The Eigenvectors of the Transition Matrix as Predictors of the Dynamics of a Synchronous Boolean Network

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Abstract

The synchronous Boolean network model is a simple and powerful tool in describing, analyzing and simulating cellular biological networks. This paper seeks a complete understanding of the dynamics of such a model by utilizing conventional matrix methods, rather than scalar methods, or matrix methods employing the non-conventional semi-tensor products (STP) of matrices. The paper starts by relating the network transition matrix to its function matrix via a self-inverse (involuntary) state matrix, which has a simple recursive expression, provided a recursive ordering is employed for the underlying basis vector. Once the network transition matrix is obtained, it can be used to generate a wealth of information including its powers, characteristic equation, minimal equation, 1-eigenvectors, and 0-eigenvectors. These might be used to correctly predict both the transient behavior and (more importantly) the cyclic behavior of the network. In a short-cut partial variant of the proposed approach, the step of computing the transition matrix might be by-passed. The reason for this is that the transition matrix and the function matrix are similar matrices that share the same characteristic equation and hence the function matrix might suffice when only the partial information supplied by the characteristic equation is all that is needed. We demonstrate the conceptual simplicity and practical utility of our approach via two illustrative examples. The first example illustrates the computation of 1-eigenvectors (that can be used to

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identify loops or attractors), while the second example deals with the evaluation of 0-eigenvectors (that can be used to explore transient chains). Since attractors are the main concern in the underlying model, then analysis of the Boolean network might be confined to the determination of 1-eigenvectors only.

Keywords: Synchronous Boolean networks; transition matrix; function matrix; characteristic equation; 1-eigenvectors; cyclic behavior; 0-eigenvectors; transient behavior; self-inverse (involutary) matrix.

1 Introduction

A synchronous Boolean network constitutes the simplest possible model that mimics or captures the essential features of general regulatory networks, gene expressions, and various biological systems comprising different types of cellular networks, proteins, DNA, and RNA [1-7]. Hence, this model became a powerful tool for describing, analyzing, and simulating these systems. Though the model is generally intended to capture coarse-grained dynamics of the biological system, it usually has a particular focus on features such as steady state behavior or limiting cycles, attractors or reverberations [8-13]. One advantage of Boolean models (and of similar discrete models) is that, for small models, the entire dynamics can be explored by exhaustive enumeration of all state transitions. Since the size of the state space of a Boolean model with $n$ nodes is $2^n$, this approach becomes unfeasible for larger networks, depending on the power of the computational resources available. In fact, the problem of finding, or even counting, steady states of Boolean networks is NP-hard [14-17], so that any algorithm for this problem will eventually encounter serious limitations.

A Synchronous Boolean network is a set of $n$ interconnected nodes, each of which is either activated (in state 1, or On) or deactivated (in state 0, or Off) at any given instance of time $t$. The network operates on discrete (clock) time such that its state at a present-time point $t$ uniquely determines its state at the next-time point $(t+1)$. Each node is updated at time $(t+1)$ by inputs from a fixed subset of the overall set of nodes (usually comprising neighboring nodes). The update takes place according to some specific logical rule, expressed as a set of next-state scalar functions. Since the number of network states is finite ($2^n$) and the network is a deterministic one, given an arbitrary initial state, the sequence of states succeeding this initial one must necessarily encounter a state it had previously occupied. Thereafter, the network must repeat the intermediate subsequence of states that it traversed from its earlier encounter with this repetitive state till its latter encounter with it. Such a subsequence of states is a cycle, and the number of distinct states in this cycle is its length. For any given network, some states (at least one state) are cyclic but others may be transient occurring during a run-in prior to cycling. For any given network, there may be different cycles of (possibly) varying lengths. If there are transient states, then some of them are first states (also called garden-of-Eden or isle-of-Eden states). Since a first state is a source state or a repelling state, it has no predecessor and does not serve as a next state for any current state. This means that if the network did not start initially in a first state, the network would never encounter that state at any time. In summary, all possible trajectories of the network consist of either cycles (loops or attractors) of any length from size one (a fixed point) to a maximum length of $2^n$ (when the whole trajectory is simply a single loop), or transient states leading eventually to a cycle.

A total description of a synchronous Boolean network is typically achieved by solving a matrix equation [18-20], or by algorithms in which a matrix equation is implicit [21,22]. Typically, matrix methods employed a novel matrix method utilizing a new matrix product, called the semi-tensor product (STP) of matrices [23-42]. A simpler description of a synchronous Boolean network is possible when the matrix equations of the network are replaced by scalar equations or reduced scalar equations [43,44]. Unfortunately, the scalar-equation technique suffers from several shortcomings and limitations [17,19,45-47]. Other candidate methods that might be employed in the analysis of synchronous Boolean networks include solution of Diophantine equations [17,46-51], solution of the Boolean satisfiability problem (SAT) [22,52-57], solution of Boolean equations [58-71], and integer linear programming [22].
The purpose of this paper is to derive the transition matrix \([T]\) of the synchronous Boolean network, independently from any STP formulations or derivations. This matrix is then analyzed to deduce full information about the transient behavior and (more importantly) the cyclic behavior of the network. In fact, subtle inferences about the network behavior are made without drawing the state diagram by exploring some mathematical properties of \([T]\), namely its characteristic equation, minimal equation, 1-eigenvectors and 0-eigenvectors.

The organization of the remainder of this paper is as follows. Section 2 presents our algorithm for computing the transition matrix \([T]\) of a synchronous Boolean network, while Section 3 explains how \([T]\) can be used to deduce the cyclic and transient behavior of the network without resort to a full construction of the network state diagram. Section 4 and 5 amplify our results, by presenting two illustrative examples of synchronous Boolean networks previously studied in the literature. Both Sections illustrate the mathematical techniques employed in deriving necessary related entities such as the characteristic equation, minimal equation, 1-eigenvectors, and 0-eigenvectors. The example of Section 4 deals mainly with the computation of 1-eigenvectors, as a prelude to predicting cyclic behavior. By contrast, the example of Section 5 deals mainly with the computation of 0-eigenvectors, as a step towards exploring transient behavior. Our matrix approach for computing the network transition matrix is superior to scalar techniques which demand cumbersome manipulations and might fail to predict the exact network behavior. In addition, our algorithm replicates in clear, visible and succinct steps the results obtained by the STP methodology. Our transition-matrix predications of network transient and cyclic behavior are also in full agreement with those obtained via a full construction of the network state diagram. In Section 6, we digress a little bit to make a brief discussion, while Section 7 concludes the paper.

2 Construction of the Transition Matrix

This section outlines an algorithm for constructing the transition matrix \([T]\). To understand the mathematical structure of this matrix, we first note that functions used in this paper are functions over the simplest finite or Galois field GF(2), also known as the binary field or mod-2 field [18,19,72,73]. The field has only two elements: the additive identity \((0)\) and the multiplicative identity \((1)\). The field addition (+) and multiplication (\(\times\)) operations are defined by the following axioms:

\[
\begin{align*}
0 + 0 &= 1 + 1 = 0, \\
1 + 0 &= 0 + 1 = 1, \\
0 \times 0 &= 0 \times 1 = 1 \times 0 = 0, \\
1 \times 1 &= 1.
\end{align*}
\] (1a) (1b) (1c) (1d)

Note that the addition (+) operation is a modulo-2 operation that resembles the exclusive-OR operation (\(\oplus\)) in switching algebra (two-valued Boolean algebra) [74-78]. Any function of \(n\) variables over GF(2) is a polynomial of \(2^n\) terms (Reed-Müller polynomial [19,58,72-74]), and hence can be represented by a vector of length \(2^n\), whose elements are the binary coefficients of the \(2^n\) terms in the polynomial. This representation is also called a linear or Boolean-ring representation [58]. In the sequel, we will use two isomorphic representations (the one over GF(2) [72] and that of the Boolean ring [58]), interchangeably, and in particular our (+) sign is equivalently understood to mean modulo-2 addition or XOR operation (1a and 1b), and our (\(\times\)) sign (to be omitted and replaced simply by juxtapositioning) is equivalently understood to mean 1-bit multiplication or AND operation (1c and 1d).

The binary field GF(2) shares many of the familiar properties of other fields such as those of the rational numbers and real numbers, including the existence of an additive identity \((0)\) and a multiplicative identity \((1)\), the existence of an additive inverse for every element and a multiplicative inverse for every element except 0, that addition and multiplication are commutative and associative and that multiplication is
distributive over addition. However, GF(2) possesses features that lack counterparts in the rational and real number systems, including two properties that can be deduced from (1) for every element $x$ of GF(2), namely (a) additive annihilation ($x + x = 0$), and (b) multiplicative idempotency ($x \times x = x$). An important consequence of these two properties is that in GF(2) a vector with an even number of 1-elements is self-orthogonal. We stress that the binary matrices to be considered herein are called GF(2)-matrices and not called Boolean matrices. Brad [79] makes a clear distinction between the two types of matrices denoted by these two names. He bases this distinction on the notion that element multiplication is basically an exclusive-OR operation for GF(2)-matrices, while it is an inclusive-OR operation for Boolean matrices.

In the sequel, we employ a recursively-ordered vector of $2^n$ elements as a basis for all functions of $n$ variables over GF(2) or equivalently all switching functions of $n$ variables (viewed over the Boolean ring), in the sense that any of these functions equals the (scalar) dot product of the vector of binary coefficients representing it with the afore-mentioned basis vector. This basis vector is given explicitly in [19] as

$$\vec{B}_n = \begin{bmatrix} 1 & x_1 & x_2 & x_1x_2 & x_3 & x_1x_3 & x_2x_3 & \cdots & x_n & x_1x_n & x_2x_n & x_1x_2x_n & \cdots & x_1x_2x_3 & \cdots & x_n \end{bmatrix}^T.$$ (2)

Equivalently, it can be defined by the simple recursive relation:

$$\vec{B}_n = \begin{bmatrix} \vec{B}_{n-1} \\ \vec{B}_{n-1} \lor x_n \end{bmatrix},$$ (3)

together with the boundary condition:

$$\vec{B}_0 = [1].$$ (4)

Next, we define the exact state vector $\vec{Y}(t)$ as a binary column vector of dimension $2^n$, whose elements are all 0 except one element that is of value 1. This particular element of value 1 corresponds to the position where the product depicting the network state occurs in the basis vector $\vec{B}_n$. We also define the transition matrix $[T]$ as a $2^n \times 2^n$ permutation matrix having exactly a single 1 in each column and with 0 elements otherwise. The transition matrix may be projective, i.e., there may be more than one element 1 in any row, and (hence) as many rows with all 0's. This transition matrix represents the state transition diagram of the network. The particular structure of $[T]$ asserts that the network is in only one state at a time and proceeds to a unique next state in the next instant of time. The transition matrix $[T]$ relates the exact next-state vector $\vec{Y}(t+1)$ to the exact present-state one via [18,19]:

$$\vec{Y}(t+1) = [T] \vec{Y}(t).$$ (5)

Equation (5) is a restatement of the fact that element $t_{ij}$ in row $i$ and column $j$ of $[T]$ is 1 if and only if present state $j$ leads to next state $i$ (state $i$ is successor to state $j$), and 0 otherwise. We also define the function matrix $[A]$ as a $2^n \times 2^n$ matrix that has as its rows the vector representations of the $2^n$ products of the $n$ scalar next-state functions, taken at a time ($0 \leq k \leq n$). The transition matrix $[T]$ is related to the function matrix $[A]$ via the following similarity transformation, which involves the state matrix $[S_n]$ [18,19]:

$$[A][S_n] = [S_n][T].$$ (6)

$$[A] = [S_n][T][S_n]^{-1} = [S_n][T][S_n].$$ (7)

$$[T] = [S_n]^{-1}[A][S_n] = [S_n][A][S_n].$$ (8)

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where the State Matrix \([S_n]\) is a \(2^n \times 2^n\) upper triangular binary matrix. The recursive ordering of the basis \(\bar{B}_n\) introduced in [19] allows the matrix \([S_n]\) to have the recursive definition [19]:

\[
[S_0] = \begin{bmatrix} 1 \end{bmatrix},
\]

\[
[S_n] = \begin{bmatrix} [S_{n-1}] & [S_{n-1}] \\ [0_{n-1}] & [S_{n-1}] \end{bmatrix}, \quad n > 0,
\]

where \([0_{n-1}]\) is the zero matrix of dimensions \(2^{n-1} \times 2^{n-1}\). This recursive definition of \([S_n]\) is reminiscent of the Preparata Transformation between the linear (Reed-Müller) representation and the minterm (truth-table) representation of a switching function [80-84]. Matrix \([S_n]\) is an involutory (self-inverse) matrix, i.e.,

\[
[S_n]^{-1} = [S_n],
\]

\[
[S_n]^2 = [S_n][S_n] = [S_n][S_n]^{-1} = [I_n],
\]

where \([I_n]\) is the identity matrix of \(2^n \times 2^n\) elements. As a check, the resulting \([T]\) should have a single element of value 1 in every column, with the remaining elements being all 0s. The column vectors of \([T]\) constitute a subset (with possibly repetitive elements) of a set forming an ortho-normal basis of the \(2^n\)-dimensional vector space. For the case \([S_n]\), the matrix \([S_3]\) is given by:

\[
[S_3] = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 & 1 \\
0 & 0 & 1 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 1 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1
\end{bmatrix}
\]

This section is summarized in Fig. 1, which presents a flow chart for the computation of the transition matrix of a synchronous Boolean network, given the scalar next-state functions of its nodes.

![Flow chart](image)

**Fig. 1. A flow-chart for the construction of the matrix \([T]\)**
3 Utilization of the Transition Matrix in Predicting Network Dynamics

This section demonstrates how the transition matrix \([T]\) could be utilized in predicting network behavior via its powers, characteristic equation, minimal equation, 1-eigenvectors and 0-eigenvectors. A state of the network \(\vec{Y}(t)\) is called cyclic if \([18,19]\): \[
\vec{Y}(t + m) = [T]^m \vec{Y}(t) = \vec{Y}(t), \quad \text{for some } m > 0.
\] (13a)

Otherwise it is called transient when: \[
\vec{Y}(t + m) = [T]^m \vec{Y}(t) \neq \vec{Y}(t), \quad \text{for all } m > 0.
\] (13b)

A set of cyclic states that map into one another are called a cycle. In particular, the \(k\)-element set defined by \(C = \{\vec{Y}(t), [T] \vec{Y}(t), \ldots, [T]^{k-1} \vec{Y}(t)\}\) is a cycle of length \(k\) if \([T]^k \vec{Y}(t) = \vec{Y}(t)\) and the elements of \(C\) are distinct \([28, p. 108]\). For \(k = 1\), the set \(C\) is the singleton \(\{\vec{Y}(t)\}\), and the cycle becomes of length 1, i.e., a fixed point. A cycle is therefore definable as a \([T]\)-invariant subspace \([28,85,86]\), since the matrix \([T]\) maps \(C\) to itself \(([T]C = C)\). A state into which no state maps is called a first state (a garden-of-Eden or isle-of-Eden state), i.e., a first state has no predecessor and does not serve as a next state for any current state, and hence the row corresponding to it in the transition matrix \([T]\) is an all-0 row. A set of transient states that can be reached from a certain first state are called a transient chain. Note that a state is transient if it is a first state or it can be reached only from a first state or from some other transient states.

By analogy to characteristic equations of real matrices \([87,88]\), Cull \([18]\) introduced the concept of the binary characteristic equation of a binary matrix \([T]\). He defined it as \(\det([T] - \lambda[I]) = 0\), where the operations are carried out in the binary field, so that subtraction (−) and addition (+) are indistinguishable. In fact, subtraction is not even defined on GF(2). Hence, the characteristic equation becomes \(\det([T] + \lambda[I]) = 0\). This equation will take the form \([18,19]\): \[
\det ([T] + \lambda[I]) = \lambda^m(\lambda^{r_1} + 1)\cdots(\lambda^{r_t} + 1) = 0,
\] (14)

where \(m\) is the total number of transient states, while the subscripted \(r\)’s are the lengths of the various cycles. We note that the eigenvalues of the matrix \([T]\) are the roots of its characteristic equation (14). In GF(2), the only possible eigenvalues are \(\lambda = 1\) (corresponding to one-eigenvectors that represent cycles) and \(\lambda = 0\) (corresponding to zero-eigenvectors that represent transient chains). The factorization of the binary characteristic equation is not always unique \([18,19]\). In fact, \[
(\lambda^r + 1) = (\lambda + 1)^r,
\] (15)

for \(r\) being a power of 2, so that one cannot specify all cycles exactly by specifying the characteristic equation \([3]\). Now, we observe that since matrices \([A]\) and \([T]\) are similar, they have the same characteristic equation \([18,19]\): \[
\det ([A] + \lambda[I]) = \det([T] + \lambda[I]) = 0
\] (16)

One reason why we prefer to transform to the matrix \([A]\) to \([T]\) is that the task of determining the characteristic polynomial of a permutation matrix such as \([T]\) is particularly simple, since it has a single non-zero entry per column. By contrast, the determination of the characteristic polynomial of \([A]\) is somewhat cumbersome since many entries of \([A]\) are non-zero. The Cayley-Hamilton theorem (which states in the continuous case that any matrix satisfies its own characteristic equation) is still applicable in this finite case, i.e., \[
[T]^m([T]^{r_1} + [I])\cdots([T]^{r_t} + [I]) = [0].
\] (17)
\[ [A]^m([T]^r_1 + [I]) \cdots ([T]^r_1 + [I]) = [0]. \]  

(18)

Cull [18] asserted that there is an equation of lowest degree that \([A]\) satisfies; which is the minimal equation \([89-92]\) of \([A]\), namely:

\[ [A]^{r_0}([A]^{r_1} + [I]) \cdots ([A]^{r_g} + [I]) = [0]. \]  

(19)

Here, \(r_0\) is the length of the longest transient chain and \(r_1, \ldots, r_g\) are lengths of distinct cycles such that all other cycle lengths divide one of the \(r_i\)s with no remainder [18].

The cyclic behavior of a synchronous Boolean network can also be obtained from one-eigenvectors of the function matrix \([A]\) or the one-eigenvectors of the transition matrix \([T]\). In fact, the cycles of the network are linearly independent one-eigenvectors of \([T]\) and the one-eigenvectors of \([T]\) are cycles or the union of cycles [18,19].

Similarly, the zero-eigenvectors can be used in the study of the transient chains [18,19]. There are as many independent 0-eigenvectors as there are chains [18,19]. Each of these eigenvectors is of the form \(\vec{Y}_i + \vec{Y}_j\), where \(\vec{Y}_i \neq \vec{Y}_j\). At least one of the states \(\vec{Y}_i\) and \(\vec{Y}_j\) is the last state of a transient chain, \(i.e.,\) a state that is not on a cycle, but whose next state is on a cycle [19].

Gelfand [4] observed that the trace (usual arithmetic sum of diagonal elements) of \([T]^m\) is equal to the number of states on cycles of length \(\kappa\) which is a divisor of the integer \(m\). Hence, the number of fixed points is equal to the trace of \([T]\) itself. If we use \(N\) to denote \(2^n\), then \(Tr(T^N)\) equals the number of states on cycles and \((n - Tr(T^N))\) equals the number of transient states, where \(N!\) denotes the factorial of \(N = 2^n\).

### 4 Example Dealing with 1-eigenvectors

This example was analyzed earlier by Cull [18] and Rushdi and Al-Otaibi [19]. Consider a network of 3 elements whose next-states are given by:

\[ f_1 = 1 + x_2 + x_1x_2 + x_1x_3 + x_1x_2x_3, \]  

(20a)

\[ f_2 = 1 + x_2 + x_1x_2 + x_3 + x_1x_3 + x_1x_2x_3, \]  

(20b)

\[ f_3 = 1 + x_1 + x_1x_2 + x_3 + x_2x_3 + x_1x_2x_3. \]  

(20c)

Now, the products of these functions (two at a time and three (all) at a time) are:

\[ f_1f_2 = 1 + x_2 + x_1x_2 + x_3 + x_2x_3 + x_1x_2x_3, \]  

(20d)

\[ f_1f_3 = 1 + x_1 + x_2 + x_1x_2x_3, \]  

(20e)

\[ f_2f_3 = 1 + x_1 + x_2 + x_3 + x_2x_3 + x_1x_2x_3, \]  

(20f)

\[ f_1f_2f_3 = 1 + x_1 + x_2 + x_3 + x_1x_3 + x_2x_3. \]  

(20g)

Noting that the product of zero functions (conveniently called \(f_0\)) is the multiplication identity (1), we construct the function matrix \([A]\),
matrix is that it provides a more efficient means for computing the characteristic equation, and it supplies
the information via its powers. The result in (24) is self-checking, since each matrix column is a unit of all-0 entries with exactly a single exception of a unique 1 element. The abbreviation $\delta_6$ in (24) is a convenient way of representing the transition matrix by specifying the row number (from 0 to 7) in which the sole 1 (the only non-zero value) in a column is located. The characteristic equation for $[T]$ (or for $[A]$) is:

$$\det ([T] + \lambda [I]) = \det ([A] + \lambda [I]) = \lambda (\lambda^4 + 1)(\lambda^3 + 1).$$

In this case the minimal equation is identical to the characteristic equation, i.e., it is

$$[T]([T]^4 + [I])([T]^3 + [I]) = [0].$$

These facts tell us that the system has a transient chain of length 1, a cycle of length 4, and another cycle of length 3. We would have obtained these results by computing $[A]$ only without computing $[T]$, since the two matrices $[T]$ and $[A]$ are similar and share the same characteristic equation. This possibility hints at the existence of a short-cut partial variant of our proposed approach, in which the step of computing the transition matrix might be skipped. The function matrix might suffice when only the partial information supplied by the characteristic equation is all that is needed. The reason we opted to work with the transition matrix is that it provides a more efficient means for computing the characteristic equation, and it supplies extra information via its powers.

$$[A] = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 \\
1 & 0 & 1 & 1 & 1 & 1 & 0 & 1 \\
1 & 0 & 1 & 1 & 1 & 0 & 1 & 1 \\
1 & 1 & 0 & 1 & 0 & 1 & 1 & 1 \\
1 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\
1 & 1 & 1 & 0 & 1 & 0 & 1 & 1 \\
1 & 1 & 1 & 0 & 1 & 1 & 1 & 0
\end{bmatrix}.$$ (21)
Now, we let \( \vec{\Psi} = [y_0 \ y_1 \ y_2 \ y_3 \ y_4 \ y_5 \ y_6 \ y_7]^T \) be a 1-eigenvector of \([T]\), i.e., \([T]\vec{\Psi} = (1)\vec{\Psi}\), then:

\[
y_0 = 0, \ y_1 = y_7, \ y_2 = y_6, \ y_3 = y_1, \ y_4 = y_2, \ y_5 = y_4, \ y_6 = y_5, \ y_7 = y_0 + y_3 = y_3
\]

which combine to give \( y_0 = 0, \ y_1 = y_3 = y_7 = \alpha, \ y_2 = y_4 = y_5 = y_6 = \beta. \) Hence, the generalized eigenvector of \([T]\) is:

\[
\vec{\Psi} = [0 \ \alpha \ \beta \ \alpha \ \beta \ \beta \ \alpha]^T.
\]

Table 1 shows all four possible values for \( \vec{\Psi} \), out of which only two \( \vec{\Psi}_b \) and \( \vec{\Psi}_c \) are linearly independent. The first linearly-independent 1-eigenvector \( \vec{\Psi}_b \) identifies a cycle of period 4 with cycle states 2, 4, 5, and 6 (referenced in the basis \( \vec{B}_3 \)). These are states \( x_2, x_3, x_1x_3, \) and \( x_2x_3 \), or equivalently \((010),(001),(101),\) and \((111)\) when identified by values of 3-tuple \((x_1x_2x_3)\). The second linearly-independent 1-eigenvector \( \vec{\Psi}_c \) identifies another cycle of period 3 with cycle states 1, 3, and 7 (again referenced in the basis \( \vec{B}_3 \)). These are states \( x_3, x_1x_2, \) and \( x_2x_2x_3 \), or equivalently \((100),(110),\) and \((111)\) again when representing \((x_1x_2x_3)\) values. Out of the 8 network states, 7 states are on cycles, and the remaining single state \((000)\) is a transient state.

To finalize this example, we verify our findings via the Karnaugh-map representation of the three next-state functions \( f_1, f_2, \) and \( f_3 \) in Fig. 2, from which we draw the full state-diagram of the network in Fig. 3. In passing, we remark that we found it more convenient to study this example via 1-eigenvectors rather than 0-eigenvectors since most of its states are cycle states rather than transient ones.

![Fig. 2. A Karnaugh-map representation for the next-state functions \( \{f_1, f_2, f_3\} \) of the network in the example of Sec. 3.](image201x270to220x276)

![Fig. 3. The state diagram for the example of Sec. 3 with states designated by the binary values of the 3-tuple \( \{x_1x_2x_3\} \).](image208x270to219x276)

| \( \alpha \) | \( \beta \) | \( \vec{\Psi} \) | Comment |
|---|---|---|---|
| 0 | 0 | \( \vec{\Psi}_b = [0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0 \ 0]^T \) | trivial |
| 0 | 1 | \( \vec{\Psi}_a = [0 \ 0 \ 1 \ 0 \ 1 \ 1 \ 1 \ 0]^T \) | independent |
| 1 | 0 | \( \vec{\Psi}_c = [0 \ 1 \ 0 \ 1 \ 0 \ 0 \ 0 \ 1]^T \) | independent |
| 1 | 1 | \( \vec{\Psi}_d = [0 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1 \ 1]^T \) | \( \vec{\Psi}_d = \vec{\Psi}_b + \vec{\Psi}_c \) |
5 Example Dealing with 0-Eigenvectors

This example was analyzed earlier by Heidel et al. [43] and Rushdi and Al-Otaibi [19]. Consider a network of 3 elements whose next-states are given by:

\[ f_1 = x_2 \lor x_3 = x_2 + x_3 \times x_2 x_3, \quad (28a) \]
\[ f_2 = x_1 \lor x_3 = x_1 + x_3 \times x_1 x_3, \quad (28b) \]
\[ f_3 = x_1 \lor x_2 = x_1 + x_2 \times x_1 x_2. \quad (28c) \]

Now, the products of these functions are:

\[ f_1 f_2 = x_1 x_2 + x_3 + x_1 x_2 x_3, \quad (28d) \]
\[ f_1 f_3 = x_2 + x_1 x_3 + x_1 x_2 x_3, \quad (28e) \]
\[ f_2 f_3 = x_1 + x_2 x_3 + x_1 x_2 x_3, \quad (28f) \]
\[ f_1 f_2 f_3 = x_1 x_2 + x_1 x_3 + x_1 x_2 x_3. \quad (28g) \]

Then, we construct the function matrix \([A]\) using the strategy of the previous section:

\[
[A] = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\
0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 1
\end{bmatrix}. \quad (29)
\]

The transition matrix \([T]\) is given by:

\[
[T] = [S_3][A][S_3] = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 1 & 1 & 1
\end{bmatrix} = \tilde{E}_0[0, 6, 5, 7, 3, 7, 7, 7]. \quad (30)
\]

This transition matrix \([T]\) has two non-0 diagonal elements, corresponding to fixed points at states 0 and 7 (expressed as \((000)\) and \((111)\)). Now, the two powers \([T]^2\) and \([T]^4\) are given by:

\[
[T]^2 = [T]^4 = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{bmatrix} = \tilde{E}_0[0, 7, 7, 7, 7, 7, 7, 7]. \quad (31)
\]
Equation (31) says that the longest transient trajectory is of length 2. After two time periods all network states (except state 0) are attracted to state 7 (111). The characteristic equation of $[T]$ is:

$$
\text{det} ([T] + \lambda [I]) = \text{det} ([A] + \lambda [I]) = \lambda^6 (\lambda + 1)^2,
$$

and hence the system has 6 transient states and two cycles of length 1. The factor $(\lambda + 1)^2$ should not be replaced by $(\lambda^2 + 1)$ which represents a single cycle of length 2 (see Equation (15)). Here, the minimal equation is not identical to the characteristic equation, but is given by:

$$
[A]^2([A] + [I])^2 = [0],
$$

which means that the longest transient chain is of length 2. In fact, equations (7), (8), (11) and (31) can be used to obtain $[A]^4 + [A]^2 = [0]$, which can be recast in the form (33) since $([A]^2 + [I])$ must be replaced by its equivalent form $([A] + [I])^2$, as required by the characteristic equation.

Fig. 4. Possible values for the 0-eigenvectors for the example of Sec. 4.

To study the transient behavior of the network, we find all the independent 0-eigenvectors of the network by solving $[T] \vec{y} = \vec{0}$. This produces three identities $\vec{0} = 0$ plus the five constraints:

$$
y_0 = y_1 = y_2 = y_4 = 0, \quad y_3 + y_5 + y_6 + y_7 = 0,
$$

(34)
which reduces the eigenspace to a 3-dimensional one. This means that there are eight 0-eigenvectors of \([T]\), as shown in the Karnaugh-map of Fig. 4, where cells violating the even parity condition on \(y_2, y_5, y_6, and y_7\) are rejected. Out of these eigenvectors only three are linearly independent, e.g., the vectors \((\vec{\delta}_3 + \vec{\delta}_5), (\vec{\delta}_6 + \vec{\delta}_7), and (\vec{\delta}_6 + \vec{\delta}_7)\). This means that there are three transient chains in the network state diagram. In fact, we can identify the start states for these chains as the ones corresponding to all-0 rows in \([T]\). These are states 1 (100), 2 (010), and 4 (001). Our knowledge about the linearly-independent 0-eigenvectors indicates that each of the four states 3, 5, 6, and 7 is either the last state of a transient chain or on a cycle. Since we have three transient chains, then we know that three of the states 3, 5, 6, and 7 are the last states of transients, with the fourth state being on a cycle. With our earlier observation that states 0 and 7 are 1-period cycles (fixed points), we realize that states 3, 5, and 6 are transient end states.

To finalize this example, we verify our findings via the Karnaugh-map representation of the three next-state functions \(f_1, f_2, and f_3\) in Fig. 5, from which we draw the full state-diagram of the network in Fig. 6.

![Karnaugh-map representation for the next-state functions](image)

**Fig. 5.** A Karnaugh-map representation for the next-state functions \((f_1 f_2 f_3)\) of the network for the example of Sec. 4

![State diagram](image)

**Fig. 6.** The state diagram for the example of Sec. 4 with states designated by the binary values of the 3-tuple \(\{x_1 x_2 x_3\}\)

### 6 Discussion

Boolean network models are one of the simplest models to study complex dynamic behavior in biological systems. There are three major paradigms (synchronous, asynchronous and probabilistic) for the mode of transition of a Boolean network from a present state to a succeeding one [93]. We have only considered the synchronous paradigm, in which all nodes of the network take an equivalent amount of time (the clock period) to change their value. Consequently, the dynamics of the Boolean network are deterministic, and each state of the network has one successor. Our main concern herein was the study of these networks using the eigenvectors of the transition matrix. Some of our concepts translate to other paradigms of Boolean networks with other types of matrices.
Real networks exhibit heterogeneous nature with nodes playing different roles in structure and function. A non-trivial task is to identify vital nodes associated with some certain structural or functional objectives \([94,95]\). The concept of ‘centrality’ is forwarded to characterize the importance of a node according the network structure \([96-99]\). Generally speaking, a centrality measure assigns a real value to each node in the network, where the values produced are expected to provide a ranking of nodes subject to their importance. An interesting measure of centrality is that of eigenvector centrality \([99,100,101]\), which has advantages over graph-theoretic centrality measures like degree, betweenness, and closeness centrality \([99]\). Eigenvector centrality supposes that the influence of a node is not only determined by the number of its neighbors, but also determined by the influence of each neighbor \([97]\). The centrality of a node is proportional to the summation of the centralities of the nodes to which it is connected \([94]\). We are particularly interested in the case where eigenvector centrality pertains to Boolean networks (see, e.g., \([102,103]\)). Ghanbarnejad and Klemm \([102]\) consider synchronous networks with deterministic update and asynchronous networks with stochastic update. They quantify the dynamical impact of a node as the probability of damage spreading after switching the node’s state. They assert that the leading or principal eigenvector of the adjacency matrix is a good predictor of dynamical impact in the case of long-term spreading. This eigenvector centrality measure is a good predictor of how a node’s initial state perturbs the attractor the system eventually arrives at. The quality of prediction is further improved when eigenvector centrality is based on the weighted matrix of activities rather than on the unweighted adjacency matrix.

7 Conclusions

To analyze a synchronous Boolean network, we start from the scalar next-state equations of the network so as to write its function matrix \([A]\). Next, we obtain the transition matrix \([T]\) via its similarity relation with \([A]\), a step which involves pre-multiplying and post-multiplying \([A]\) with the state matrix \([S_n]\). This step is self-checking, since it must produce a matrix \([T']\) whose column vectors are unit vectors. We utilize certain properties of \([T']\) to make useful deductions about network behavior without drawing the state diagram. We use the characteristic and minimal equations for \([T]\), its 1-eigenvectors, and 0-eigenvectors as advocated by Cull \([18]\) and later by Rushdi and Al- Otaibi \([19]\), as well as by Li et al. \([10]\). The predictions made by the various methods are self-consistent and are in full agreement with results obtained earlier, notably via the STP machinery. These predictions also coincide exactly with those deduced from the full state diagram. We note that there is a relation between our current matrix method and the method of describing the network via reduced scalar equations \([43,44,47]\). Contrary to earlier assumptions and assertions that appeared in \([43,44]\), the reduced scalar equations are not necessarily the same for all variables, and the true or minimal scalar equation (for the worst-case variable) must be sought in order to give a correct information about the transient behavior of the network \([46,47]\). We stress that the method reported herein is, indeed, superior to the scalar techniques in \([43,44]\). In fact, scalar techniques use ad-hoc cumbersome heuristics, and might fail to predict the exact network behavior, especially its transient one \([46,47]\). Cheng et al. \([28]\) reported a disparity in the assessment of the maximum length of a transient chain as obtained by their matrix method, and the scalar methods of \([43,44]\). Since the matrix method is a complete one, there was no doubt that its assessment was the correct one. Intrigued by the reason of fallibility of the scalar approach, Rushdi & Alsogati \([46]\) and Rushdi \([47]\) took pains to correct the way the scalar approach is implemented, so as to reconcile its output with that of matrix methods.

The current paper is a serious attempt to make the matrix analysis of synchronous Boolean networks independent of any particular implementation, such as that of the semi-tensor products (STP) of matrices. We produce results that exactly replicate those of the STP approach, but achieve that without sophisticated ambiguity or unwarranted redundancy. We stress that we perform binary (Boolean) computations on GF(2), while usual STP computations involve real numbers and real operations. However, we must admit that the STP methodology comprises an ingenious paradigm shift that might considerably mitigate the ‘curse of dimensionality’ in a variety of fields, including the present one of synchronous Boolean networks. All we are asking for, is that when STP handles logic or Boolean expressions, then it should be constrained to the use of Boolean operations.
Competing Interests

Authors have declared that no competing interests exist.

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