Pair Diagram and Cyclic Properties
Characterizing the Inverse of Reversible Automata

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Received: November 1, 2006. Accepted: February 1, 2007.

Professor Harold V. McIntosh has realized deep and elegant contributions in the analysis and understanding of cellular automata. Inspired in his work about applying graph and algebraic tools in the study of reversible automata, this paper implements some of his ideas and results for characterizing the features of the inverse rule for a reversible one-dimensional cellular automata. In particular, we use the pair diagram for knowing the size of the inverse neighborhood and the position of its evolution and we take advantage of the cyclic behavior in finite configurations for obtaining the inverse local rule.

Keywords: Reversible cellular automata, pair diagram, cyclic evolutions.

1 INTRODUCTION

Since their conceptualization by von Neumann [16], cellular automata have represented a relevant knowledge field both by their relevant practical applications in physics, chemistry, biology, computer science, etc [1,4,17], and by the interesting theoretical questions about the complexity raised from dynamical systems rules by simple local interactions.

In the last case several paths have been taken in the analysis of cellular automata looking for a deep comprehension of their properties and searching

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the characterization of special types of cellular automata showing well-defined and significant behaviors; one of them has been the analysis of reversible automata. For the one-dimensional case, there are classic references describing their local features from a topological [6] and graphical [12] point of view, characterizing their global behavior by permutations [8] and establishing precise bounds for the inverse local behavior [5].

The previous references have been part of the inspiration in the work developed by McIntosh for bringing a deeper understanding of the reversible phenomena in cellular automata through the application of graphic and matrix tools, in particular investigating in detail the properties of de Bruijn diagrams in order to obtain computational algorithms and analytic tools for studying and classifying different kinds of reversible automata [9–11, 13–15]. Some of the results provided for these papers and other ones proposed by Boykett [2] and Kari [7] for simulating every one-dimensional cellular automata by another with neighborhood size 2 will be combined for providing an algorithm for calculating the size, position and description of an inverse rule for a given reversible one-dimensional cellular automaton.

In particular we shall use the pair diagram, a graph produced from the cartesian product of the de Bruijn diagram, and we shall prove that its features are useful for knowing the size and the mapping position of the inverse rule. From this characterization we shall apply the cyclic properties of the global mapping of reversible automata over finite configurations to calculate the complete inverse rule.

The paper is organized as follows: section 2 provides the basic concepts of reversible one-dimensional cellular automata, section 3 gives the definition and properties of the pair diagram and how these ones characterize the inverse rule. Section 4 explains the cyclic properties of reversible automata and their application to establish the inverse rule, section 5 gives an example of the results obtained in the paper and the section 6 exposes the concluding remarks of the manuscript. Finally, section 7 explains the nomenclature utilized during the development of the study.

2 BASIC CONCEPTS

A one-dimensional cellular automaton $A = \{m_k, m, M_\varphi\}$ consists of a finite set of states $K$ where $|K| = m_k$, form $m \in \mathbb{Z}^+$ let $K^m$ be the set of sequences with $m$ states, let $E$ be the empty word where $K^0 = \{E\}$; for $w \in K^m$ and $n \in \mathbb{Z}^+$ let $w^n$ be the sequence formed by $n$ repetitions of $w$ and for $\{w_1, w_2\} \subseteq K^m$ let $w_1w_2 \in K^{2m}$ be the usual concatenation of sequences. When needed, the elements of $w \in K^m$ will be indexed from left to right starting from 0 by means of brackets; thus for $0 \leq i < j < m$, $w[i,j]$ is the state placed at position $i$ and $w[i,j]$ is the block of states in $w$ from $i$ to $j$.

The dynamics of the automaton is specified by a mapping $\varphi: K^{mn} \rightarrow K$ where each $w \in K^{mn}$ is a neighborhood, $m \in \mathbb{Z}^+$ is the neighborhood size.
and $\varphi$ is the evolution rule of the automaton; for the non-trivial case we take $m_n > 1$. The evolution rule can be represented by a matrix $M$, where the row and column indices are the sequences in $K^{m_n-1}$ and for each $\{a, b\} \subseteq K$ and every $w \in K^{m_n-2}$, the entry with indices $(aw, wb) = \varphi(aw, wb) \in K$.

The previous matrix is known as the de Bruijn matrix of the automaton [9].

The definition of the evolution rule can be extended for larger sequences; for each $n \geq m_n$ and every $w \in K^n$, $\varphi(w)$ means to apply the rule over all the overlapping neighborhoods in $w$, that is, $\varphi(w) = v \in K^{n-m_n+1}$.

In this paper we shall use finite global states for the automata; form, $c \in Z^+$ an initial global state or configuration $c^0 \in K^mc$ is taken; the upper index indicates the current time of the automaton and when it is understood, the configuration will be only defined by $c$. Similar to the case of sequences, for $i, j \in \mathbb{N}$ with $j > i$ let $c_{[i]}$ be the state at position $c_{[i]}$ where $i' = i \mod m_c$; and let $c_{[i,j]}$ be the sequence of states comprised from $c_{[i]}$ to $c_{[j]}$.

For every $i \in \{0, \ldots, m_c\}$, we have that $c^0_{[i]} = \varphi(c^0_{[i,i+m_n-1]})$ where $c^0_{[i]}$ is placed centered below of the sequence $c^0_{[i,i+m_n-1]}$. We take periodic boundary conditions concatenating $c^0_{[0]}$ with $c^0_{[m_c-1]}$ forming a ring; in this way every cell $c^0_{[i]}$ has a complete neighborhood. The simultaneous application of $\varphi$ over all the neighborhoods in $c^0$ yields a new configuration $c^1 \in K^mc$; this process is indefinitely repeated producing a global function $\Phi : K^mc \rightarrow K^mc$ establishing the dynamics of the automaton.

Taking advantage of the features previously described we can take any pair $\{w_1, w_2\} \subseteq K^{m_n-1}$, hence $\varphi(w_1w_2) = w_3 \in K^{m_n-1}$.

We can take a new set of states $S$ such that $|S| = m_k^{m_n-1}$ and define any bijection $r : S \rightarrow K^{m_n-1}$; then $\tau^{-1}(w_1w_2) \in S^2, \tau^{-1}(w_3) \in S$ and the evolution rule can be also defined as $\varphi : S^2 \rightarrow S$. This result is described by Boykett [2] and Kari [7] and shows that every one-dimensional cellular automaton can be simulated by another with neighborhood size 2; for every $A = \{m_k, 2, M_i\}$, the indices of $M_i$ are the states of $K$ and for every pair $\{a, b\} \subseteq K$, the entry $(a, b) = \varphi(ab)$. In this way all the results obtained for this kind of automata are extensive for all the other cases and therefore in the rest of this paper we shall only study examples with neighborhood size 2.

Given a cellular automaton $A = \{m_k, 2, M_i\}$, for every $m \in Z^+$ and each $w \in K^m$, let $\Lambda(w) = \{v \mid v \in K^{m+1}, \varphi(v) = w\}$; that is, $\Lambda(w)$ is the set of sequences or ancestors evolving into $w$. For every $w \in K^m$ and each $0 \leq i \leq m$, $\Lambda_i(w) = \{a \in K \mid$ there exist $w_1 \in K^i$ and $w_2 \in K^{m-i}$ such that $\varphi(w_1aw_2) = w\}$; that is, $\Lambda_i(w)$ is the set of states at position $i$ in the ancestors of $w$. For $w \in \Lambda(w)$, if $v_{\{0\}} = v_{\{m\}}$, then a cyclic ancestor of $w$ is defined as $v' = v_{\{0,m-1\}}$ where periodic boundary conditions can be taken over $v'$ for obtaining an ancestor of $w$ with the same length.

A special kind of cellular automata is the one where the global dynamics is invertible, this type of automata is called reversible. A reversible one-dimensional cellular automaton $A_R = \{m_k, 2, M_i, m_l, m\}$ is characterized
for the existence of another inverse automaton $A_R^{-1} = \{m_k, m_n^{-1}, \varphi^{-1}, m_l^{-1}, m_r^{-1}\}$ (commonly $m_n^{-1} > 2$) such that for each $m \geq m_n^{-1}$, every sequence in $K^m$ has one and only one cyclic ancestors in $A_R^{-1}$. This implies the existence of an inverse function $\Phi^{-1}(c^i+1) = c^i$ for every $i \in \mathbb{Z}$. Reversible one-dimensional cellular automata are locally characterized from a topological and graph-theoretical viewpoint in the papers by Hedlund [6] and Nasu [12]; from these works three main properties are formalized:

**Property 1.** For every $m \in \mathbb{Z}^+$ and each $w \in K^m$, $|\Lambda(w)| = m_k$.

**Property 2.** For every $m \geq m_n^{-1}$, each $w \in K^m$ and for some $0 < i < m$; we have that $|\Lambda_0(w)| = m_l$, $|\Lambda_i(w)| = 1$ and $|\Lambda_m(w)| = m$, holding that $m_l m_r = m_k$. Values $m_l$ and $m_r$ are called the left and right Welch indices.

**Property 3.** For every $m \geq m_n^{-1}$ and each pair $\{w_1, w_2\} \subseteq K^m$; we have that $|\Lambda_m(w_1) \cap \Lambda_0(w_2)| = 1$. Set $\Lambda_m(w_1) \subseteq K$ is the right Welch set of $w_1$ and $\Lambda_0(w_2)$ is the left Welch set of $w_2$.

The previous properties show that in a reversible automaton, the ancestors of every sequence with the appropriated size have their differences at the extremes, sharing a common state at the same position defining the inverse evolution rule. In the next section we shall use a special diagram for knowing the size and position of the inverse mapping.

### 3 Pair Diagram

The pair diagram is a tool used by McIntosh for knowing if a given one-dimensional cellular automaton is reversible [9, 10]; in this paper we shall use this diagram and its matrix representation for developing our results. For a reversible automaton $A_R = \{m_k, 2, m_l, m_r\}$, let $P_\varphi$ be its pair matrix, where the row and column indices are the elements in $K \times K$ and for every entry $\omega = \{ (a_1, a_2), (b_1, b_2) \} \subseteq K \times K$ we have that:

$$\alpha = \begin{cases} 1 & \text{if } \varphi(a_1 b_1) = \varphi(a_2 b_2) \\ 0 & \text{otherwise} \end{cases}$$

Thus $P_\varphi$ relates pairs of states where the concatenation between corresponding elements evolve into the same state. For every $\{a, b\} \subseteq K$ with $a \neq b$, $(a, a)$ is a basic index and $(a, b)$ is a composed index of $P_\varphi$. Let $P_\varphi(a, b)$ be the element in $P_\varphi$ at position $(a, b)$; a null row in $P_\varphi$ is a row where all its elements are 0, analogously a null column is defined. Let $d_r$ be a $0 \rightarrow 1$ vector with $m_k^2$ elements; for $0 \leq i < m_k^2$, $d_r(i)$ is the i-th element in $d_r$ where:

$$d_r(i) = \begin{cases} 1 & \text{if } i \text{ is not a null row in } P_\varphi \\ 0 & \text{otherwise} \end{cases} \quad (1)$$
similarly, vector $d_c$ and elements $d_c(i)$ are specified. Matrix $P$, represents an adjacency matrix corresponding to the pair diagram $D = \{ V_{D_\Phi}, E_{D_\Phi} \}$, where the nodes of the diagram are described by $V_{D_\Phi} = K \times K$ and the directed edges are presented by $E_{D_\Phi} \subseteq V_{D_\Phi} \times V_{D_\Phi}$ where for $(d_0, d_1) \in E_{D_\Phi}$, there is a directed link $l^1 \in E_{D_\Phi}$ from $d_0$ into $d_1$ if $p, (d_0, d_1) = 1$; where $l^1_0 = d_0$ and $l^1_1 = d_1$. If $d_0 = (a_0, a_1)$ and $d_1 = (b_0, b_1)$, then the directed edge $l^1$ is labeled by the state $a = \varphi(a_0b_0)$.

Generalizing, for every $m \in \mathbb{Z}^+$, each path $l^m$ has an associated label $w \in K^m$ and for $0 \leq i \leq m$, let $l^m_i \in V_{D_\Phi}$ be the $i$-th node in $l^m$. For $0 \leq i < j < m$, a cycle $l^m_i$ is a path in $D$, such that $l^m_{\lambda,0} = l^m_{\lambda,m}$. Let $V_{D_\Phi}^b = \{ d \in V_{D_\Phi} \mid d = (a, a) \}$ be the set of basic nodes and let $V_{D_\Phi}^c = \{ d \in V_{D_\Phi} \mid d = (a, b) \}$ be the set of composed nodes in $D$. Properties of the pair diagram shall be explored for characterizing the inverse rule of a reversible automaton; part of the next results are based on those obtained by McIntosh \cite{9, 10, 13}.

**Lemma 1.** Given a reversible automaton $A_R = \{ m_k, 2, M_\varphi, m_I, m_r \}$, for every $m \in \mathbb{Z}^+$ and $0 \leq i \leq m$, there is not a path $l^m_i$ such that $l^m_{\lambda,i} \in V_{D_\Phi}^c$.

**Proof.** Suppose the contrary, that there exists $l^m_i$ such that $l^m_{\lambda,i} = (a, b)$ where $a \neq b$ for some $i \in \{0 \ldots m\}$. The cycle has a label $v \in K^m$ and the nodes forming it determine two distinct ancestors $\{ w_0, w_1 \} \subseteq \Lambda(v)$. Thus we have that $w_0[0] = w_0[m]$ and $w_1[0] = w_1[m]$; therefore two cyclic ancestors $u_0 = w_0[0, m-1]$ and $u_1 = w_1[0, m-1]$ can be defined where for $j = i \mod m$ we have that $u_0[j] \neq u_1[j]$. Hence for every $n \in \mathbb{Z}^+$, $u_0^n$ and $u_1^n$ are cyclic ancestor of $v^n$, contradicting the definition of $\Phi^{-1}$.

A direct result from Lemma 1 is established as follows:

**Corollary 1.** Given a reversible automaton $A_R = \{ m_k, 2, M_\varphi, m_I, m_r \}$, for every $m \in \mathbb{Z}^+$ and $0 \leq i_1 < i_2 < i_3 \leq m$, there is not a path $l^m$ in $D_\Phi$ such that $\{ l^m_{i_1}, l^m_{i_3} \} \subseteq V_{D_\Phi}^b$ and $l^m_{i_2} \in V_{D_\Phi}^c$.

**Proof.** Suppose the contrary; for $l^m_{i_1} = \{ a_1, a_1 \}$ and $l^m_{i_2} = \{ a_2, a_2 \}$ we have that $\varphi(a_2, a_1) = a_3 \in K$. Therefore for $n_1 = i_3 - i_1 + 1$ and $n_2 = i_2 - i_1$, there exists a cycle $l^m_{\lambda,0} = l^m_{\lambda,n_1} = 1$ and $l^m_{\lambda,n_2} = l^m_{i_2}$; but $l^m_{i_2} \in V_{D_\Phi}^c$, contradicting Lemma 1.

Paths in the pair diagram indicate if a cellular automaton is reversible or not; but more information can be obtained of them. Let $m_i = \max\{ m \mid m \in \mathbb{Z}^+, \text{ for } 0 \leq i < m, l^m_i \in V_{D_\Phi}^c \text{ and } l^m_i \in V_{D_\Phi}^b \}$ and let $m_o = \max\{ m \mid m \in \mathbb{Z}^+, \text{ for } 0 < i \leq m, l^m_i \in V_{D_\Phi}^b \text{ and } l^m_i \in V_{D_\Phi}^c \}$. Using $m_i$ and $m_o$ the next results can be formulated:

**Theorem 1.** Given a reversible automaton $A_R = \{ m_k, 2, M_\varphi, m_I, m_r \}$, $m_n^{-1} \leq m_i + m_o$. 

Proof. Let us take $n = m_i + m_o$ and every path $l^n$ in $D^*$; for each $m_1 \leq m_i$ and $0 \leq i_1 < m_1$, if $l^n_{i_1} \in V^b_{D^0}$ and $l^n_{m_1} \in V^b_{D^0}$; by Lemma 1 and the maximality of $m_o$, for $m_2 = m_i - m_1$ and $0 \leq i_2 \leq m_2$ we have that $l^n_{i_2} \in V^b_{D^0}$. In the same way, for each $m_1 \leq m_o$ and $0 \leq i_1 < m_1$, if $l^n_{m_o - i_1} \in V^b_{D^0}$ and $l^n_{m_o - m_1} \in V^b_{D^0}$; by Lemma 1 and the maximality of $m_i$, for $m_2 = m_o - m_1$ and $0 \leq i_2 \leq m_2$ we have that $l^n_{m_o - m_1 - i_2} \in V^b_{D^0}$. Therefore for each $w \in K^n$, $|\Lambda m_i(w)| = |\Lambda n - m_o(w)| = 1$ and $m_o^{-1} \leq m_i + m_o$. 

Proof of Theorem 1 assures the following results:

Corollary 2. For every $w \in K^{m_i + m_o}$; $|\Lambda m_i(w)| = 1$, defining an inverse mapping yielding a global invertible behavior.

Corollary 3. For a reversible automaton $A_R = \{m_k, 2, M_\varphi, 1, m_k\}, m_o^{-1} = m_o$.

Corollary 4. For a reversible automaton $A_R = \{m_k, 2, M_\varphi, m_k, 1\}, m_i^{-1} = m_i$.

Theorem 1 proves that only values $m_i$ and $m_o$ are needed for establishing an adequate length to define an inverse mapping. In this sense the problem is now to find a way for calculating such values; we shall resolve this question through a numerical procedure based on Warshall’s algorithm over the matrix $P$. Since we are only interested in paths where the initial or the final node is a basic one and all the others are composed ones, all the links between basic nodes will be omitted in order to obtain a correct computation of $m_i$ and $m_o$.

Pseudocode 1 (Calculating $m_i$ and $m_o$).

$m_i = m_o = 0$ Initializing values according to Welch indices

$IF (m_i = 1) THEN m_o = 1$
$IF (m_o = 1) THEN m_i = 1$

FOR ($i \in V^b_{D^0}$) Removing links between basic nodes

FOR ($f \in V^b_{D^0}$)

$p_\varphi(i, f) = 0$

FOR ($t \in V^b_{D^0}$) Choosing intermediate nodes

$IF (d(t, i) = 1) THEN$ Avoiding isolated nodes

FOR ($i \in V^b_{D^0}$) Choosing initial nodes

$IF (t \neq i AND p_\varphi(i, t) > 0) THEN$

FOR ($f \in V^b_{D^0}$) Choosing final nodes

$IF (d_c(f) = 1) THEN$

$IF (t \neq f AND i \neq f AND p_\varphi(t, f) > 0) THEN$

$IF (p_\varphi(i, f) < p_\varphi(i, t) + p_\varphi(t, f)) THEN$

$p_\varphi(i, f) = p_\varphi(i, t) + p_\varphi(t, f)$

$IF (f \in V^b_{D^0} AND m_i < p_\varphi(i, f)) THEN$

$m_i = p_\varphi(i, f)$

$IF (i \in V^b_{D^0} AND m_o < p_\varphi(i, f)) THEN$

$m_o = p_\varphi(i, f)$
The results obtained in this section will be complemented with the cyclic properties of a reversible automaton over finite configurations in order to obtain an explicit calculation of its inverse behavior.

4 CYCLIC PROPERTIES IN REVERSIBLE AUTOMATA

In the study of dynamical systems ruled by an invertible mapping, a common option is to investigate cyclic behaviors in correspondence to the mapping in order to characterize the system. This is the case of reversible automata; this section shall take their cyclic properties to find an adequate inverse mapping for a given evolution rule. In the case of a reversible automaton with finite neighborhood size, for every \( m \geq m \), and each \( w \in K^m \) the global mapping iteratively applied over \( w \) yields a cyclic evolution represented by the sequence \( C = \{c_0, c_1, \ldots, c_t\} \); where for \( 0 \leq i < t \), \( \Phi(c_i) = c_{i+1} \) and \( \Phi(c_t) = c_0 = w \).

For each \( j \in \mathbb{N} \), \( 0 \leq i < m \), \( n = (i + j) \mod m \) and any \( w \in K^m \), let \( s_j(w) = v \in K^m \) where \( w_i = v_n \); thus \( w \) is a shift operator over \( w \). Indeed, every \( w \in K^m \) may represent at most \( m \) different sequences \( \{s_0(w), s_1(w), \ldots, s_{m-1}(w)\} \); where it is clear that \( s_0(w) = w \). In this way; applying the shift operator, a cyclic evolution may also represent at most \( m \) distinct cyclic evolutions. In this sense we shall expand our notation of a cyclic evolution, so that if \( C = \{c_0, c_1, \ldots, c_t\} \) then \( C = \{s_t(c_0), s_i(c_1), \ldots, s_i(c_t)\} \); therefore \( C = C^0 \).

Due to the finiteness of \( K^m \), there exists \( n \in \mathbb{Z}^+ \) such that for some \( i \in \{0, \ldots, n-1\} \) and for some \( j \in \{0, \ldots, m-1\} \) there is a family \( \mathcal{F}^m = \{C_0^1, C_0^2, \ldots, C_{n-1}^m\} \) where for every \( w \in K^m \) we have that \( w \in C_i^j \). Given a reversible automaton \( A_R \), \( \mathcal{F}^m \) induces an equivalence relation \( f^m \) over \( K^m \); for any pair \( \{w_1, w_2\} \subseteq K^m \), \( w_1 f^m w_2 \) if there exists a pair \( \{j_1, j_2\} \subseteq \{0, \ldots, m-1\} \) and some \( C_i^j \in \mathcal{F}^m \) holding that \( s_{j_1}(w_1) = s_{j_2}(w_2) \in C_i^j \). Therefore, the invertible global behavior of \( A_R \) yields that \( f^m \) be a partition of \( K^m \); so we can use this family in order to find the inverse evolution rule.

**Theorem 2.** Given a reversible automaton \( A_R = \{m_k, 2, M_\varphi, m_1, m_r\} \), for \( m = m_i + m_o \); an inverse evolution rule \( \varphi^{-1} \) can be calculated using \( f^m \).

**Proof:** For each \( w \in K^m \), there exists \( c_i^i \in C_j^i \in \mathcal{F}^m \) where \( n_1 = |C_j^i| \) such that \( w f^m c_i^i \) for some \( i_1 \in \{0, \ldots, n_1 - 1\} \). In this way \( \Phi_{n_1}(w) = w \); hence \( \Phi_{n_1-1}(\Phi(w)) = w \) implying that \( \Phi_{n_1-1} = \Phi^{-1} \). Thus \( c_i^i \) is a cyclic ancestor of \( c_i^i \) and for \( i_2 \in \{0, \ldots, m-1\} \) we have that \( s_{i_2}(w) = c_i^i \). By Corollary 2, \( |\Lambda_{m_i}(c_i^i)| = 1 \); therefore \( \varphi^{-1}(w) = c_{i_2}^{i_2+1} \). \( \square \)

**Proof of Theorem 2** reflects a constructive process for obtaining the inverse rule of a reversible automaton. First we have to calculate all the cyclic evolutions in \( \mathcal{F}^m \) form \( m = m_i + m_o \) and form a vector \( t \) keeping the inverse mapping for every sequence \( w \in K^m \). For every \( i \in \mathbb{N} \), let \( i_{\text{base}}(m_i) \) be the mapping
taking $i$ into its corresponding number in base $m_k$; with this, the indices of $t$ are defined by $b_{m_k}(w) = i$ where $i_{\text{base}(m_k)} = w$; with $b_{m_k}^{-1}(i) = w$.

**Pseudocode 2 (Inverse mapping for each $w \in K^m$).**

```
m = m_i + m_o
FOR ($i_1 \in \{0, \ldots, m_k - 1\}$) Initializing the vector
    $t_{i_1} = -1$
    $j_1 = 0$
WHILE ($j_1 < m_k^m$) Taking all the sequences in $K^m$
    $j_2 = 0$
    WHILE ($t_{j_2} \neq -1$) Finding the first free sequence
        $j_2 = j_2 + 1$
        $w = b_{m_k}^{-1}(j_2)$
    DO Calculating the cyclic evolution
        $v = \Phi(w)$
        FOR ($i_1 \in \{0, \ldots, m - 1\}$) Taking all the shifts for $v$
            $i_2 = b_{m_k}(s_{i_1}(w))$
            IF ($t_{i_2} = -1$) Checking for a free sequence
                $u = s_{i_1}(w)$
                $t_{i_2} = um_i$
                $j_1 = j_1 + 1$
            Setting the inverse mapping of $v$
            $w = v$
        WHILE ($b_{m_k}(v) \neq j_2$)
```

The algorithm has order $O(2m_k^m)$ since for each sequence we have at most two operations, one reviewing if the sequence has been selected and other calculating the corresponding cyclic evolution. An example showing the results developed in the work will be depicted in the next section.

5 **ILLUSTRATIVE EXAMPLE**

In this section we shall expose the results obtained in the work taking a reversible automaton with four states and with both Welch indices equal to 2. The matrix representing the pair diagram of the automaton will be constructed, then Algorithm 1 will be used for obtaining a valid inverse neighborhood size and Algorithm 2 will be applied for obtaining the mapping of the neighborhoods associated with the inverse rule. Finally we depict an example showing the evolution of the automaton from a random configuration taking periodic boundary conditions, both in the original and in the inverse sense applying the evolution rule obtained by Algorithm 2. Let us take the automaton
\[ \mathcal{A}_R = \{4, 2, M_\varphi, 2, 2\} \] where the matrix \( M_\varphi \) is defined as follows:

\[
M_\varphi = \begin{bmatrix}
0 & 1 & 0 & 1 \\
1 & 0 & 1 & 0 \\
2 & 2 & 3 & 2 \\
3 & 3 & 2 & 2 \\
\end{bmatrix}
\]

For \( M_\varphi \), the matrix \( P_\varphi \) representing the pair diagram of \( \mathcal{A}_R \) can be constructed following the steps described in Section 3.

\[
P_\varphi = \begin{bmatrix}
(00) & (01) & (02) & (03) & (10) & (11) & (12) & (13) & (20) & (21) & (22) & (23) & (30) & (31) & (32) & (33) \\
00 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 \\
01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 \\
02 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 \\
03 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 \\
10 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 \\
11 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 \\
12 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 \\
13 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 \\
20 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 \\
21 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 \\
22 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 \\
23 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 \\
30 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 \\
31 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 & 01 \\
32 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 \\
33 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 & 00 \\
\end{bmatrix}
\]

From \( P_\varphi \), we have \( d_\varphi = \{1100110000110011\} \) and \( d_c = (111111111101101) \). With these vectors, Algorithm 1 produces an appropriate matrix for calculating a valid inverse neighborhood size; let us remember that links between simple nodes have been removed from \( D_\varphi \) for yielding a right calculation of \( m_i \) and \( m_o \).
From matrix $P$, obtained by Algorithm 1 we can see that $m_i = 2$ which is obtained observing the longest length of the paths going from composed to simple nodes, in the same way we have that $m_o = 1$ which is the longest length from paths going from simple to composed nodes in $D_i$. Other entries in $P$, are equal to 3; they represent paths in $D$, starting from composed nodes, reaching a simple one and leaving it for ending in another composed node.

Taking $m_i = 2$ and $m_o = 1$ we have that a valid inverse neighborhood size is $m_n^{-1} = 3$; therefore the set $K^3$ will be taken for obtaining an inverse evolution rule $A^{-1}$. Using Algorithm 2 we obtain the following cyclic evolutions (with no shift applied on them yet): $C_0^0 = \{000\}, C_1^0 = (001, 010, 100), C_2^0 = \{002\}, C_3^0 = (003, 013, 113, 112, 103, 012, 102), C_4^0 = (011, 110, 101), C_5^0 = \{022\}, C_6^0 = \{023, 033, 133, 132, 123, 032, 122\}, C_7^0 = \{111\}, C_8^0 = \{200\}, C_9^0 = \{201, 210, 300, 301, 310, 211, 310\}, C_{10}^0 = \{202\}, C_{11}^0 = (203.212, 302, 303, 313, 213, 312), C_{12}^0 = \{222\}, C_{13}^0 = (223,232,3221, C_{14}^0 = (233,332,3231, C_{15}^0 = \{333\}.

The previous 16 cyclic evolutions consider 48 of the 64 possible sequences in $K^3$; showing that there is no need of calculating all the evolutions for every sequence. The rest of inverse mappings can be obtained taking an adequate shift over the cyclic evolutions presented before. In this way the table presenting the inverse evolution rule is the following one:

<table>
<thead>
<tr>
<th>$w$</th>
<th>$\varphi^{-1}(w)$</th>
<th>$w$</th>
<th>$\varphi^{-1}(w)$</th>
<th>$w$</th>
<th>$\varphi^{-1}(w)$</th>
<th>$w$</th>
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<tr>
<td>000</td>
<td>0</td>
<td>100</td>
<td>0</td>
<td>200</td>
<td>0</td>
<td>300</td>
<td>0</td>
</tr>
<tr>
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<td>101</td>
<td>0</td>
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<td>0</td>
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<td>0</td>
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<td>002</td>
<td>2</td>
<td>102</td>
<td>2</td>
<td>202</td>
<td>2</td>
<td>302</td>
<td>2</td>
</tr>
<tr>
<td>003</td>
<td>2</td>
<td>103</td>
<td>2</td>
<td>203</td>
<td>2</td>
<td>303</td>
<td>2</td>
</tr>
<tr>
<td>010</td>
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<td>110</td>
<td>1</td>
<td>210</td>
<td>1</td>
<td>310</td>
<td>1</td>
</tr>
<tr>
<td>011</td>
<td>1</td>
<td>111</td>
<td>1</td>
<td>211</td>
<td>1</td>
<td>311</td>
<td>1</td>
</tr>
<tr>
<td>012</td>
<td>3</td>
<td>112</td>
<td>3</td>
<td>212</td>
<td>3</td>
<td>312</td>
<td>3</td>
</tr>
<tr>
<td>013</td>
<td>3</td>
<td>113</td>
<td>3</td>
<td>213</td>
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<td>3</td>
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<tr>
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<td>1</td>
<td>220</td>
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<td>320</td>
<td>1</td>
</tr>
<tr>
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<td>0</td>
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<td>1</td>
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<td>1</td>
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<td>2</td>
</tr>
<tr>
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<td>130</td>
<td>0</td>
<td>230</td>
<td>1</td>
<td>330</td>
<td>0</td>
</tr>
<tr>
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<td>131</td>
<td>0</td>
<td>231</td>
<td>1</td>
<td>331</td>
<td>0</td>
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<tr>
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<td>132</td>
<td>3</td>
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<td>3</td>
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<td>3</td>
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<tr>
<td>033</td>
<td>3</td>
<td>133</td>
<td>3</td>
<td>233</td>
<td>3</td>
<td>333</td>
<td>3</td>
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TABLE 1
Inverse mappings defined by the cyclic evolutions
In Table 1 we can see that every state has as many ancestors as all the others, holding with Property 1. As we mentioned in Section 3, meanwhile we used centered evolutions in the original sense from the neighborhoods in every reversible cellular automaton with neighborhood size 2; this is not the case for the inverse evolution of every neighborhood considered in Table 1; in this case for every neighborhood $c_{[i,i+2]}^t$ the inverse mapping will be placed in $c_{[i+2]}^t$ since $m_i = 2$.

An example of the evolution of $A_R$ from a random configuration with 12 cells in 24 steps is presented in Figure 1. Periodic boundary conditions are taken in every step forming a ring for every configuration, and a cylinder is defined joining all the configurations in the temporal sense. In Figure 1, arrows indicate both the cells taken into account for each neighborhood and the direction for producing the next state in the following configuration.

In Figure 1, states are described by gray tones for facilitating their graphic presentation. We shall apply now the inverse evolution rule in Table 1 over the

![Figure 1: Evolution of $A_R$ from a random configuration.](image-url)
last configuration in the figure in order to return the evolution of the automaton backwards for obtaining the initial condition of the system (Figure 2), or the first configuration in Figure 1. Let us notice that this process can be continued without restriction, obtaining ancestor configurations for the initial one showed in the evolution.

It is clear in Figure 2 that the inverse rule returns to the system into the initial configuration, showing that the original information of the automaton is conserved during the temporal evolution of the same. In this case more cells by neighborhood are needed in the inverse direction for establishing the adequate state in the previous configuration.

6 CONCLUDING REMARKS

Reversible cellular automata represents one of the most interesting and studied cases in cellular automata theory; the approach fomented by McIntosh applying graph tools for obtaining a deep and intuitive comprehension of the
features of these systems has been one of the most important branches in the development of results for the reversible case.

Further work implies to take results from graph theory for complementing the actual ones; other perspective is to join the current results with those in group theory for achieving a careful characterization of these systems. The last direction has been explored by Boykett [3] with promising results.

7 NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
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</thead>
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<tr>
<td>$\mathcal{A}$</td>
<td>cellular automata</td>
</tr>
<tr>
<td>$k$</td>
<td>set of states</td>
</tr>
<tr>
<td>$m_k$</td>
<td>number of states</td>
</tr>
<tr>
<td>$m_n$</td>
<td>neighborhood size</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>evolution rule</td>
</tr>
<tr>
<td>$M_\varphi$</td>
<td>de Bruijn Matrix</td>
</tr>
<tr>
<td>$c^i$</td>
<td>configuration at time $i$</td>
</tr>
<tr>
<td>$m_c$</td>
<td>configuration size</td>
</tr>
<tr>
<td>$\Phi$</td>
<td>global mapping</td>
</tr>
<tr>
<td>$\Lambda (w)$</td>
<td>ancestors of $w$</td>
</tr>
<tr>
<td>$P_\varphi$</td>
<td>pair matrix</td>
</tr>
<tr>
<td>$p^b_{\varphi}$</td>
<td>Element of $V_{D_\varphi}$</td>
</tr>
<tr>
<td>$m_i$</td>
<td>Size of the largest path ending in a basic node</td>
</tr>
<tr>
<td>$C$</td>
<td>Cyclic evolution</td>
</tr>
<tr>
<td>$s_i (w)$</td>
<td>Shift operator over $w$</td>
</tr>
<tr>
<td>$a_{\text{base}} (b)$</td>
<td>Number a base $b$</td>
</tr>
<tr>
<td>$b^b_{\varphi} (w)$</td>
<td>Representation of $w$ base $b$</td>
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</table>

REFERENCES


