Optimising attractor computation in Boolean automata networks

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Abstract

This paper details a method for optimising the size of Boolean automata networks in order to compute their attractors under the parallel update schedule. This method relies on the formalism of modules introduced recently that allows for (de)composing such networks. We discuss the practicality of this method by exploring examples. We also propose results that nail the complexity of most parts of the process, while the complexity of one part of the problem is left open.

1 Introduction

Boolean automata networks (BANs) are studied for their capacity to succinctly expose the complexity that comes with the composition of simple entities into a network. They belong to a wide family of systems which include cellular automata and neural networks, and can be described as cellular automata with arbitrary functions and on arbitrary graph structures.

Understanding and predicting the dynamics of computing with BANs has been a focus of the scientific community which studies them, in particular since their applications include the modelling of gene regulatory networks [12, 20, 13, 5, 6]. In those applications, fixed points of a BAN are often viewed as cellular types and limit cycles as biological rhythms [12, 20]. It follows that most biological studies relying on BANs require the complete computation of their dynamics to propose conclusions. The complete computation of the dynamics of BANs is an exponentially costly process. Indeed, for $n$ the size of a BAN, the size of its dynamics is precisely $2^n$. The dynamics of a BAN is usually partitionned in two sorts of configurations: the recurring ones that are parts of attractors and either belong to a limit cycle or are fixed points; the others that evolve towards these attractors and belong to their attraction basins. The questions of
characterising, computing or counting those attractors from a simple description of the network have been explored \[8, 1, 9, 7, 14, 2\], and has been shown to be difficult problems \[8, 16, 3, 4, 15\].

In this paper, we propose a new method for computing the attractors of a BAN under the parallel update schedule. For any input network, this method generates another network which is possibly smaller and which is guaranteed to possess attractors isomorphic to those of the input network. Computing the dynamics of this smaller network therefore takes as much time as needed to compute the dynamics of the input networks, divided by some power of two.

This method uses tools and results developed in previous works by the authors \[17, 18\]. These works involve adding inputs to BANs, in a generalisation called modules that proposes in some cases the study of the computational capabilities of the network as the computation in terms of the inputs. In particular, a result states that two networks that have equivalent such computations share isomorphic attractors.

Section 2 starts by exposing all the definitions needed to read this paper. Section 3 explores the question of obtaining an acyclic module from a BAN. Section 4 explains how to extract so called output functions from a module. Section 5 details how to generate a minimal module from a set of output functions. Finally Section 6 shows the final step of the method, which implies constructing a BAN out of an acyclic module and computing its dynamics. Each section explores complexity results of the different parts of the process, and details examples along the way. An illustrative outline of the paper can be found in Figure 1.
2 Definitions

2.1 Boolean functions and their encodings

In this paper, we consider a Boolean function as any function \( f : A \to \mathbb{B} \), for \( A \) a finite set. An affectation \( x \) of \( f \) is a vector in \( \mathbb{B}^A \). We consider two different encodings of Boolean functions.

A Boolean circuit of \( f \) is an acyclic digraph in which nodes without incoming edges are labelled by an element in \( A \), and every other node by a Boolean gate in \( \{\land, \lor, \neg\} \), with a special node marked as the output of the circuit. The evaluation \( f(x) \) is computed by mapping \( x \) to the input nodes of the circuit, and propagating the evaluation along the circuit using the gates until the output node is reached.

Boolean formulae are a restriction of Boolean circuits on trees. They are often represented as propositional formulae instead of graphs.

2.2 Boolean automata networks and acyclic modules

2.2.1 Boolean automata networks

BANs are composed of a set \( S \) of automata. Each automaton in \( S \), or node, is at any time in a state in \( \mathbb{B} \). Gathering those isolated states into a vector of dimension \( |S| \) provides us with a configuration of the network. More formally, a configuration of \( S \) over \( \mathbb{B} \) is a vector in \( \mathbb{B}^S \). The state of every automaton is bound to evolve as a function of the configuration of the entire network. Each node has a unique function, called a local function, that is predefined and does not change over time. A local function is thus a function \( f \) defined as \( f : \mathbb{B}^S \to \mathbb{B} \). Formally, a BAN \( F \) is a set that assigns a local function \( f_s \) over \( S \) for every \( s \in S \).

Example 1. Let \( S_A = \{a, b, c, d\} \). Let \( F_A \) be the BAN defined by \( f_a(x) = x_d \), \( f_b(x) = f_c(x) = x_a \), and \( f_d(x) = \neg x_b \lor \neg x_c \). The interaction digraph of this BAN is depicted in Figure 2 (left panel).

Example 2. Let \( S_B = \{St, Sl, Sk, Pp, Ru, S9, C, C25, M, C^*\} \). Let \( F_B \) be the BAN defined by \( f_{St}(x) = \neg x_{St} \), \( f_{Sl}(x) = \neg x_{Sl} \lor x_{C^*} \), \( f_{Sk}(x) = x_{Sl} \lor \neg x_{Sk} \), \( f_{Pp}(x) = x_{Sl} \lor \neg x_{Pp} \), \( f_{Ru}(x) = f_{S9}(x) = \neg x_{Sk} \lor x_{Pp} \lor \neg x_C \lor \neg x_{C^*} \), \( f_C(x) = \neg x_{Ru} \lor \neg x_{S9} \lor \neg x_{Sl} \), \( f_{C25}(x) = \neg x_{Pp} \lor x_C \), \( f_{M}(x) = x_{Pp} \lor \neg x_C \), and \( f_{C^*}(x) = \neg x_{Ru} \lor \neg x_{S9} \lor x_{C25} \lor \neg x_{M} \). The interaction digraph of this BAN is depicted in Figure 2 (right panel).

In the scope of this paper, BANs (and modules) are updated according to the parallel update schedule. Formally, for \( F \) a BAN and \( x \) a configuration of \( F \), the update of \( x \) under \( F \) is denoted by configuration \( F(x) \), and defined as for all \( s \) in \( S \), \( F(x)_s = f_s(x) \).

Example 3. Consider \( F_A \) of Example 1 and \( x \in \mathbb{B}^{S_A} \) such that \( x = 1001 \). We observe that \( F_A(x) = 1111 \). Configurations 1000 and 0111 are recurring and
form a limit cycle of size 2, as well as configurations 0000, 0001, 1001, 1111, 1110 and 0110 that form a limit cycle of size 6.

2.2.2 Interaction digraph

BANs are usually represented by the influence that automata hold on each other. As such the visual representation of a BAN is a digraph, called an interaction digraph, whose nodes are the automata of the network, and arcs are the influences that link the different automata. Formally, \( s \) influences \( s' \) if and only if there exist two configurations \( x, x' \) such that for all \( r \) in \( S \), \( r \neq s \) if and only if \( x_r = x'_r \) and \( f_s(x) \neq f_{s'}(x') \).

2.2.3 Dynamics

Finally, we define the dynamics of a BAN \( F \) as the digraph with \( B^S \) as its set of vertices. There exists an edge from \( x \) to \( y \) if and only if \( F(x) = y \). Computing the dynamics of a BAN from the description of its local function is an exponential process. See [19] for a more throughout introduction to BANs and related subjects.

2.2.4 Modules

Modules were first introduced in [17]. A module \( M \) is a BAN with added inputs. It is defined on two sets: \( S \) a set of automata, and \( I \) a set of inputs, with \( S \cap I = \emptyset \). Similarly to standard BANs, we can define configurations as vectors in \( B^S \), and we define input configurations as vectors in \( B^I \). A local function of a module updates itself based on a configuration \( x \) and an input configuration \( i \), concatenated into one configuration. Formally, a local function is defined from \( B^{S \cup I} \) to \( B \). The module \( M \) defines a local function for every node \( s \) in \( S \).

Example 4. Let \( M_e \) be the module defined on \( S_e = \{p, q, r\} \) and \( I = \{\alpha, \beta\} \), such that \( f_p(x) = x_\alpha \), \( f_q(x) = \neg x_p \), and \( f_r(x) = x_q \lor \neg x_\beta \).
We represent modules with an interaction digraph, in the same way as for BANs. The interaction digraph of a module has added arrows that represent the influence of the inputs over the nodes; for every node \( s \) and every input \( \alpha \), the node \( s \) of the interaction digraph has an ingoing arrow labelled \( \alpha \) if and only if \( \alpha \) influences \( s \), that is, there exists two input configurations \( i, i' \) such that for all \( \beta \in I \), \( \beta \neq \alpha \) if and only if \( i_\beta = i'_\beta \), and \( x \) a configuration such that \( f_s(x \cdot i) \neq f_s(x \cdot i') \), where \( \cdot \) denotes the concatenation operator.

A module is acyclic if and only if its interaction digraph is cycle-free.

2.2.5 Recursive wirings

A recursive wiring over a module \( M \) is defined by a partial function \( \omega : I \rightarrow S \).

The result of such a wiring is denoted \( \mathcal{R}_\omega M \), a module defined over sets \( S \) and \( I \setminus \text{dom}(\omega) \), in which the local function of node \( s \) is denoted \( f'_s \) and defined as

\[
\forall x \in B^{|I|},
\quad f'_s(x) = f_s(x \circ \hat{\omega}),
\quad \text{with } \hat{\omega}(i) = \begin{cases} 
\omega(i) & \text{if } i \in \text{dom}(\omega) \\
 i & \text{if } i \in I \setminus \text{dom}(\omega) 
\end{cases}.
\]

2.2.6 Output functions

Output functions were first introduced in [18] and present another way of computing the evolution of an acyclic module. In the Boolean case, those functions are defined on \( B^{I \times \{1, \ldots, D\}} \rightarrow B \), for \( I \) the input set of the module, and \( D \) some integer. We interpret an input in \( B^{I \times \{1, \ldots, D\}} \) as an evaluation over \( B \) of a set of variables \( I \times \{1, \ldots, D\} \), and for \( \alpha \in I \) and \( d \leq D \), we denote this variable by \( \alpha_d \). In the context of an acyclic module \( M \), \( \alpha_d \) is referring to the evaluation of the input \( \alpha \) on the \( d \)th update of the module. A vector \( j \in B^{I \times \{1, \ldots, D\}} \) simply describes an evaluation of all the inputs of the network over \( D \) iterations. With such a vector, and \( x \in B^S \), it is easy to see that the acyclic module \( M \) can be updated \( k \) times in a row, for any \( k \leq D \). The result of this update is denoted by \( M(x, j[1, \ldots, k]) \). The delay of an output function \( O \) is the maximal value in the set of all the \( d \in \mathbb{N} \) for which there exists \( \alpha \in I \) such that variable \( \alpha_d \) has an influence on the computation of \( O \). Finally, for \( M \) an acyclic module defined on the sets \( S \) and \( I \), for \( D \) a large enough integer, for \( x \in B^S \) and \( j \in B^{I \times \{1, \ldots, D\}} \) some vectors, and for \( s \) a node in \( S \), we define the output function of \( s \), denoted \( O_s \), as the output function with minimal delay \( d \) such that \( O_s(j) = M(x, j[1, \ldots, k])_s \). Such a function always exists and is always unique.

3 From BANs to AMs

The first step of our process is to unfold a BAN into an AM. This simply requires the removal of any cycle in the interaction digraph of the BAN, and their replacement by inputs. In the scope of this paper, the number of inputs generated is required to be minimal. This is justified by the fact that the
complexity of most of the problems addressed in the pipeline highly depends on the number of inputs of the considered AM.

- Acyclic Unfolding Functional Problem
  
  **Input:** A Boolean automata network $F$, an integer $k$.
  
  **Output:** An acyclic module $M$ with at most $k$ inputs and a recursive wiring $\omega$ such that $\circlearrowright_{\omega} M = F$.

**Theorem 1.** The Acyclic Unfolding Functional Problem is in FNP.

**Proof.** Consider the following simple non-deterministic algorithm: first guess a module $M$ and a wiring $\omega$; then check that the number of inputs in $M$ is no more than $k$ and that $\circlearrowright_{\omega} M$ syntactically equals $F$.

This algorithm operates in polynomial non-deterministic time since the recursive wiring is a simple substitution of variables, and thanks to the fact that one only needs to compare $\circlearrowright_{\omega} M$ and $F$ at a syntactical level. Indeed, if any solution exists, then a solution exists with the same number of nodes, the same inputs, the same wirings, and such that the substitution operated by $\omega$ on $M$ leads to the local functions of $F$ written identically: because all local functions are equal on a semantic level, this is always possible, by starting from the local functions of $F$ and operating variable substitutions that are then reversed by the recursive wiring $\omega$ (remark that this last “reversed” construction is not required to be computable in polynomial time).

**Theorem 2.** The Acyclic Unfolding Functional Problem is NP-hard.

**Proof.** Let us provide a reduction from the Feedback Arc Set problem. We provide $f$ a function that for any instance $(G, k)$ of the Feedback Arc Set problem, provides an instance $(F, k)$ of the Optimal Acyclic Unfolding Problem where $S = V(G)$ and $f_s$ is a XOR function of exactly every node $s'$ such that $(s', s) \in A(G)$. This construction is explicitly designed so that the interaction digraph of $F$ is isomorphic to $G$. Clearly $f$ is computable in polynomial time. We also provide $g$ a function that for $(G, k)$ an instance of the Feedback Arc Set problem, and $M$ a solution to the Optimal Acyclic Unfolding Problem, checks if $S = V(G)$, and then deduces the solution for $(G, k)$ the following way: $s$ is part of the feedback arc set if and only if every exiting edge of $s$ has been replaced by a unique consistent input in $M$. This means that the variable $x_s$ has been replaced in every local function in $M$ by the same input variable. Finally $g$ checks that the size of the obtained set is not greater than $k$. It is clear that $g$ is polynomial.

From the definition of $f$ and $g$, it follows that the Feedback Arc Set problem reduces in polynomial time to the Optimal Acyclic Unfolding Problem, which implies the result.

**Example 5.** Consider $S_A$ and $F_A$ of Example 4. Let us define $I_A = \{\alpha\}$. Let $M_A$ be the acyclic module that defines $f'_a(x) = x_\alpha$, $f'_b(x) = f'_c(x) = x_\alpha$, and $f'_d(x) = \neg x_b \lor \neg x_c$. The module $M_A$ is a valid answer to the instance $F_A$, $k = 1$ of the Acyclic Unfolding Functional Problem. The interaction digraph of this module is represented in Figure 3 (left panel).
Example 6. Consider $S_B$ and $F_B$ of Example 2. Let us define $I_B = \{\alpha_{St}, \alpha_{Sl}, \alpha_{Sk}, \alpha_{Pp}, \alpha_{C}, \alpha_{C^*}\}$. Let $M_B$ be the acyclic module that defines $f'_{St}(x) = \neg \alpha_{St}$, $f'_{Sl}(x) = \neg \alpha_{Sl} \lor \neg \alpha_{C^*}$, $f'_{Sk}(x) = \alpha_{Sk}$, $f'_{Pp}(x) = \alpha_{Pp}$, $f'_{Ru}(x) = f'_{S9}(x) = \alpha_{Ru}$, and $f'_{C}(x) = \alpha_{C^*}$. The module $M_B$ is a valid answer to the instance $F_B, k = 6$ of the Acyclic Unfolding Functional Problem. The interaction digraph of this module is represented in Figure 3 (right panel).
Theorem 3. The Output Circuit Computation Problem is in FP.

Proof. First we will assume that every local function in $M$ is provided as a Boolean circuit which does not possess redundant variables. This allows us to deduce the interaction digraph of $M$ in polynomial time.

To compute $X$, we provide an algorithm to compute the output function circuit of any node $s \in S$ in polynomial time.

The algorithm first constructs a list of requirements. This list is initially $R_0 = \{(s, 0)\}$, which can be interpreted to say that we require the construction of the output function of $s$ with added delay 0.

We construct the next list the following way: $(t', d') \in R_{k+1}$ if and only if there exists some $(t, d) \in R_k$ such that $t'$ influences $t$ in $M$.

The total list $R$ is simply defined as $R = \bigcup_{k \in \mathbb{N}} R_k$.

Claim 1. $R$ is computable in polynomial time in the size of $M$.

To see that this is true, consider that for $D$ the maximal depth of $M$, the maximal $d$ such that $(t, d) \in R_k$ for any $k$ is $D$. Indeed since the interaction digraph of $M$ is acyclic, the maximal delay value can only be obtained by following the longest path in $M$. As such we can conclude that the size of any $R_k$ is bounded by $D \times n$, for $n$ the size of the network $M$. Finally, by a similar argument, consider that the list $R$ converges after a maximum of $D$ steps. This implies that the list $R$ is computed after $D$ steps of a $D \times n$ costly process, and $R$ can therefore be computed in polynomial time.

We can construct the Boolean circuit from $R$ in the following way: for every pair $(t, d) \in R$, take an instance of the Boolean circuit which encodes the local function of $t$. Combine all of these instances the following way: any input variable in $I$ is replaced by its delayed counterpart with delay $1+d$. For example, if a variable $\alpha$ appeared in the local function of node $t$, substitute it by the variable $\alpha_{d+1}$. Then, for any gate displaying an input variable $t' \in S$, replace it with the same gate, which rather than taking the value of variable $t'$, takes the value of the output of the circuit that computes the local function of the node $t'$ with added delay $d+1$. By definition of $R$ this circuit will always be in $R$. The obtained circuit computes the output function of the node $s$.

Repeat this process for every $s \in X$. 

In the rest of this paper, output functions are always considered encoded as Boolean circuits. The following example uses Boolean formulae instead for the sake of readability.

Example 7. Consider $M_A$ of Example 3. Let $X_A = \{d\}$ be an instance of the Output Circuit Computation Problem. The circuit $O_d = \alpha_3$ is a valid answer to that instance.

Example 8. Consider $M_B$ of Example 6. Let $X_B = \{St, Sk, Sl, Pp, C, C\}$ be an instance of the Output Circuit Computation Problem. The circuits $O_{St} = \neg \alpha_{sl,1}$, $O_{Sl} = \neg \alpha_{sl,1} \lor \alpha_{C,1}$, $O_{Sk} = \alpha_{sl,1} \lor \neg \alpha_{sk,1}$, $O_{Pp} = \alpha_{sl,1} \lor \neg \alpha_{pp,1}$, $O_C = \alpha_{sk,2} \land \neg \alpha_{pp,2} \land \alpha_{c,2} \land \alpha_{C,2}$, $\neg \alpha_{sl,1}$ and $O_{C\neg} = \alpha_{C,2} \lor \neg \alpha_{pp,2}$ taken altogether are a valid answer to that instance.
5 Optimal acyclic module synthesis

5.1 Module Synthesis

This part of the process takes in a set of output functions and generates a module that realizes these functions with an hopefully minimal number of nodes. In this part the actual optimisation of the pipeline, if any, can be directly observed. It is also the part of the pipeline which is the most computationally costly.

Module Synthesis Problem

**Input:** A set $I$ of input labels, a finite set of output functions $O$, encoded as Boolean circuits, defined on those labels, and $k$ an integer.

**Output:** An acyclic module $M$ with at most $k$ nodes such that every function in $O$ is the output function of at least one node in $M$.

5.2 Complexity results

**Theorem 4.** The Module Synthesis Problem is coNP-hard.

**Proof.** Consider $f$ an instance of the Tautology problem, with $I$ the set of propositional variables contained in $f$. We define $f_2$ as the output function defined on the labels $I$ such that $f'$ is obtained from $f$ by substituting all variables $\alpha \in I$ by their equivalent of delay 1, $\alpha_1$. Let us also define 1 as the constant output function of delay 0 which value is always 0. We compose an instance of the Module Synthesis Problem with $I$ the set of input labels, $O = \{f', 1\}$ and $k = 0$. This instance has a solution if and only there exists an acyclic module with only one node such that the output function of this node is equivalent to all the output functions in $O$. This implies that, if the problem has a solution, $f'$ is equivalent to 1, which proves that $f'$ is a tautology. Therefore computing the output of the Module Synthesis Problem requires solving a coNP-hard decision problem. \qed

**Theorem 5.** The Module Synthesis Problem is in $FNP^{coNP}$.

**Proof.** Consider the following algorithm. First, guess an acyclic module $M$, with size $k$. Compute every output function of the network, which is in FP. Then simply check that every function in $O$ is equivalent to at least one output function in $M$, which requires at most $|M| \times |O|$ calls to a coNP oracle. \qed

5.3 Refining the complexity bounds

It is unclear whether the synthesis problem can be proven to be in FcoNP or to be NPcoNP-hard. An attempt has been made to prove the former by using a greedy algorithm which would fuse nodes in an acyclic module, starting from a trivially large enough module. This method requires solving the following problem:
Module Local Fusion Problem

**Input:** An acyclic module $M$ defined on sets $S$ and $I$, and $a$, $b$ two different nodes.

**Question:** Is there a local function $f_c$ such that there exists some acyclic module $M'$ defined on the node set $S \cup \{c\} \setminus \{a, b\}$ and input set $I$, such that $f_c \equiv f'_c$ and $O_s \equiv O'_s$ for $s \in S \setminus \{a, b\}$?

This problem formalises the idea of replacing two nodes by one in an acyclic module, such that every other output function in the module is conserved. Assuming the removed nodes are not considered outputs of the network is an important step of any greedy algorithm that would try to optimise the size of an acyclic module.

It is rather simple to prove that this problem is coNP-hard, since its computation requires checking the equivalence of multiple pairs of Boolean circuits. It is also rather easy to see that it is in NP$^{\text{coNP}}$, as one can guess $f_c$ and $M'$ in polynomial time and verify the solution using a polynomial amount of calls to a coNP oracle, one for every equivalence check.

The function $f_c$ could be composed as a binary function of the results of $f_a$ and $f_b$, as it is intuitive to suppose that assuming such a fusion is possible, then every node influenced by $a$ or $b$ should be computable from such a composition of $a$ and $b$. The issue however is that this process requires modifying every node influenced by $a$ or $b$ such that their output functions match the output functions in $M$.

It is unclear that there should exist a method in coNP to ensure this modification such that the output functions are conserved. This leads us to believe that a greedy algorithm wouldn’t prove the Optimal Module Synthesis Problem to be in FcoNP.

Similarly, it is interesting to consider the open question of whether or not the Module Synthesis Problem can be proven NP$^{\text{coNP}}$-hard. This implies to prove, between other things, that the problem is NP-hard. This is, to us, another open problem as the Module Synthesis Problem does not seem equipped to compute the satisfaction of a Boolean formula or circuit.

### 5.4 Similarities to other optimisation problems

This open question bears strong ressemblance to another open problem that concerns Boolean circuits. The Circuit Minimisation Problem is a problem that asks to provide a Boolean circuit below a given size such that it computes a Boolean function given as a truth table as the input of the problem [11]. The problem is trivially in NP but it is not known whether the problem is in P or NP-hard, as both possibilities imply proving other results which seem beyond the currently known techniques. The same problem has been found to be NP-complete in both restricted (DNFs) and generalised (unrestricted Boolean circuits) variations of the Boolean circuit model [10].

There are strong similarities between acyclic modules and Boolean circuits. Both are defined on acyclic digraphs, have inputs and outputs, and compute
Boolean functions. It is important to note that this analogy is misleading when talking about the optimisation of their size. Optimising a Boolean circuit requires the optimisation of a Boolean function in terms of the number of gates that computes it. Optimising an acyclic module, however, requires the optimisation of a network of functions with respect to a notion of delay of the inputs, whereas in this case one node may contain an arbitrary Boolean function. As such these problems seem too independent to provide any reduction between them.

5.5 Examples

Example 9. Consider the output function $O_d$ defined in Example 7. Let us define $M'_A$ as the module defined on $S'_A = \{a, b, d\}$ and $I_A = \{\alpha\}$, such that $f'_a = x_\alpha$, $f''_a = x_\alpha$ and $f_d = \neg x_b$. The module $M'_A$ is a valid answer to the instance $I_A, \{O_d\}, k = 3$ of the Module Synthesis Problem. The interaction digraph of this module is depicted in Figure 4 (left panel).

Example 10. Consider the output functions $O_B = \{O_{St}, O_{Sl}, O_{Sk}, O_{Pp}, O_{C}, O_{C^*}\}$ defined in Example 8. Let us define $M'_B$ as the module defined on $S'_B = \{St, Sl, Sk, Pp, Ru, C25, C^*\}$ and $I_B = \{\alpha_{St}, \alpha_{Sl}, \alpha_{Sk}, \alpha_{Pp}, \alpha_C, \alpha_{C^*}\}$, such that $f'_{St}(x) = \neg x_{\alpha_{St}}, f''_{St}(x) = \neg x_{\alpha_{St}} \lor x_{\alpha_{C^*}}, f''_{Sl}(x) = x_{\alpha_{Sl}} \lor \neg x_{\alpha_{sk}}, f''_{Sk}(x) = x_{\alpha_{Sl}} \lor \neg x_{\alpha_{Sk}}, f''_{Pp}(x) = x_{\alpha_{Sl}} \lor \neg x_{\alpha_{Pp}}, f''_{Ru}(x) = \neg x_{\alpha_{Sl}} \lor x_{\alpha_{Pp}} \lor \neg x_{\alpha_{C}} \lor \neg x_{\alpha_{C^*}}, f''_{C25}(x) = \neg x_{\alpha_{Ru}} \lor \neg x_{\alpha_{Sl}}$, $f''_{C^*}(x) = x_{C25}$, and $f''_{C}(x) = x_{C25}$. The module $M'_B$ is a valid answer to the instance $I_B, O_B, k = 8$ of the Module Synthesis Problem. The interaction digraph of this module is depicted in Figure 4 (right panel).

6 Final wiring and analysis

The final step in the pipeline is simply to wire the module obtained in Section 5 so that the obtained networks hold isomorphic attractors to the input network.
This is ensured by application of the following result.

**Theorem 6 (18).** Let $M$ and $M'$ be two acyclic modules, with $T$ and $T'$ subsets of their nodes such that $|T| = |T'|$. If there exists $g$ a bijection from $I$ to $I'$ and $h$ a bijection from $T$ to $T'$ such that for every $s \in T$, $O_s$ and $O'_{h(s)}$ have same delay, and for every input sequence $j$ with length the delay of $O_s$,

$$O_s(j) = O'_{h(s)}(j \circ g^{-1})$$

then for any function $\omega : I \to T$, the networks $\circ_\omega M$ and $\circ_{h^{-1}} M'$ have isomorphic attractors (up to the renaming of automata given by $h$).

Applying this theorem to the current problem is simple: the module $M$ is the module obtained in Section 3 and the module $M'$ is the module obtained in Section 5. The set $T$ is the set of nodes which are substituted by new inputs in the process described in Section 3. The set $T'$ is the set of nodes in $M'$ which are considered as the output of the module, for example when the module $M'$ is obtained as the result of the application of the functional problem defined in Section 5.

As modules $M$ and $M'$ are defined over the same set of inputs, the bijection $g$ is the identity. The bijection $h$ is directly constructed so that for all $s \in T$, $h(s)$ in $M'$ has an equivalent output function as $s$ in $M$, which is always possible thanks to the careful structure of our pipeline. It follows quite clearly that for any $s \in T$, and for any input sequence $j$, $O_s(j) = O'_{h(s)}(j \circ g^{-1})$ holds, and the theorem applies.

**Example 11.** Consider $M'_A$ of Example 10 Let $\omega_A(\alpha) = d$. The AN $\circ_\omega A M'_A$ is defined over $S'_A = \{a, b, d\}$ such that $f''_a(x) = x_d$, $f''_b(x) = x_a$, $f''_d(x) = \neg x_b$. The interaction digraph of this module is depicted in Figure 5 (left panel).

**Example 12.** Consider $M'_B$ of Example 10 Let $\omega_B(\alpha_s) = s$, for all $s \in X_B$. The AN $\circ_\omega B M'_B$ is defined over $S'_B = \{St, Sl, Sk, Pp, Ru, C25, C\}$ such that $f''_{St}(x) = \neg x_{St}$, $f''_{Sl}(x) = \neg x_{Sl} \lor x_C$, $f''_{Sk}(x) = x_{Sl} \lor \neg x_{Sk}$, $f''_{Pp}(x) = x_{St} \lor \neg x_{Pp}$, $f''_{Ru}(x) = \neg x_{St} \lor x_{Pp} \lor x_C \lor \neg x_C$, $f''_{C25}(x) = \neg x_{St} \lor \neg x_{Sl} \lor x_{C25}$. The interaction digraph of this module is depicted in Figure 5 (right panel).

This allows us to compute the attractors of any BAN by computing the dynamics of another BAN with possibly less nodes, thus dividing the number of computed configurations by some power of two. Examples throughout this paper showcase the application of the pipeline over two initial examples.

Examples 1, 5, 7, 9, 11 and 13 show the optimisation of a simple four nodes network into a three nodes equivalent network. The optimisation proceeds here by ‘compacting’ two trivially equivalent nodes, $b$ and $c$, into one. The resulting BAN has dynamics $2^1$ times smaller than the initial network, with isomorphic attractors. Examples 2, 11, 10, 100 and 11 show the optimisation of a larger, more intricate network which is drawn from a model predicting the cell cycle sequence of fission yeast [10]. This practical example, processed through our
pipeline, reduces from 10 nodes to 8. This implies a reduction in dynamics size of $2^2$, while keeping isomorphic attractors. Both sets of examples are illustrated throughout the paper in Figures 2, 3, 4 and 5.

7 Conclusion

The present paper showcases an innovative way of reducing the cost of computing the attractors of Boolean automata networks. The method provides better optimisation on networks showing structural redundancies, which are removed by the pipeline. The limitations of this method are still significant; it requires solving a problem that is at least coNP-hard, and believed to be FNP$^{coNP}$-complete. As it presently stands, this method is not as much a convincing practical tool as it is a good argument in favor of the powerfulness of acyclic modules, their output functions, and the approaches they allow together towards the computation of BAN dynamics.

Future perspectives include finding better Complexity bounds to the Module Synthesis Problem, and generalising the formalism of output functions and the optimisation pipeline to different update schedules distinct from the parallel one.

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