negative for any subgraph of G, then any attractor is a fixed point. Elsewhere, when there exists some G' such that the parameter is non-negative, it is always possible to find a threshold vector such that the network admits a cycle of period two. It is important to point out that odd circuits and loops tend to freeze the dynamics (convergence to fixed points). For instance, for every graph such that it admits two connected vertices without loops we proved that there exists always a threshold vector in order to exhibit two-cycles. Further, every bipartite graph (with or without loops) such that it admits a circuit has the same two cycle behavior.

The computation of parameter $\alpha(G)$ is not easy, because we have to compute, p, the minimum number of edges to remove in order to obtain a maximum bipartite graph. This problem is known in the literature as the MAX-CUT problem which is NP-complete (Garey & Johnson, 1979). It is important to point out that it becomes polynomial for planar graphs (Hadlock, 1975). Further, the optimization of the quadratic expression $\varphi(y) = -\frac{1}{2}y^t W^* y$; for $y \in \{-1, 1\}^n$ is related with the problem of finding the ground state of the spin glass model. In this context the problem to compute the maximum of the previous quadratic expression is polynomial over undirected graphs (see Moore & Mertens, 2011). By extending the weights to the set $\{-1, 0, 1\}$ it continues to be polynomial in a two-dimensional grid and NP-hard in a three dimensional one (Barahona, 1982). As an example, we exhibit in Fig. D.12 (Appendix D) the value of $\alpha(G)$ for every graph such that $n = |V| \leq 5$.

Furthermore, previous results, for the parallel updating scheme, can be directly extended to any block-sequential update by applying Theorem 3.1 to each block of the partition. But in this case, when, for some partition I_k, $\alpha(G(I_k)) \geq 0$ the situation is largely more interesting, because for partitions taking into account only two connected vertices without loops, non-polynomial cycles and transients appear. Further, it is the minimum partition size case (remember for partitions of size one the sequential iteration converges to fixed points independently of the threshold vector (Corollary 2.1(b)).

It is important to remark Corollary 3.2 about the convergence to fixed points, when $diag(W) = \vec{1}$, and the size of partitions ≤ 5. In this context, for partitions of size 4 and 5, four-circuits without cords as well as the graph given in Fig. 7(a) are forbidden. This result may be extended for bigger partitions but, of course by adding more forbidden graphs. For instance, if we consider also

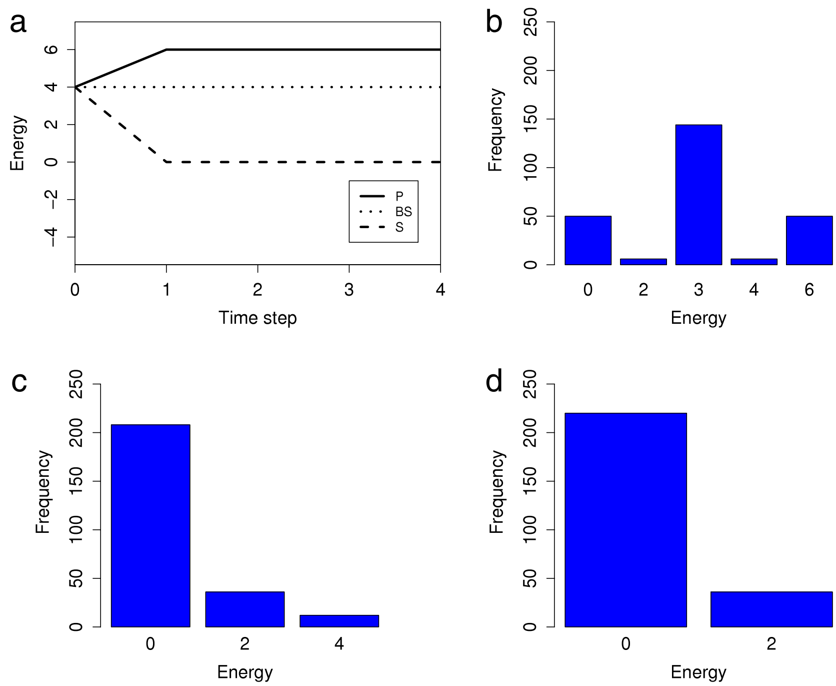

Fig. 10. (a) Energy plot for a particular initial configuration of the staircase model in Fig. 9, where P is the parallel update, BS is a block sequential update, and S is a sequential update. Histogram of the energy values where the staircase model converges to using all the 256 initial configurations for the (b) parallel update, (c) block sequential update, and (d) sequential update.

partitions of size 6, we have to forbid also six-circuits without cords and graphs like those of Fig. 7(d) and (e).

The non-polynomial periodic and transient behavior gives us an insight about the possibility to adapt a monotone operator driving the dynamics for more general updating schemes. For instance, the parallel or the sequential update on undirected graphs. As we discussed in the introduction their dynamics are driven by an energy operator. Furthermore, since the entries of the connection matrix are 0's and 1's and $|\Delta E| \geq 1/2$ then the convergence time is $O(|V|^2)$, which implies that the algorithmic complexity to know the state of a site at a given step $T \geq 0$, is polynomial. Since we proved that for other block-sequential updating schemes there exist non-polynomial transients, then it is not possible to determine a polynomial energy operator driving its dynamics, and also, the complexity class where these decision problems belong may change depending on the updating scheme (Goles & Montealegre-Barba, in press-a).

The use of the energy operator defined in (2) has been studied extensively for discrete neural networks in Cosnard and Goles (1997). These kinds of operators only apply for, essentially undirected graphs, or in the most general case directed acyclic graphs (DAGs) where each node may be an undirected connected graph, or a Hopfield network (undirected weighted graph). Looking for instance at a feedforward neural network, where in the forward propagation, its like a tree, so in this kind of step, an energy operator can be used. Nevertheless, during the training, there is also back propagation (to adjust the weights), which then forbids the definition of an energy operator.

The existence of a decreasing energy operator is associated essentially to the fact that there is no direct circuits and the fact, for instance, that in undirected graphs (like the staircase model) where cycles appear, is due to the different updating schemes, that tend to simulate a directed graph as studied in Goles and Matamala (1993), by imposing an order of how the nodes are updated, thus not allowing a decreasing energy.

The prediction problem of knowing whether or not an arbitrary node of a network may change its state (from 0 to 1, or vice versa), for planar majority networks, has been studied in Goles and Montealegre-Barba (in press-b). It is shown that it is a difficult problem (P-complete), and in general, in a large network, even with a subset of nodes fixed to certain values, the problem is still P-complete. Although, the problem can be solved in polynomial time, it cannot be accelerated to polylogarithmic time, unless P = NC (problems decidable in polylogarithmic time on a parallel computer with a polynomial number of processors).

The construction to obtain non-polynomial cycles is done over a very simple connected network, where most of the nodes have degree three and the joints between staircases degree four. Further, the Heaviside function is also simple: the local majority. The same kind of construction for non-polynomial cycles and transients can be easily obtained for other local functions and updating schemes. For instance by using only AND and OR functions (Goles & Montealegre-Barba, in press-a). Finally in Appendix E we illustrate our convergence results on a neural network with six nodes, iterated under different updating schemes.

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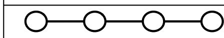
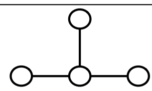
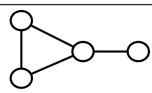
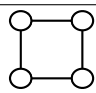
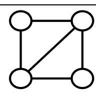
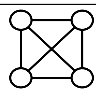
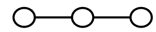
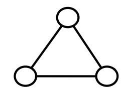
Appendix A. Proof of Eq. (9)

Proof. Clearly:

$$\varphi(y) = -\frac{1}{2}\sum_{(i,j)\in E} y_i y_j = -\frac{1}{2}\sum_{\substack{(i,j)\in E\\ i<j}} 2y_i y_j = -\sum_{\substack{(i,j)\in E\\ i<j}} y_i y_j \qquad (A.1)$$

such that $y_i y_j = -1$ if $y_i \neq y_j$ (+1 otherwise). Suppose in general that G has q odd circuits: $C_1, \ldots, C_q$. By assigning +1 or −1 (the value of y_i) to each vertex, it is direct that there exists at least one edge (a, b) in each odd circuit C_l such that $y_a y_b = 1$. On the other hand, by cutting an edge in each odd circuit, we obtain a bipartite graph. So one may assign $y_i \in \{-1, 1\}$ such that they alternate its value for neighboring vertices. This gives the maximum value of φ over the subgraph where we have not considered the set of q edges,

	$\alpha(G)<0$ Fixed points	$\alpha(G)\geq 0$ Two-cycles
	$3\leq d\leq 4$	$0\leq d\leq 2$
	$3\leq d\leq 4$	$0\leq d\leq 2$
	$1\leq d\leq 4$	$d=0$
	$\emptyset$	$0\leq d\leq 4$
	$3\leq d\leq 4$	$0\leq d\leq 2$
	$1\leq d\leq 4$	$d=0$

	$\alpha(G)<0$ Fixed points	$\alpha(G)\geq 0$ Two-cycles
	$2\leq d\leq 3$	$0\leq d\leq 1$
	$0\leq d\leq 3$	$\emptyset$

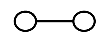
	$\alpha(G)<0$ Fixed points	$\alpha(G)\geq 0$ Two-cycles
	$1\leq d\leq 2$	$d=0$

Fig. B.11. All the possible connected graphs with $n\leq 4$, $d=$ the number of loops.

$X=\{v_1,\ldots,v_q\}$ which cut off every odd circuit. Hence:

$\forall(a,b)\in E\setminus X\Longrightarrow z_az_b=-1.$

So, for any edge $v_i=(\alpha,\beta)\in X$, we have $z_\alpha z_\beta=+1$, then $\varphi(z)=(m-q)-q=m-2q$. Since $p\leq q$, we conclude that $\varphi(z)\leq m-2p$. Further, by taking a set $\tilde{X}=\{v_1,\ldots,v_p\}\subseteq E$ which realizes the minimum cardinality, p, of edges to be deleted such that $E\setminus\tilde{X}$ is a maximum bipartite graph, we have:

$\varphi(y)=m-2p.$ □

Appendix B. Proof of Corollary 3.1

Proof. For partitions of size one we have by hypothesis that every vertex has a loop, so $w_{ii}=1>0$ and the conclusion is direct from Corollary 2.1. For partitions of size two it is direct that $-4\leq\alpha(G')\leq -2$, for any $G'\subseteq G$. Similarly, for graphs of size three we have that $-6\leq\alpha(G')\leq -2$ (see Fig. B.11). So, for any partition with cardinality less than or equal to three $\alpha(G')\leq 0$ for any $G'\subseteq G$. We conclude by applying the main theorem.

For the case when there exist a partition of size four or more, we can show that there exist graphs and thresholds such that at least two periodic cycles appear. Let us consider a graph, given by the following incidence matrix

$$W=\begin{pmatrix}1&1&0&1&1&1\\1&1&1&0&0&0\\0&1&1&1&0&0\\1&0&1&1&0&0\\1&0&0&0&1&1\\1&0&0&0&1&1\end{pmatrix}$$

and the threshold vector

$\Theta=(3/2,3/2,3/2,3/2,3/2,3/2).$

It is direct that the neural network $(W,\Theta,\{\{1,2,3,4\},\{5,6\}\})$ admits the two-cycle $(0,1,0,1,0,0)\longleftrightarrow(1,0,1,0,0,0)$. □

Appendix C. Proof of Corollary 4.1

Proof. We consider the graph of the l interconnected staircases as above and we add four new vertices, a,b,c,d. Let us denote $y(t)=(x(t),y_a(t),y_b(t),y_c(t),y_d(t))$, the configuration of the new network at step t. The role of these vertices is the following:

Vertex a: must be in 0 during the steps $t=1,2,\ldots,T-1,T$ of the cycle of staircases and to become 1 when the configuration of staircases is $x(T)=x(0)$.
Vertex b: has to be fixed at state 1 and connected exactly to the same vertices of staircases as vertex a (so, while $y_a=0$, since $y_b=1$, they do not change the value of the majority functions updates on the dynamics of the staircases).
Vertex c: must be at value 0 during the steps $t=1,2,\ldots,T-1,T$ of the cycle of the staircases and becomes 1 when $y_a(T+1)=1$. When it is at state 1 it has to force vertices $\{n_1-1,(n_1-1)'\}$ of the first staircase to become fixed at state 1.
Vertex d: has to be always at state 1. It is connected to the same two vertices of the staircases as c. For $t<T+1$, since they have a different value, they do not change the internal majority dynamics of the staircases.

Vertices c and d are connected to two contiguous staircases's sites, n_1-1, $(n_1-1)'$, such that when both are at state 1 they force these sites to become also fixed at state 1. So the new set of vertices is the old one (staircases's vertices) together with $\{a,b,c,d\}$:

$$\begin{aligned}V^*&=V\cup\{a,b,c,d\}\\&=\{1,1',2,2',\ldots,n_1,n_1'\}\cup\{n_1+1,(n_1+1)',\ldots,n_2,n_2'\}\\&\quad\cup\cdots\cup\{n_{(l-1)}+1,(n_{(l-1)}+1)',\ldots,n_l,n_l'\}\cup\{a,b,c,d\}.\end{aligned}$$

The new connections for each new vertex are the following:
Connections associated to vertices $r\in\{a,b\}$:

$E(r)=\{(r,n_1),(r,n_2),\ldots,(r,n_l),(c,r),(d,r)\}.$

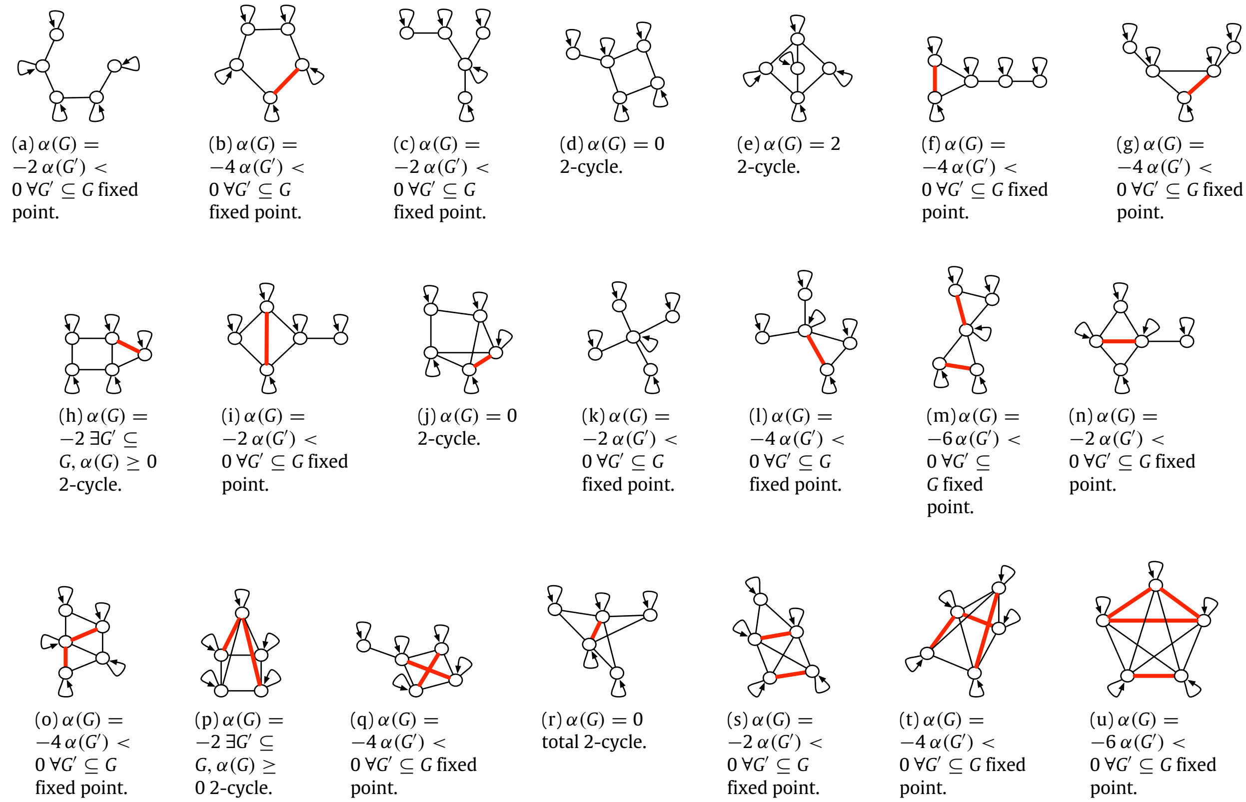
Connections associated to vertices in $\{c,d\}$:

$$E(c)=\{(c,a),(c,b),(c,c),(c,d),(c,(n_1-1)'),(c,(n_1-1))\}$$
$$E(d)=\{(d,a),(d,b),(d,d),(d,c),(d,(n_1-1)'),(d,(n_1-1))\}.$$

Therefore, the set of edges is

$E^*=E\cup E(a)\cup E(b)\cup E(c)\cup E(d).$

The updating mode of the network is for staircases the same as in the cycle construction below but, after finishing the set of par-



(a) $\alpha(G) = -2\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(b) $\alpha(G) = -4\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(c) $\alpha(G) = -2\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(d) $\alpha(G) = 0$ 2-cycle.
(e) $\alpha(G) = 2$ 2-cycle.
(f) $\alpha(G) = -4\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(g) $\alpha(G) = -4\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(h) $\alpha(G) = -2\ \exists G' \subseteq G, \alpha(G) \geq 0$ 2-cycle.
(i) $\alpha(G) = -2\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(j) $\alpha(G) = 0$ 2-cycle.
(k) $\alpha(G) = -2\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(l) $\alpha(G) = -4\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(m) $\alpha(G) = -6\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(n) $\alpha(G) = -2\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(o) $\alpha(G) = -4\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(p) $\alpha(G) = -2\ \exists G' \subseteq G, \alpha(G) \geq 0$ 2-cycle.
(q) $\alpha(G) = -4\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(r) $\alpha(G) = 0$ total 2-cycle.
(s) $\alpha(G) = -2\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(t) $\alpha(G) = -4\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.
(u) $\alpha(G) = -6\ \alpha(G') < 0\ \forall G' \subseteq G$ fixed point.

Fig. D.12. Evaluation of the expression $\alpha(G) = -2n + 2m - 4p$ for all the strongly connected graphs (with loops in each node) for $n = 5$. The thicker red edges are the edges that can be removed. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

titions we update two new blocks $\{a, b\}$ and $\{c, d\}$: $\{\tau^1, \ldots, \tau^l, \{a, b\}, \{c, d\}\}$. The Heaviside functions for the new vertices are the following:

$$f_a(y) = \mathbf{H}\left(\sum_{j\in\{k\in V/x_k(T)=1\}} x_j + y_c + y_d - (|\{k \in V/x_k(T) = 1\}|) - \frac{1}{2}\right)$$

$$f_b(y) = \mathbf{H}\left(\sum_{j\in\{k\in V/x_k(T)=1\}} x_j + y_c + y_d - \frac{1}{2}\right)$$

$$f_c(y) = \mathbf{H}\left(y_d + y_a + y_b + x_1 + x_1' - \frac{7}{2}\right)$$

$$f_d(y) = \mathbf{H}\left(y_c + y_a + y_b + x_1 + x_1' - \frac{1}{2}\right).$$

Let us consider the initial configuration

$$y(0) = (x(1), y_a, y_b, y_c, y_d) = (x(1), 0, 1, 0, 1).$$

Clearly, for any $t \geq 0$, $y_b(t) = y_d(t) = 1$ (by construction of the cycle $\{x(t)\}_{t\in\{0,\ldots,T-1\}}$ for every step $t \geq 0$, $\sum_{j\in\{k\in V/x_k(T)=1\}} x_j \geq 1$ and $x_j + x_{j'} = 1$). Since every configuration on the cycle $\{x(0), \ldots, x(T)\}$ has the same number of ones, then for $t < T + 1$ there is only one configuration, $x(T) = x(0)$, such that the ones are exactly in the staircases' connections with vertex a, then:

$$y_a(t) = \begin{cases} 0 & \text{for any } t \in \{1, 2, \ldots, T\} \\ 1 & \text{for } t \geq T + 1. \end{cases}$$

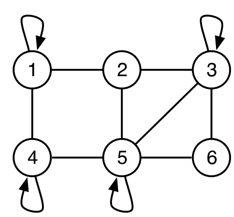


Fig. E.13. An undirected graph.

Hence, just at step $t = T + 1$, the variable y_a changes to 1, and after that, also we will have $x_c(t) = x_d(t) = 1$ for every $t \geq T + 2$. So, vertices n_1 and $n_{1'}$ have at least three vertices at value one among five so they become fixed at 1 for every $t \geq T + 2$. Then it is enough to conclude that the network admits a transient time $T^* \geq T + 1$, and from the previous theorem we conclude that the transient time is exponential. □

Appendix D

Fig. D.12 shows all the strongly connected graphs (with loops on each node) for $n = 5$. For each graph, we analyze the value of the expression $\alpha(G)$ (to see if it is negative, zero, or positive) and the possibility to have two-cycles for the parallel updating scheme.

Appendix E

For the graph in Fig. E.13 with

$$\Theta = [1.5, 1.5, 2.5, 1.5, 1.5, 1.5]$$

the state transition graphs for different updating schemes are shown in Fig. E.14.

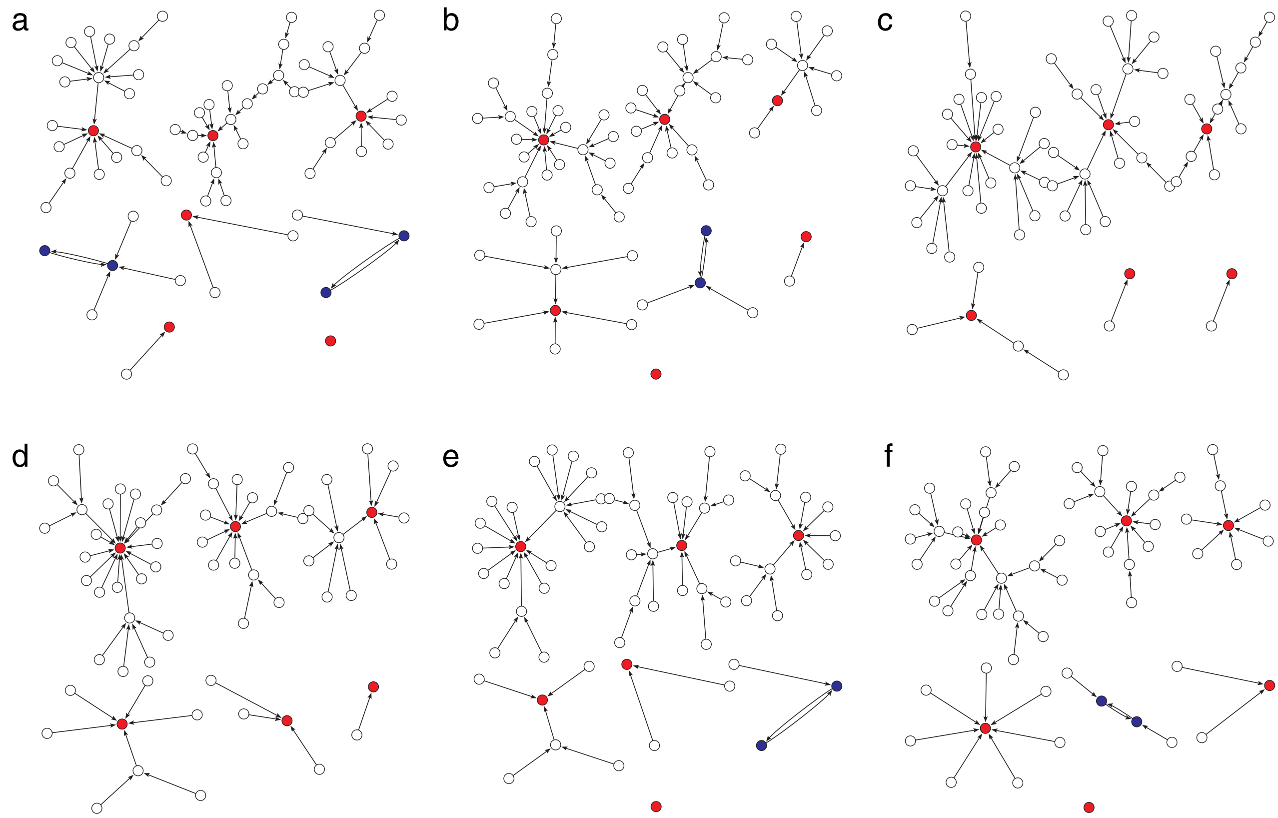


Fig. E.14. State transition graphs for the graph in Fig. E.13, for the updates (a) parallel (b) (1245)(36) (c) (124)(356) (d) (134)(256) (e) (14)(2356) (f) (145)(236). The red circles represent the fixed point states, and the blue circles represent the states that belong to the limit cycles. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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