# Welch sets for random generation and representation of reversible one-dimensional cellular automata ${ }^{\text {ar }}$ 

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#### Abstract

Reversible one-dimensional cellular automata are studied from the perspective of Welch Sets. This paper presents an algorithm to generate random Welch sets that define a reversible cellular automaton. Then, properties of Welch sets are used in order to establish two bipartite graphs describing the evolution rule of reversible cellular automata. The first graph gives an alternative representation for the dynamics of these systems as block mappings and shifts. The second graph offers a compact representation for the evolution rule of reversible cellular automata. Both graphs and their matrix representations are illustrated by the generation of random reversible cellular automata with 6 and 18 states.


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## 1. Introduction

Cellular automata are discrete dynamical systems able to generate complex behavior based on simple local interaction among their components. Reversible cellular automata are characterized to produce an invertible global behavior provoked by a set of local mappings which are not reversible.

In the one-dimensional case, reversible cellular automata have been widely investigated in order to understand their topological, combinatorial and dynamical properties.

Due to their property of keeping the original information of the system, concepts and alternative definitions of reversible cellular automata have been employed in the specification of different cyphering systems [2,8,9,11,19,20,22], and error-correcting codes [13].

Recent works have presented different procedures to characterize reversible behavior in cellular automata. For instance: the generalization of reversibility defined by linear rules over the binary field case under null boundary conditions is explained in [21]. Reversibility of elementary cellular automata rule number 150 is described by circulant matrices in [14]. Reversibility in cellular automata with memory has been studied in [1] and [17].

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Fig. 1. Evolution of sequence $v$ with four cells for $r=1$, in this case $\varphi(v)$ has two cells..

Thus, there is a continuous investigation to characterize the properties of reversible cellular automata, both for theoretical research and practical application.

The first topological study of reversible cellular automata is developed by Hedlund in [10] establishing important concepts for the one-dimensional case such as the uniform multiplicity of ancestors and Welch sets. Several investigations followed this paper using Welch sets to define new graphs representing the local behavior inducing global reversibility [15], and using their vector representation to give a maximum bound for the minimum information needed to obtain global invertibility [7]. Another topic of interest has been to enumerate all the possible cases of reversible one-dimensional cellular automata $[3,4,18]$, the last two references taking reversible automata as groupoids with algebraic properties. In this sense, references [6] and [5] establish the properties of these groupoids and their relation with isotopy and Cayley graphs.

Based on this previous work, the aim of this paper is to present an algorithm to create random Welch sets to define reversible one-dimensional cellular automata. From these Welch sets, we define two bipartite graphs, both for representing the forward and reverse local mappings of the associated reversible cellular automaton. We give examples showing that the former graph provides an alternative representation for the dynamics of reversible automata by block mappings and shifts firstly demonstrated by Kari in [12], and the latter needs less space than the original evolution rule.

The paper is organized as follows: Section 2 explains the basic concepts of reversible one-dimensional cellular automata and Welch sets. Section 3 defines the properties of Welch Sets for reversible automata with neighborhood size 2. Section 4 presents the algorithm generating random Welch sets and arbitrary reversible cellular automata. Section 5 exposes the construction of a bipartite graph based on Welch elements to calculate the evolution of reversible cellular automata and represent their dynamics by block mappings and shifts. Section 6 specifies a shorter version of this graph in order to represent the evolution of reversible automata with a reduced number of elements. The last section gives the final remarks of the study.

## 2. Basic concepts of Welch sets

One-dimensional cellular automata are defined by a discrete set of states $S$, a neighborhood radius $r \in \mathbb{N}$, an initial configuration $c_{0}:\{1,2, \ldots, m\} \rightarrow S$ for some $m \in \mathbb{N}$, and an evolution rule $\varphi: S^{2 r+1} \rightarrow S$. The dynamics is given applying the evolution rule over every cell in $c_{0}$, thus $c_{1}(i)=\varphi\left(c_{0}(i-r) \ldots c_{0}(i+r)\right)$ taking periodic boundary conditions. In general $c_{t+1}(i)=\varphi\left(c_{t}(i-r) \ldots c_{t}(i+r)\right)$.

For simplicity we shall represent $\varphi(c(i-r) \ldots c(i+r))$ just as $\varphi(c(i))$. Thus, for a string $v \in S^{m}$ with $m \geq 2 r+1$, we define $\varphi(v)$ as follows:

$$
\begin{align*}
\varphi(v) & =\varphi(v(r+1)) \varphi(v(r+2)) \ldots \varphi(v(m-r)) \\
& =w(1) w(2) \ldots w(m-2 r)=w \tag{1}
\end{align*}
$$

where $w$ is the evolution of $v$. Eq. (1) shows that $\varphi(v)$ has $2 r$ cells less than $v$. Fig. 1 illustrates the case for a sequence of four cells and $r=1$; in this work we are using centered evolutions.

In order to simplify our study, we take the simulation of every cellular automaton by another with neighborhood size 2. By Eq. (1), for $v=c_{t}(i-2 r+1) \ldots c_{t}(i+2 r)$ we have that $\varphi(v)=w=c_{t+1}(i-r+1) \ldots c_{t+1}(i+r)$. Then $|v|=4 r$ and $|w|=2 r$. Let us define a new set of states $S^{\prime}$ such that $\left|S^{\prime}\right|=|S|^{2 r}$; thus, we can define a bijection from $S^{\prime}$ to $S^{2 r}$. With this, there are bijections $v \rightarrow s_{1} s_{2}$ and $w \rightarrow s_{3}$ for $s_{i} \in S^{\prime}$ such that:

$$
\begin{equation*}
\varphi^{\prime}\left(s_{1} s_{2}\right)=s_{3} \tag{2}
\end{equation*}
$$

Eq. (2) shows that the original evolution of a cellular automaton can be simulated by another evolution rule $\varphi^{\prime}$ with neighborhood size 2 (or radius $1 / 2$ ) and an extended set of states. Fig. 2 describes this simulation for a cellular automaton with $r=1$; where $t$ indicates time step.

A cellular automaton is reversible if there exists an integer $r^{\prime} \in \mathbb{N}$ and an inverse mapping $\varphi^{-1}: S^{2 r^{\prime}+1} \rightarrow S$ such that $c_{t}(i)=\varphi^{-1}\left(c_{t+1}(i)\right)$. This implies that $\varphi^{-1}\left(\varphi\left(c_{t}(i)\right)\right)=c_{t}(i)$.

A reversible cellular automaton can be simulated by another with $r=1 / 2$ for both invertible rules, taking $r^{\star}=\max \left(r, r^{\prime}\right)$ and using an extended set of states $S^{\star}$ with $\left|S^{\star}\right|=|S|^{2 r^{\star}}$. Therefore, we have to study only reversible cellular automata with neighborhood size 2 in both invertible rules in order to understand the other cases.


Fig. 2. Evolution of a cellular automaton with $r=1$ represented by another with $r=1 / 2$ according to Eq. (2).

The main properties of reversible cellular automata were firstly defined in the seminal works of Hedlund [10] and Nasu [15]. A detailed explanation of how these properties generate reversible behavior for reversible automata with neighborhood size 2 can be consulted in [18].

The features of reversible one-dimensional cellular automata are summarised in three main properties:

1. Uniform multiplicity of ancestors. For every string $w \in S^{n}$ there is a set of strings $A \subset S^{n+1}$ such that $|A|=|S|$ and each $v \in A$ holds that $\varphi(v)=w$. Each $v$ is an ancestor of $w$.
2. Welch indices. There exist $o_{L}, o_{R} \in \mathbb{N}$ such that for every state $s \in S$ there are sets $L_{S}, R_{S} \subset S$ with $\left|L_{S}\right|=o_{L}$ and $\left|R_{S}\right|=o_{R}$ such that $\varphi(a b)=s$ for each $a \in L_{S}$ and every $b \in R_{s}$, and the product $o_{L} o_{R}=|S|$. These $o_{L}, o_{R}$ are calledWelch indices.
3. Unique intersection. Every pair of states $a, b \in S$ holds that $\left|R_{a} \cap L_{b}\right|=\left|R_{b} \cap L_{a}\right|=1$.

Properties 2 and 3 define that the ancestor strings of any sequence of 2 or more states share a common central part and their differences are at the ends. These properties assure the existence of an inverse evolution rule able to revert the global dynamics of the automaton.

The sets $L_{S}$ and $R_{S}$ are the Welch sets associated with state $s \in S$. Notice that indices $o_{L}$ and $o_{R}$ are independent of the state defining $L_{s}$ and $R_{s}$. That is, $\left|L_{S}\right|=o_{L}$ and $\left|R_{S}\right|=o_{R}$ for all $s \in S$.

Since $\varphi$ and $\varphi^{-1}$ are defined with a neighborhood size 2 , they can be represented by matrices $M_{\varphi}$ and $M_{\varphi^{-1}}$ such that entries $M_{\varphi}(a, b)=\varphi(a b)$ and $M_{\varphi^{-1}}(a, b)=\varphi^{-1}(a b)$ for every pair of states $a, b \in S$.

## 3. Properties of Welch sets

The previous properties give a particular structure for $M_{\varphi}$ and $M_{\varphi^{-1}}$. Property 1 guarantees that there are $|S|$ entries equal to $s$ in both matrices for every $s \in S$. Property 2 establishes that if $M\left(s_{1}, s_{2}\right)=M\left(s_{3}, s_{4}\right)$ then $M\left(s_{1}, s_{4}\right)=M\left(s_{3}, s_{2}\right)$ for $s_{i} \in S$. Finally, Property 3 specifies that for every state $s \in S$ there is a unique state $a \in S$ such that $M_{\varphi}(a, a)=s$. Thus, in $M_{\varphi}$ and $M_{\varphi^{-1}}$ every state has a rectangular arrangement, and both matrices define a rectangular groupoid [5].

For every reversible cellular automaton, we can define a state permutation such that $M_{\varphi}(s, s)=s$. Due to $\varphi(s s)=s$, it is hold that $\varphi(s s s)=s s$. Therefore, $\varphi^{-1}(s s)=s$ and the same state permutation implies that $M_{\varphi^{-1}}(s, s)=s$. This feature simplifies even more our study, we just need to analyze reversible cellular automata with neighborhood size 2 and diagonal elements $M_{\varphi}(s, s)=M_{\varphi^{-1}}(s, s)=s$ for every $s \in S$ because all the other cases can be represented by this one. Since $\left|L_{s}\right|=o_{L}$ and $\left|R_{S}\right|=o_{R}$, state $s$ appears in $o_{L}$ rows of $M_{\varphi}$, at the same $o_{R}$ columns.

For $a \in S$, let $M_{\varphi}\left(a,{ }^{*}\right)$ and $M_{\varphi}\left({ }^{*}, a\right)$ be the $a$-th row and the $a$-th column respectively of matrix $M_{\varphi}$. Let $D_{\varphi}(a)$ be the set of states in row $M_{\varphi}\left(a,{ }^{*}\right)$ and let $I_{\varphi}(a)$ be the set of states in column $M_{\varphi}\left({ }^{*}, a\right)$. With this, the following remark can be proved.

Remark 1. $\left|D_{\varphi}(a)\right|=o_{L}$ for each $a \in S$.
Proof. Since $M_{\varphi}\left(a,{ }^{*}\right)$ has $|S|$ columns and every state $s$ holds that $\left|R_{S}\right|=o_{R}$, then there are $|S| / o_{R}=o_{L}$ states in $M_{\varphi}\left(a,{ }^{*}\right)$.
A straightforward result from Remark 1 is the following one.
Corollary 1. $\left|I_{\varphi}(a)\right|=o_{R}$ for each $a \in S$.
A relevant property of $D_{\varphi}(a)$ and $I_{\varphi}(a)$ is the next one.
Remark 2. $D_{\varphi}(a) \cap I_{\varphi}(a)=a$ for every $a \in S$.
Proof. Since $M_{\varphi}(a, a)=a$ we have that $a \in D_{\varphi}(a)$ and $a \in I_{\varphi}(a)$. If there is another state $b \neq a$ such that $b \in D_{\varphi}(a)$ and $b \in$ $I_{\varphi}(a)$, then $a \in L_{b}$ and $a \in R_{b}$. This implies that $\varphi(a a)=b$ and therefore $M_{\varphi}(a, a)=b$, which is a contradiction.

Remark 2 says that $D_{\varphi}(a)$ and $I_{\varphi}(a)$ agree only in the diagonal state. For each $s \in S$, let $L_{s}^{-1}$ and $R_{s}^{-1}$ be the Welch sets of $s$ associated with the inverse evolution rule $\varphi^{-1}$. Accordingly, let $o_{L^{-1}}$ and $o_{R^{-1}}$ be the Welch indices related to $\varphi^{-1}$. The following remark establishes the relationship between the Welch indices of $\varphi$ and $\varphi^{-1}$.

Remark 3. $o_{L^{-1}}=o_{R}$ and $o_{R^{-1}}=o_{L}$.

Proof. For every state $s \in S$, we have that $a \in L_{i}^{-1}$ and $b \in R_{i}^{-1}$ iff $\varphi^{-1}(a b)=s$. This implies that $a \in I_{\varphi}(s)$ and $b \in D_{\varphi}(s)$, hence $L_{s}^{-1}=I_{\varphi}(s)$ and $R_{s}^{-1}=D_{\varphi}(s)$. Remark 1 and Corollary 1 indicate that $\left|I_{\varphi}(s)\right|=o_{R}$ and $\left|D_{\varphi}(s)\right|=o_{L}$. Therefore $o_{L^{-1}}=o_{R}$ and $o_{R^{-1}}=o_{L}$.

## 4. Algorithm to generate random Welch sets

For $U \subseteq S$, we can represent the elements of $U$ by a binary vector $g_{U}: S \rightarrow 0$, 1 of size $1 \times|S|$ such that $g_{U}(a)=1$ iff $a \in$ $U$; otherwise, $g_{U}(a)=0$. With this, we define two mappings $\alpha\left(g_{U}\right)=U$ and $\beta(U)=g_{U}$.

The next algorithm computes valid Welch sets for every state $s \in S$ to fill up the matrix $M_{\varphi}$ representing the evolution rule of a reversible cellular automaton. The algorithm applies the properties of Welch sets as vector and matrix operations in order to facilitate their computational implementation. The vectors and matrices used in the algorithm are defined as follows:

- $G_{L}:|S| \times|S|$ matrix representing left Welch vectors as row binary vectors.
- $G_{R}:|S| \times|S|$ matrix representing right Welch vectors as row binary vectors.
- $G_{D}:|S| \times|S|$ matrix where every binary row represents the valid states that can be placed at the same row in $M_{\varphi}$.
- $G_{I}:|S| \times|S|$ matrix where every binary row represents the valid states that can be placed at the corresponding column in $M_{\varphi}$.
- $h_{D}: 1 \times|S|$ integer vector representing the number of states used in each row of $M_{\varphi}$.
- $h_{I}: 1 \times|S|$ integer vector representing the number of states used in each column of $M_{\varphi}$.
- $E:|S| \times|S|$ matrix representing the sum of Kronecker products to validate that the Welch vectors calculated so far compose a valid evolution rule.

Let us represent the identity matrix as $\mathbf{I}$, the zero matrix as $\mathbf{0}$, and the row vector of ones as $\overline{\mathbf{1}}$. For a binary matrix $B$, let us define its negation by $\neg B$ and its transpose by $B^{T}$. With these elements, the algorithm is defined as follows:

1. Initialize limit $_{l}$, limit $_{r} \in \mathbb{N}$ (loop variables).
2. Initialize $s=1, G_{L}=G_{R}=\mathbf{I}, G_{D}=G_{I}=\neg \mathbf{I}, h_{D}=h_{I}=\overline{\mathbf{1}}$, and $M_{\varphi}=E=\mathbf{0}$. This step specifies that at the beginning each state $s \in S$ belongs to $L_{s}$ and $R_{s}$. Equally, the initialization determines that $s$ belongs to $D_{S}$ and $I_{S}$ and the rest of states are available to fill up each row $M_{\varphi}\left(s,{ }^{*}\right)$ and every column $M_{\varphi}\left({ }^{*}, s\right)$ respectively.
3. Set threshold $_{l}=0$ and flag $_{l}=1$ (control variables).
4. Calculate a candidate left Welch set $L_{s}$ taking state $s$ and $o_{L}-1$ random states from $\left\{\alpha\left(h_{D}<o_{L}\right) \cap \alpha\left(G_{D}\left(s,{ }^{*}\right)>0\right)\right\}$. Set $G_{L}(s, *)=\beta\left(L_{s}\right)$. Validate Property 3 for candidate $L_{s}$ : for $1 \leq i<s$, if any dot product $G_{R}(i, *) \cdot G_{L}(s, *) \neq 1$ then flag $_{l}=0$.
5. If $f l a g_{l}=1$, restrict the possible states for candidate $R_{s}$. By Remark 2, for every $a \in L_{s}, a \neq s$, set $G_{I}(s, a)=0$. For $1 \leq i$ $<s$, take every $i$ such that $\left|\alpha\left(G_{L}\left(i,{ }^{*}\right)\right) \cap \alpha\left(G_{L}\left(s,{ }^{*}\right)\right)\right|>0$. Then the states in the corresponding $\alpha\left(G_{R}\left(i,{ }^{*}\right)\right)$ cannot be part of $R_{s}$ to avoid that the same neighborhood has multiple evolutions. Therefore, set $G_{I}(s, a)=0$ for every $a \in \alpha\left(G_{R}\left(i,{ }^{*}\right)\right)$. Enumerate the set of possible states for the candidate right Welch set $R_{s}$ : if $\left|\left\{\alpha\left(h_{I}<o_{R}\right) \cap \alpha\left(G_{I}(s, *)>0\right)\right\}\right|<o_{R}-1$ then flag $_{l}=0$.
6. If flag $_{l}=0$, set threshold $_{l}=$ threshold $_{l}+1$. If threshold $_{l}<$ limit $_{l}$ then set flag $_{l}=1$ and return to step 4 , otherwise return to step 2.
7. Set threshold ${ }_{r}=0$ and flag $_{r}=1$ (control variables).
8. Calculate a candidate right Welch set $R_{S}$ taking state $s$ and $o_{R}-1$ random states from $\left\{\alpha\left(h_{I}<o_{R}\right) \cap \alpha\left(G_{I}\left(s,{ }^{*}\right)>0\right)\right\}$. Set $G_{R}(s, *)=\beta\left(R_{s}\right)$. Validate Property 3 for candidate $R_{s}$ : for $1 \leq i \leq s$, if any dot product $G_{R}\left(s,{ }^{*}\right) \cdot G_{L}\left(i,{ }^{*}\right) \neq 1$ then flag $_{r}=0$.
9. If flag $_{r}=1$, calculate the Kronecker product $K_{s}=G_{L}(s, *)^{T} \otimes G_{R}(s, *)$ and take $K^{\prime}=K_{s}+E$. If $K^{\prime}(i, j)>1$ for $1 \leq i \leq j \leq S$ then flag $_{r}=0$. This means that there is a neighborhood with multiple evolutions.
10. If flag $_{r}=0$ set threshold $r_{r}=$ threshold $_{r}+1$. If threshold $_{r}<$ limit $_{r}$ then set flag $_{r}=1$ and return to step 8 , otherwise go to step 4.
11. Valid Welch sets have been generated for state $s$. Update $h_{D}(a)=h_{D}(a)+1$ for each $a \in\left\{\alpha\left(G_{L}(s, *)\right)-s\right\}$, and analogously $h_{I}(b)=h_{I}(b)+1$ for each $b \in\left\{\alpha\left(G_{R}(s, *)\right)-s\right\}$. Set $E=E+K_{s}$ and $M_{\varphi}(a, b)=s$. If $s<|S|$ then $s=s+1$ and go to step 3. Otherwise return matrices $G_{L}, G_{R}$ and $M_{\varphi}$.
The associated pseudocode is presented in Algorithm 1.
In Algorithm 1, loop parameters limit $_{l}$ and limit $_{r}$ define the number of iterations to search valid Welch sets for every state $s$. In case that a valid $R_{s}$ has not been calculated after limit $r_{r}$ attempts, a new $L_{s}$ is calculated to restart the search of an appropriate $R_{s}$. If a valid $L_{s}$ has not been calculated after limit ${ }_{l}$ attempts, a valid $R_{s}$ has not been calculated after limit $_{l} *$ limit $_{r}$ iterations. This implies that the previous calculated Welch sets could not be so adequate to specify a reversible automaton, especially for large values of limit $_{l}$ and limit $_{r}$. Therefore, the search restarts from $s=1$. Notice that parameters limit $_{l}$ and limit $_{r}$ are not directly related to the number of cells in the configuration of the reversible automaton.

The aim of the algorithm proposed in this paper is not to enumerate reversible automata but only to generate a random instance for a larger number of states. In fact, the algorithm has been able to calculate random Welch sets for reversible automata up to 30 states, with any combination of Welch indices.

```
Algorithm 1 Generate reversible automata by random Welch sets.
Require: Number of states \(|S|, s=1\), and loop parameters limit \(_{l}\), limit \(_{r} \in \mathbb{N}\);
    while \(s<=|S|\) do
        if \(\mathrm{s}=1\) then \(\quad\) Initialize data structures
            \(G_{L}=G_{R}=\mathbf{I}, G_{D}=G_{I}=\neg \mathbf{I}, h_{D}=h_{I}=\overline{\mathbf{1}}\), and \(M_{\varphi}=E=\mathbf{0} ;\)
        end if
        threshold \(_{l}=0 ; \quad \triangleright\) Set loop variable to find a valid \(L_{S}\)
        while threshold \(_{l}<=\) limit \(_{l}\) do
            \(L_{s} \leftarrow o_{L}-1\) random states in \(\left\{\alpha\left(h_{D}<o_{L}\right) \cap \alpha\left(G_{D}(s, *)>0\right)\right\} ; \quad \triangleright\) Validate Remark 1
            \(G_{L}(s, *)=\beta\left(L_{s}\right) ;\) flag \(_{l}=1\);
if \(G_{R}(i, *) \cdot G_{L}(s, *) \neq 1\) for \(1 \leq i<s\) then flag \(_{l}=0\);
            end if
            if flag \(_{l}=1\) then
                \(G_{I}(s, a)=0\) for every \(a \in L_{s}, a \neq s ; \quad \triangleright\) Restrict states for \(R_{s}\) to hold Remark 2
                for all \(i \in\{1 \ldots s-1\}\) such that \(\left|\alpha\left(G_{L}(i, *)\right) \cap \alpha\left(G_{L}(s, *)\right)\right|>0\) do
                    \(G_{I}(s, a)=0\) for \(a \in \alpha\left(G_{R}(i, *)\right)\);
                \(\triangleright\) To avoid neighborhoods with multiple evolutions
                    end for
                if \(\left|\left\{\alpha\left(h_{I}<o_{R}\right) \cap \alpha\left(G_{I}(s, *)>0\right)\right\}\right|<o_{R}-1\) then flag \(_{l}=0\)
                else \(\quad\) Enough available states for \(R_{S}\)
                            threshold \(_{r}=0\); \(\quad \triangleright\) Set loop variable to find a valid \(R_{S}\)
                    while threshold \({ }_{r}<=\) limit \(_{r}\) do
                        \(R_{S} \leftarrow o_{R}-1\) random states in \(\left\{\alpha\left(h_{I}<o_{R}\right) \cap \alpha\left(G_{I}(s, *)>0\right)\right\} ; \quad \triangleright\) Validate Cor. 1
                        \(G_{R}(s, *)=\beta\left(R_{s}\right) ;\) flag \(_{r}=1\);
                            \(\triangleright\) Validate Property 3 for \(R_{s}\)
                        if \(G_{R}(s, *) \cdot G_{L}(i, *) \neq 1\) for \(1 \leq i<=s\) then flag \(_{r}=0\);
                        end if
                        if flag \(_{r}=1\) then \(G_{R}(s, *) ; K^{\prime}=K_{s}+E . \quad \triangleright\) Kronecker product to check neighborhoods already taken
                        \(K_{s}=G_{L}(s, *)^{T} \otimes G_{R}(s, *) ; K^{\prime}=K_{s}+E ;\)
                            if \(K^{\prime}(i, j)>1\) for \(1 \leq i \leq j \leq S\) then \(\operatorname{flag}_{r}=0\);
                    else
                            \(h_{D}(a)=h_{D}(a)+1\) for \(a \in\left\{\alpha\left(G_{L}(s, *)\right)-s\right\} ;\)
                            \(h_{I}(b)=h_{I}(b)+1\) for \(b \in\left\{\alpha\left(G_{R}(s, *)\right)-s\right\} ;\)
                            \(E=E+K_{s} ;\)
                    for all \(a \in\left\{\alpha\left(G_{L}(s, *)\right)\right\}\) and \(b \in\left\{\alpha\left(G_{R}(s, *)\right)\right\}\) do
                            \(M_{\varphi}(a, b)=s\)
                    end for
                            if \(s<|S|\) then \(\quad \triangleright\) There are more states remaining
                                    \(s=s+1 ;\)
                                    \(\triangleright\) Advance to the next state
                                    threshold \(_{r}=\) limit \(_{r}+1 ;\) threshold \(_{l}=\) limit \(_{l}+1 ;\)
                                    \(\triangleright\) Break while loops
                                    else return \(G_{L}, G_{R}\) and \(M_{\varphi}\)
                                    end if
                                    end if
                                    end if
                                    if flag \(_{r}=0\) then threshold \(_{r}=\) threshold \(_{r}+1 ; \quad \quad \triangleright\) Incorrect \(R_{s}\), search again
                    end if
                    end while
                end if
            end if
            if flag \(_{l}=0\) then threshold \(_{l}=\) threshold \(_{l}+1 ; \quad \triangleright\) Incorrect \(L_{s}\), search again
                threshold \(_{l}>\) limit \(_{l}\) then \(s=1\);
            end if
            end if
        end while
    end while
```

This algorithm can be classified as a constrained random local search [16], in the same category as random search heuristics or evolutionary algorithms. Random local search are applied to problems whose structure is not well-understood, as well as to hard combinatorial problems, like the enumeration of reversible automata.

This enumeration is still an open problem. In fact, a set of formulas or a general algorithm to enumerate all reversible automata with $r=1 / 2$ and any number of states have not been defined yet. The maximum number of states reported for any procedure so far is 12 [3,18].

Properties of reversible automata are implicit in the generation of the Welch vectors $G_{L}\left(s,{ }^{*}\right)$ and $G_{R}\left(s,{ }^{*}\right)$ in lines 8 and 21 for each $s \in S$. We have that the Welch sets $\left|\alpha\left(G_{L}(s, *)\right)\right|=o_{L}$ due to lines 3 and 7 , and $\left|\alpha\left(G_{R}(s, *)\right)\right|=o_{R}$ due to lines 3 and 20, holding Property 2 (Welch indices). Property 1 (Uniform multiplicity of ancestors) is fulfilled in lines 31-33 where $|S|$ ancestors are specified for every s. Lines 9 and 22 validate Property 3 for all the products between left and right Welch sets. Thus, the obtained matrix $M_{\varphi}$ satisfies Properties 1, 2 and 3 and therefore generates a reversible automaton.

One important point in the algorithm is the set of restrictions implemented to validate and reduce the search space. In particular, in the algorithm, Remark 1 in line 7, Remark 2 in line 12, discard multiple evolutions for the same neighborhood in line 14, enough available states for $R_{S}$ in line 16 and Corollary 1 in line 20, are implemented to restrict the random search of Welch sets, making possible the generation of reversible automata with larger number of states. Property 3 and Kronecker product validate the obtained Welch sets in lines 9, 22 and 26.


Fig. 3. Flow chart to generate random Welch sets.
The associated flow chart is presented in Fig. 3. Several examples of reversible automata generated with the previous algorithm are displayed in Fig. 5 using limit $_{l}=$ limit $_{r}=100$. The corresponding Welch indices are presented below each image.

## 5. First representation: bipartite graph with Welch elements

For $s \in S$ and its left Welch set $L_{s}$, a left Welch element is a pair $(a, s)$ such that $a \in L_{s}$. Analogously, a right Welch element is a pair ( $s, a$ ) such that $a \in R_{s}$.

Given the matrices $G_{L}, G_{R}$ and $M_{\varphi}$, we can define a bipartite graph $P=N_{L} \times N_{R}$ where $N_{L}$ is the set of left Welch elements and $N_{R}$ is the set of right Welch elements for every state in $S$.

Every left Welch element $(a, b) \in N_{L}$ holds that $a \in L_{b}$ for $a, b \in S$. Analogously, every right Welch element $(d, e) \in N_{R}$ holds that $e \in R_{d}$ for $d, e \in S$. There is a directed edge from $(a, b)$ to ( $d, e$ ) labeled by $\varphi^{-1}(b d)$. Similarly, the directed edge from ( $d, e$ ) to $(a, b)$ is labeled by $\varphi(e a)$. Fig. 4 presents two examples of the bipartite graphs associated with a reversible automaton of 3 states, $o_{L}=1$ and $o_{R}=3$ (left side); and a reversible automaton of 4 states, $o_{L}=2$ and $o_{R}=2$. Edges are colored according to $\varphi^{-1}$ from $N_{L}$ to $N_{R}$, and using $\varphi$ from $N_{R}$ to $N_{L}$. Since the graphical representation can be very complicated for larger values of number of states and Welch indices, a matrix definition will be used for further analysis.


Fig. 4. Digraphs $P$ related to reversible automata of 3 and 4 states respectively..

For $p_{L}=(a, b) \in N_{L}$ let us define $\gamma\left(p_{L}\right)=a$ and $\delta\left(p_{L}\right)=b$. In the same way, for $p_{R}=(d, e) \in N_{R}$ let us define $\gamma\left(p_{R}\right)=e$ and $\delta\left(p_{R}\right)=d$. Thus, the directed edge $\left(p_{L}, p_{R}\right)$ is labeled by $\mu\left(p_{L}, p_{R}\right)=\varphi^{-1}\left(\delta\left(p_{L}\right) \delta\left(p_{R}\right)\right)$ and the directed edge $\left(p_{R}, p_{L}\right)$ is labeled by $\eta\left(p_{R}, p_{L}\right)=\varphi\left(\gamma\left(p_{R}\right) \gamma\left(p_{L}\right)\right)$.
$P$ can be represented by a matrix $M_{P}$ with row indices $N_{L}$ and column indices $N_{R}$. Every position $M_{P}\left(p_{L}, p_{R}\right)$ has two entries, $\mu\left(p_{L}, p_{R}\right)$ and $\eta\left(p_{R}, p_{L}\right)$. With this, the following result can be established.

Theorem 1. For every $s \in S$ and fixed states $a, e \in S$, there is a unique pair of nodes $\left(p_{L}, p_{R}\right)$ in $P$ with $\gamma\left(p_{L}\right)=a$ and $\gamma\left(p_{R}\right)=e$ such that $\mu\left(p_{L}, p_{R}\right)=s$.

Proof. Every string in $S^{3}$ is represented by a directed edge from a node in $N_{L}$ to other node in $N_{R}$. By Property 2 and Remark 1, for every $a \in S$ there is a subset $N_{L}^{\prime} \subset N_{L}$ with $\left|N_{L}^{\prime}\right|=o_{L}$ such that $\gamma\left(p_{L}\right)=a$ for each $p_{L} \in N_{L}^{\prime}$. Analogously, for every $e \in S$ there is a subset $N_{R}^{\prime} \subset N_{R}$ with $\left|N_{R}^{\prime}\right|=o_{R}$ such that $\gamma\left(p_{R}\right)=e$ for each $p_{R} \in N_{R}^{\prime}$. Thus there are $o_{L} o_{R}=|S|$ directed edges in $P$ to represent all the sequences ase for fixed states $a, e$ and every $s \in S$. Since there are exactly $|S|$ strings ase, there is a unique pair ( $p_{L}, p_{R}$ ) with $p_{L} \in N_{L}^{\prime}$ and $p_{R} \in N_{R}^{\prime}$ such that $\mu\left(p_{L}, p_{R}\right)=s$.

Direct results from Theorem 1 is the next one.
Corollary 2. For every $s \in S$ and fixed states $d, b \in S$, there is a unique pair of nodes $\left(p_{R}, p_{L}\right)$ in $P$ with $\delta\left(p_{R}\right)=d$ and $\delta\left(p_{L}\right)=b$ such that $\eta\left(p_{R}, p_{L}\right)=s$.

Corollary 3. For every $s \in S$ and fixed states $e, a \in S$, there are $|S|$ pairs of nodes $\left(p_{R}, p_{L}\right)$ in $P$ with $\gamma\left(p_{R}\right)=e, \gamma\left(p_{L}\right)=a$ such that $\eta\left(p_{R}, p_{L}\right)=s$.

Proof. For every $e \in S$ there is a subset $N_{R}^{\prime} \subset N_{R}$ with $\left|N_{R}^{\prime}\right|=o_{R}$ nodes such that $\gamma\left(p_{R}\right)=e$ for each $p_{R} \in N_{R}^{\prime}$. Besides, for every $a \in S$ there is a subset $N_{L}^{\prime} \subset N_{L}$ with $\left|N_{L}^{\prime}\right|=o_{L}$ such that $\gamma\left(p_{L}\right)=a$ for each $p_{L} \in N_{L}^{\prime}$. Thus there are $o_{R} o_{L}=|S|$ directed edges in $P$ to represent the neighborhood ea such that $\eta\left(p_{R}, p_{L}\right)=s$.

As an illustrative example, Table 1 presents a reversible cellular automata with $|S|=6, o_{L}=3$ and $o_{R}=2$ with Welch sets generated at random applying the algorithm in the previous section.

Fig. 6 displays some evolution examples of this automaton. The matrix $M_{P}$ associated with this rule is presented in Table 2.


Fig. 5. Different reversible cellular automata with $6,16,24$ and 30 cell-states generated by the algorithm. Every example is specified by a distinct combination of Welch indices with 100 cells evolving in 120 steps. Cell-state colors are presented on the right side of every evolution.

## Table 1

Random reversible cellular automata with 6 cell-states. Indexes of $M_{\varphi}$ are implicitly defined, thus $M_{\varphi}(a, b)$ indicates the evolution of the neighborhood $a b$.

| Evolution rule $M_{\varphi}$ | State s | $L_{s}$ | $R_{\text {s }}$ |
| :---: | :---: | :---: | :---: |
| 414166 | 1 | 126 | 24 |
| 315135 | 2 | 345 | 24 |
| 325235 | 3 | 235 | 15 |
| 424266 | 4 | 146 | 13 |
| 325235 | 5 | 235 | 36 |
| 414166 | 6 | 146 | 56 |



Fig. 6. Evolution examples of the reversible automaton described in Table 1 for 100 cells in 100 time steps.
Table 2
Matrix $M_{P}$ for the evolution rule and Welch elements presented in Table 1. For row and column indices $p \in N_{L}$ and $q \in N_{R}$ respectively, $\gamma(p)$ and $\gamma(q)$ are in bold. In the same way, every $\mu(p, q)$ is in bold too.

| $N_{L} / N_{R}$ | $(1,2)$ | $(1,4)$ | $(2,2)$ | $(2,4)$ | $(3,1)$ | $(3,5)$ | $(4,1)$ | $(4,3)$ | $(5,3)$ | $(5,6)$ | $(6,5)$ | $(6,6)$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $(1,1)$ | $(2,3)$ | $(2,4)$ | $(4,3)$ | $(4,4)$ | $(2,4)$ | $(2,3)$ | $(4,4)$ | $(4,3)$ | $(2,3)$ | $(2,4)$ | $(4,3)$ | $(4,4)$ |
| $(2,1)$ | $(2,1)$ | ( 2,2) | $(4,1)$ | $(4,2)$ | $(2,1)$ | ( 2,2) | $(4,1)$ | $(4,2)$ | $(2,2)$ | $(2,1)$ | $(4,2)$ | $(4,1)$ |
| $(6,1)$ | $(2,5)$ | $(2,6)$ | $(4,5)$ | $(4,6)$ | $(2,6)$ | $(2,5)$ | $(4,6)$ | $(4,5)$ | $(2,5)$ | $(2,6)$ | $(4,5)$ | $(4,6)$ |
| $(3,2)$ | $(2,5)$ | $(2,4)$ | $(4,5)$ | $(4,4)$ | ( 2,4) | $(2,5)$ | $(4,4)$ | $(4,5)$ | $(2,5)$ | $(2,4)$ | $(4,5)$ | $(4,4)$ |
| $(4,2)$ | $(2,1)$ | $(2,2)$ | $(4,1)$ | $(4,2)$ | $(2,1)$ | $(2,2)$ | $(4,1)$ | (4,2) | $(2,2)$ | $(2,1)$ | $(4,2)$ | $(4,1)$ |
| $(5,2)$ | $(2,3)$ | $(2,6)$ | $(4,3)$ | $(4,6)$ | $(2,6)$ | $(2,3)$ | $(4,6)$ | $(4,3)$ | $(2,3)$ | $(2,6)$ | $(4,3)$ | $(4,6)$ |
| $(2,3)$ | $(1,1)$ | $(1,2)$ | $(5,1)$ | $(5,2)$ | $(5,1)$ | $(5,2)$ | $(1,1)$ | $(1,2)$ | $(5,2)$ | $(5,1)$ | $(1,2)$ | $(1,1)$ |
| $(3,3)$ | ( 1,5 ) | ( 1,4) | $(5,5)$ | $(5,4)$ | $(5,4)$ | $(5,5)$ | ( 1,4 ) | $(1,5)$ | $(5,5)$ | $(5,4)$ | $(1,5)$ | ( 1,4 ) |
| $(5,3)$ | $(1,3)$ | $(1,6)$ | $(5,3)$ | $(5,5)$ | $(5,6)$ | $(5,3)$ | $(1,6)$ | $(1,3)$ | $(5,3)$ | $(5,6)$ | $(1,3)$ | $(1,6)$ |
| $(1,4)$ | $(1,3)$ | ( 1,4 ) | $(3,3)$ | $(3,4)$ | $(3,4)$ | $(3,3)$ | ( 1,4 ) | $(1,3)$ | $(3,3)$ | $(3,4)$ | $(1,3)$ | $(1,4)$ |
| $(4,4)$ | $(1,1)$ | $(1,2)$ | $(3,1)$ | $(3,2)$ | $(3,1)$ | $(3,2)$ | $(1,1)$ | $(1,2)$ | $(3,2)$ | $(3,1)$ | $(1,2)$ | $(1,1)$ |
| $(6,4)$ | $(1,5)$ | $(1,6)$ | $(3,5)$ | $(3,6)$ | $(3,6)$ | $(3,5)$ | $(1,6)$ | $(1,5)$ | $(3,5)$ | $(3,6)$ | $(1,5)$ | $(1,6)$ |
| $(2,5)$ | $(6,1)$ | $(6,2)$ | $(3,1)$ | $(3,2)$ | $(3,1)$ | $(3,2)$ | $(6,1)$ | $(6,2)$ | $(3,2)$ | $(3,1)$ | $(6,2)$ | $(6,1)$ |
| $(3,5)$ | $(6,5)$ | $(6,4)$ | $(3,5)$ | $(3,4)$ | $(3,4)$ | $(3,5)$ | $(6,4)$ | $(6,5)$ | $(3,5)$ | $(3,4)$ | $(6,5)$ | $(6,4)$ |
| $(5,5)$ | $(6,3)$ | $(6,6)$ | $(3,3)$ | $(3,6)$ | $(3,6)$ | $(3,3)$ | $(6,6)$ | $(6,3)$ | $(3,3)$ | $(3,6)$ | $(6,3)$ | $(6,6)$ |
| $(1,6)$ | $(6,3)$ | $(6,4)$ | $(5,3)$ | $(5,4)$ | $(5,4)$ | $(5,3)$ | $(6,4)$ | $(6,3)$ | $(5,3)$ | $(5,4)$ | $(6,3)$ | $(6,4)$ |
| $(4,6)$ | $(6,1)$ | $(6,2)$ | $(5,1)$ | $(5,2)$ | $(5,1)$ | $(5,2)$ | $(6,1)$ | $(6,2)$ | $(5,2)$ | $(5,1)$ | $(6,2)$ | $(6,1)$ |
| $(6,6)$ | $(6,5)$ | $(6,6)$ | $(5,5)$ | $(5,6)$ | $(5,6)$ | $(5,5)$ | $(6,6)$ | $(6,5)$ | $(5,5)$ | $(5,6)$ | $(6,5)$ | $(6,6)$ |

Based on the proof of Theorem 1, matrix $M_{P}$ can be used to obtain the evolution of a reversible cellular automaton in both senses. For an initial configuration $c$ with $|c|=m$ and $1 \leq i \leq m$, the forward evolution is obtained following the next steps:

1. For every $i$ with modulus $\bmod (i, 3)=1$, take every state $c(i)$ and the set of rows $N_{i}^{\prime} \subseteq N_{L}$ such that $\gamma(p)=c(i)$ for each $p \in N_{i}^{\prime}$.
2. For every $i$ with $\bmod (i, 3)=0$, take every state $c(i)$ and the set of columns $N_{i}^{\prime} \subseteq N_{R}$ such that $\gamma(q)=c(i)$ for each $q \in N_{i}^{\prime}$.
3. For every $i$ with $\bmod (i, 3)=2$ and from the previous row and column sets, take the unique pair holding that $\mu\left(p_{i-1}, q_{i+1}\right)=c(i)$ where $p_{i-1} \in N_{i-1}^{\prime}$ and $q_{i+1} \in N_{i+1}^{\prime}$. The evolution of $c(i-1) c(i) c(i+1)$ is given by $\delta\left(p_{i-1}\right) \delta\left(q_{i+1}\right)$.
4. For every $i$ with $\bmod (i, 3)=0$ and $j$ with $\bmod (i+1,3)=1$, the evolution of $c(i) c(j)$ is obtained taking the directed edge $\eta\left(q_{i}, p_{j}\right)$.

The backwards evolution is calculated as follows:

1. For every $i$ with $\bmod (i, 3)=1$, take every state $c(i)$ and the set of columns $N_{i}^{\prime} \subseteq N_{R}$ such that $\delta(q)=c(i)$ for each $q \in N_{i}^{\prime}$.
2. For every $i$ with $\bmod (i, 3)=0$, take every state $c(i)$ and the set of columns $N_{i}^{\prime} \subseteq N_{L}$ such that $\delta(p)=c(i)$ for each $p \in N_{i}^{\prime}$.
3. For every $i=\bmod (i, 3)=2$ and from the previous rows and columns, take the unique pair with $\eta(q i-1, p i+1)=c(i)$. The inverse evolution of $c(i-1) c(i) c(i+1)$ is given by $\gamma\left(q_{i-1}\right) \gamma\left(p_{i+1}\right)$.
4. For every $i$ with $\bmod (i, 3)=0$ and $j$ with $\bmod (i+1,3)=1$, the inverse evolution of $c(i) c(j)$ is obtained taking the directed edge $\mu\left(p_{i}, q_{j}\right)$.

Fig. 7 describes how the previous algorithms are able to calculate the forward and backwards evolution from a given random configuration.

In this figure, for the forward direction, every sequence $w \in S^{3}$ is mapped into a pair of nodes $(p, q)$ such that $\gamma(p)=$ $w(1), \gamma(q)=w(3)$ and $\mu(p, q)=w(2)$ (bold font). Then the evolution of $w$ is given by $\delta(p) \delta(q)$ (italic font). In the second part of the process, the missing cell-states are obtained taking every directed edge $\eta(q, p)$ (italic font) in order to calculate the complete evolution. The backward evolution can be analogously described. Notice that the last state in the evolution is repeated to represent periodic boundary conditions.


Fig. 7. Forward and backward evolution obtained by means of the bipartite graph $P$.
Table 3
Bijections from Welch elements of $L_{s}$ and $R_{s}$ into $X$ and $Y$ respectively.

| $L_{S}$ | Symbol | $L_{\text {s }}$ | Symbol | $L_{S}$ | Symbol | $R_{\text {S }}$ | Symbol | $R_{s}$ | Symbol |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $(1,1)$ | $X_{1}$ | $(2,3)$ | $X_{7}$ | $(2,5)$ | $X_{13}$ | $(1,2)$ | $Y_{1}$ | $(4,1)$ | $Y_{7}$ |
| $(2,1)$ | $X_{2}$ | $(3,3)$ | $X_{8}$ | $(3,5)$ | $X_{14}$ | $(1,4)$ | $Y_{2}$ | $(4,3)$ | $Y_{8}$ |
| $(6,1)$ | $X_{3}$ | $(5,3)$ | $X_{9}$ | $(5,5)$ | $X_{15}$ | $(2,2)$ | $Y_{3}$ | $(5,3)$ | $Y_{9}$ |
| $(3,2)$ | $X_{4}$ | $(1,4)$ | $X_{10}$ | $(1,6)$ | $X_{16}$ | $(2,4)$ | $Y_{4}$ | $(5,6)$ | $Y_{10}$ |
| $(4,2)$ | $X_{5}$ | $(4,4)$ | $X_{11}$ | $(4,6)$ | $X_{17}$ | $(3,1)$ | $Y_{5}$ | $(6,5)$ | $Y_{11}$ |
| $(5,2)$ | $X_{6}$ | $(6,4)$ | $X_{12}$ | $(6,6)$ | $X_{18}$ | $(3,5)$ | $Y_{6}$ | $(6,6)$ | $Y_{12}$ |

Although the previous algorithms are more technical and complicated than using the matrix $M_{\varphi}$ to obtain the evolution of a reversible automata, their relevance is to show that invertible evolution rules can be represented by a bipartite graph, which opens a future direction of research.

With the nodes of $P$ we can obtain a reinterpretation of Kari's proof about the representation of the dynamics of reversible cellular automata by block permutations and shifts [12]. The original proof demonstrates that the evolution of a reversible cellular automata is equivalent to mapping blocks of $6 r$ states into other blocks with the same length, and from these blocks, apply a shift of $3 r$ places and a second mapping to other blocks of $6 r$ states. This demonstration is completely based on the properties of Welch indices and only takes the case when $o_{L}=1$.

Suppose that we have a reversible automaton with $r=1 / 2$ and $|S|=4$; if $o_{L}=1$ then $\left|N_{L}\right|=4$ and $\left|N_{R}\right|=16$. This implies that we can define a bijection from $N_{L}$ to $S$ and from $N_{R}$ to $S^{2}$. Thus, a permutation from blocks $w \in S^{3}$ to blocks of the same length is easily defined.

However, if $o_{L} \neq 1$ a permutation cannot be defined. For the same case assume that $o_{L}=o_{R}=2$, hence $\left|N_{L}\right|=8$ and $\left|N_{R}\right|=8$. In order to define a permutation, we should map blocks $w$ into other blocks of the same size, such that they should have 8 different left parts and 8 distinct right parts, which is not possible. This fact does not imply that the original result is wrong, but it is required to generalize the idea that the evolution of a reversible automaton is equivalent to perform two mappings of blocks with a shift between them.

In order to obtain this generalization, the elements of $N_{L}$ and $N_{R}$ (or the nodes of $P$ ) can be mapped into two different sets of symbols $X$ and $Y$ respectively. Instead of defining that every block $w$ permutes into another block of 3 states, it is only necessary that the block maps into a block $x y$ where $x \in X$ and $y \in Y$.

Thus, it is not mandatory that the block $x y$ has the same length that $w$, therefore the set sizes $|X|$ and $|Y|$ can be arbitrarily controlled to generalize the mappings of blocks with a shift between them for any combination of $o_{L}$ and $o_{R}$ such that $o_{L} o_{R}=|S|$.

Notice that every sequence $w \in S^{3}$ maps into a unique pair ( $p_{L}, p_{R}$ ) in $P$ such that $\mu\left(p_{L}, p_{R}\right)=w(2)$. The same happens in the inverse direction, there is a unique pair $\left(p_{R}, p_{L}\right)$ in $P$ such that $\eta\left(p_{R}, p_{L}\right)=w(2)$. This implies that every left Welch element defined by $\varphi$ is a right Welch element determined by $\varphi^{-1}$.

Thus, we can define two sets of symbols $X$ and $Y$ such that $|X|=\left|N_{L}\right|=|S| o_{L}$ and $|Y|=\left|N_{R}\right|=|S| o_{R}$. Every left Welch set defined by $\varphi$ can be mapped bijectively into an element of $X$ and consequently each right Welch set can be mapped bijectively into an element of $Y$.

Then, every configuration can be partitioned in blocks of three cells and every block is represented by a pair of symbols $x y$ for $x \in X$ and $y \in Y$.Analogously, every pair $y x$ maps into a unique sequence $w \in S^{3}$ applying now the bijection from $Y$ into $N_{R}$ and from $X$ into $N_{L}$.

For the reversible cellular automaton in Table 1, let us define a set of bijections from $L_{s}$ into $X$ and from $R_{s}$ into $Y$ in Table 3.


Fig. 8. Dynamics of the reversible cellular automaton represented by block mappings and shifts.

Given a random initial configuration, Fig. 8 describes the application of block mappings for every sequence $w \in S^{3}$. First, each $w$ is mapped into its respective pair of nodes $(p, q)$ in $P$. Then each $p$ is mapped into its corresponding element in $X$ according to Table 3. The analogous process is applied for every $y$ to produce a sequence of symbols $x y x y \ldots x y$. From this sequence, each block $y x$ is mapped into its particular pair $(q, p)$ in $P$, thereafter every pair $(q, p)$ maps into a unique sequence $w \in S^{3}$. With this, we obtain the evolution of the initial configuration.

## 6. Second representation: Bipartite graph with welch sets

With the matrices $G_{L}, G_{R}$ and $M_{\varphi}$, another bipartite graph $Q=\mathcal{L} \times \mathcal{R}$ is defined where $\mathcal{L}$ is the family of left Welch sets and $\mathcal{R}$ is the family of right Welch sets. For every $s \in S$, each set $L_{s} \in \mathcal{L}$ and every $R_{s} \in \mathcal{R}$. There is a directed edge ( $L_{s}, R_{s}$ ) labeled by $s$. The directed edges from $\mathcal{R}$ into $\mathcal{L}$ are implicitly defined by Property 3 . That is, $\left(R_{a}, L_{b}\right)=R_{a} \cap L_{b}$ for each $R_{a} \in \mathcal{R}$ and every $L_{b} \in \mathcal{L}$.

Fig. 9 presents de digraphs $Q$ associated with the reversible automata previously used in Fig. 4. Bold lines describe the edges from $\mathcal{L}$ to $\mathcal{R}$. Notice that there are states with the same Welch sets in the second case, thus only one instance of each set is taken to define the graph.
$Q$ can be represented by a matrix $M_{Q}$ with row indices $\mathcal{L}$ and column indices $\mathcal{R}$. Every position $\left(L_{a}, R_{a}\right)=a$, otherwise $\left(L_{a}, R_{b}\right)=\emptyset$ for $a, b \in S, a \neq b$. Since Property 3 is accomplished by the intersection of Welch sets, there is no need to write explicitly the corresponding entries in $M_{Q}$.

The maximum order of $M_{Q}$ is the one of $M_{\varphi}(|S| \times|S|)$, but only with $|S|$ entries instead of $|S| \times|S|$. All our computational experiments, however, have shown empirically that the order of $M_{Q}$ is lesser than $|S| \times|S|$ because different states can have the same Welch sets. Therefore, $M_{Q}$ can be used as a reduced representation of $M_{\varphi}$, which would be favorable for practical applications of reversible automata in order to minimize computational resources.

Matrix $M_{Q}$ can be used as well to obtain the evolution of a reversible cellular automaton in both directions. For an initial configuration $c$ with $|c|=m$ and $1 \leq i \leq m$, the forward evolution is obtained following the next steps:

1. For every state $c(i)$, take the family $V_{L} \subseteq \mathcal{L}$ with $c(i) \in L \in V_{L}$.
2. For every $j=\bmod (i+1, m)$ and state $c(j)$, take the family $V_{R} \subseteq \mathcal{R}$ with $c(j) \in R \in V_{R}$.
3. Select the unique pair $(L, R) \neq \emptyset$ in $M_{Q}$ for $L \in V_{L}$ and $R \in V_{R}$.
4. The evolution of $c(i) c(j)$ is given by the label $(L, R)=s$.

The inverse evolution is obtained in a more direct way by Property 3.

1. For every state $c(i)$, take the unique entry in $M_{Q}$ with $\left(L_{c(i)}, R_{c(i)}\right)=c(i)$.
2. The inverse evolution of $c(i) c(i+1)$ is given by $a=R_{c(i)} \cap L_{c(i+1)}$.

As an illustrative example, Table 4 shows a reversible cellular automaton with $|S|=18, o_{L}=3$ and $o_{R}=6$ with Welch sets generated at random applying the algorithm in Section 4.

Fig. 10 depicts some evolution examples of this automaton. The Welch sets associated with this automaton are described in Table 5.

This table shows that there are only 11 different left Welch sets and 15 distinct right Welch sets. Every Welch set is enumerated according to the first state defining it. With these sets, we specify $M_{Q}$ in Table 6.


Fig. 9. Digraphs $Q$ related to reversible automata in Fig. 4.


Fig. 10. Evolution examples of the reversible automaton described in Table 4 for 100 cells in 100 time steps.

Table 4
Random reversible cellular automata with 18 cell-states. Row and column indices indicate left and right part of each neighborhood respectively.

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 9 | 6 | 9 | 6 | 6 | 7 | 9 | 7 | 7 | 9 | 6 | 7 | 7 | 6 | 6 | 9 | 9 | 7 |
| 2 | 4 | 6 | 4 | 6 | 6 | 15 | 4 | 15 | 15 | 4 | 6 | 4 | 15 | 6 | 6 | 4 | 15 | 15 |
| 3 | 13 | 14 | 14 | 12 | 14 | 12 | 14 | 13 | 12 | 13 | 13 | 13 | 12 | 14 | 14 | 13 | 12 | 12 |
| 4 | 13 | 14 | 14 | 12 | 14 | 12 | 14 | 13 | 12 | 13 | 13 | 13 | 12 | 14 | 14 | 13 | 12 | 12 |
| 5 | 9 | 1 | 9 | 1 | 1 | 1 | 9 | 2 | 2 | 9 | 1 | 2 | 2 | 2 | 1 | 9 | 9 | 2 |
| 6 | 5 | 16 | 5 | 16 | 16 | 7 | 5 | 7 | 7 | 5 | 16 | 7 | 7 | 16 | 16 | 5 | 5 | 7 |
| 7 | 11 | 8 | 11 | 8 | 10 | 10 | 11 | 10 | 10 | 11 | 10 | 10 | 8 | 8 | 8 | 11 | 11 | 8 |
| 8 | 13 | 14 | 14 | 12 | 14 | 12 | 14 | 13 | 12 | 13 | 13 | 13 | 12 | 14 | 14 | 13 | 12 | 12 |
| 9 | 4 | 6 | 4 | 6 | 6 | 15 | 4 | 15 | 15 | 4 | 6 | 4 | 15 | 6 | 6 | 4 | 15 | 15 |
| 10 | 5 | 1 | 5 | 1 | 1 | 1 | 5 | 2 | 2 | 5 | 1 | 2 | 2 | 2 | 1 | 5 | 5 | 2 |
| 11 | 11 | 8 | 11 | 8 | 10 | 10 | 11 | 10 | 10 | 11 | 10 | 10 | 8 | 8 | 8 | 11 | 11 | 8 |
| 12 | 18 | 17 | 18 | 3 | 3 | 17 | 3 | 17 | 3 | 18 | 18 | 3 | 17 | 3 | 17 | 18 | 18 | 17 |
| 13 | 11 | 1 | 11 | 1 | 1 | 1 | 11 | 2 | 2 | 11 | 1 | 2 | 2 | 2 | 1 | 11 | 11 | 2 |
| 14 | 5 | 16 | 5 | 16 | 16 | 7 | 5 | 7 | 7 | 5 | 16 | 7 | 7 | 16 | 16 | 5 | 5 | 7 |
| 15 | 18 | 17 | 18 | 3 | 3 | 17 | 3 | 17 | 3 | 18 | 18 | 3 | 17 | 3 | 17 | 18 | 18 | 17 |
| 16 | 4 | 16 | 4 | 16 | 16 | 15 | 4 | 15 | 15 | 4 | 16 | 4 | 15 | 16 | 16 | 4 | 15 | 15 |
| 17 | 18 | 17 | 18 | 3 | 3 | 17 | 3 | 17 | 3 | 18 | 18 | 3 | 17 | 3 | 17 | 18 | 18 | 17 |
| 18 | 9 | 8 | 9 | 8 | 10 | 10 | 9 | 10 | 10 | 9 | 10 | 10 | 8 | 8 | 8 | 9 | 9 | 8 |

Table 5
Welch sets for the reversible cellular automaton with 18 cell-states.

| State $s$ | $L_{s}$ | $I D$ | $R_{s}$ | ID |
| :---: | :--- | :--- | :--- | :--- |
| 1 | 51013 | $L_{1}$ | 24561115 | $R_{1}$ |
| 2 | 51013 | $L_{1}$ | 8912131418 | $R_{2}$ |
| 3 | 121517 | $L_{3}$ | 45791214 | $R_{3}$ |
| 4 | 2916 | $L_{4}$ | 137101216 | $R_{4}$ |
| 5 | 61014 | $L_{5}$ | 137101617 | $R_{5}$ |
| 6 | 129 | $L_{6}$ | 245111415 | $R_{6}$ |
| 7 | 1614 | $L_{7}$ | 689121318 | $R_{7}$ |
| 8 | 71118 | $L_{8}$ | 2413141518 | $R_{8}$ |
| 9 | 1518 | $L_{9}$ | 137101617 | $R_{5}$ |
| 10 | 71118 | $L_{8}$ | 56891112 | $R_{10}$ |
| 11 | 71113 | $L_{11}$ | 137101617 | $R_{5}$ |
| 12 | 348 | $L_{12}$ | 469131718 | $R_{12}$ |
| 13 | 348 | $L_{12}$ | 1810111216 | $R_{13}$ |
| 14 | 348 | $L_{12}$ | 23571415 | $R_{14}$ |
| 15 | 2916 | $L_{4}$ | 689131718 | $R_{15}$ |
| 16 | 61416 | $L_{16}$ | 245111415 | $R_{6}$ |
| 17 | 121517 | $L_{3}$ | 268131518 | $R_{17}$ |
| 18 | 121517 | $L_{3}$ | 1310111617 | $R_{18}$ |

Table 6
Matrix $M_{Q}$ for the reversible automaton of 18 cell-states.

| $L / R$ | $R_{1}$ | $R_{2}$ | $R_{3}$ | $R_{4}$ | $R_{5}$ | $R_{6}$ | $R_{7}$ | $R_{8}$ | $R_{10}$ | $R_{12}$ | $R_{13}$ | $R_{14}$ | $R_{15}$ | $R_{17}$ | $R_{18}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $L_{1}$ | 1 | 2 |  |  |  |  |  |  |  |  |  |  |  |  |  |
| $L_{3}$ |  |  | 3 |  |  |  |  |  |  |  |  |  |  | 17 | 18 |
| $L_{4}$ |  |  |  | 4 |  |  |  |  |  |  |  |  | 15 |  |  |
| $L_{5}$ |  |  |  |  | 5 |  |  |  |  |  |  |  |  |  |  |
| $L_{6}$ |  |  |  |  |  | 6 |  |  |  |  |  |  |  |  |  |
| $L_{7}$ |  |  |  |  |  |  | 7 |  |  |  |  |  |  |  |  |
| $L_{8}$ |  |  |  |  |  |  |  | 8 | 10 |  |  |  |  |  |  |
| $L_{9}$ |  |  |  |  | 9 |  |  |  |  |  |  |  |  |  |  |
| $L_{11}$ |  |  |  |  | 11 |  |  |  |  |  |  |  |  |  |  |
| $L_{12}$ |  |  |  |  |  |  |  |  |  | 12 | 13 | 14 |  |  |  |
| $L_{16}$ |  |  |  |  |  | 16 |  |  |  |  |  |  |  |  |  |



Fig. 11. Evolution of the reversible cellular automaton in Table 4 described by mappings and intersection between Welch sets.

Fig. 11 presents an example calculating the evolution for the reversible cellular automaton in Table 4 from a random initial configuration. Every state is mapped into the Welch sets containing it and then the only nontrivial intersection, between left and right Welch sets, is taken to calculate the evolution. Notice that the Welch sets at both ends are repeated to represent periodic boundary conditions.


Fig. 12. Reversible evolution computed by the intersection of Welch sets.

For the same automaton, the inverse evolution is easily calculated taking the intersections of the Welch sets associated with every state (Fig. 12). This case exemplifies how the forward and backwards evolution of a reversible automaton is calculated using $M_{Q}$, which has only $|S|$ elements instead of the $|S| \times|S|$ elements in the $M_{\varphi}$.

## 7. Final remarks

This paper has presented an algorithm based on the properties of Welch indices in order to calculate a random reversible cellular automaton. This algorithm is able to calculate reversible automata with tens of states.

The properties of Welch indices are employed as well to specify two types of bipartite graphs, which represent the dynamics of reversible automata.

The first graph takes as nodes the Welch elements, and the edges among them are utilized to represent the evolution in both directions of reversible automata.

The nodes of this graph are useful as well to generalize the result that the dynamical behavior of reversible automata is equivalent to perform two mappings of blocks with a shift between them.

The second graph takes every different Welch set to establish a reduced version of the evolution rule associated with a given reversible automaton. This graph can be used as well to calculate the evolution of the reversible automaton with the intersection property of Welch sets. Therefore, this graph can be useful to minimize the computational resources required in applications of reversible automata in data cyphering and error-correcting codes.

The main objective of the paper is to show the utility of Welch sets to generate and represent reversible automata by bipartite graphs. These results may open a new research area, where cellular automata and graph theory experts can utilize the properties and operations of bipartite graphs to complement the study of the structural and dynamical behavior of reversible automata in future papers.

Additional further work may imply the definition of an algorithm to calculate random reversible automata in more dimensions, or to enumerate reversible automata for a desired combination of Welch indices.

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[^0]:    Dedicated to the memory of Harold V. McIntosh (1929-2015), a leader in the development of cellular automata theory, whose teaching and knowledge were essential to this work.

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