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The Boolean constraint method application for qualitative analysis of the dynamical properties of singular Boolean networks

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Qualitative study problems of trajectories behaviour for singular Boolean networks functioning on a finite time interval are solved using the method of Boolean constraints. In the form of Boolean constraints, models are built for local dynamical properties, the periodicity property of trajectories, and the property of the reachability of the target state set from the initial state set. Depending on the property, the verification of Boolean models is reduced to the Boolean satisfiability problem or the problem of verifying the truth of a quantified Boolean formula. Several examples demonstrate the technology of qualitative analysis of dynamic properties in a microservice heterogeneous computing environment. The applied software modules for constructing a Boolean model of the dynamical property of singular Boolean networks and verifying the feasibility of the model are implemented in the form of computational microservices. The use of this approach provides independence, reproducibility, autonomy, and scalability of modules. The developed microservices are integrated into the applied microservices package. This package is intended for the qualitative study of binary dynamic systems. The rights to launch microservices are delegated to the managing agents of this package installed in the nodes of the distributed environment. The developed automation tools allow a specialist in automaton dynamics to formulate the problem statement on a computational model of the subject area in meaningful terms.

Keywords: singular Boolean networks, qualitative analysis, Boolean constraints, service-oriented solver.

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Introduction

Singular Boolean networks — singular binary dynamical systems (BDS) — are a new class of mathematical objects, similar in a certain sense to algebraic-differential systems. The systematic study of algebraic-differential systems was begun by several mathematicians in the USSR [1] and the USA [2] independently from each other. Later, centers for the study of algebraic-differential systems were opened in other countries, for example, in Germany [3]. During the construction of Boolean models of some biological and social networks, a situation arises when additional static algebraic constraints are imposed on the states of the equations of network dynamics [4].

A new class of mathematical models is emerging, which are interested both from a theoretical and practical point of view. These models are called singular Boolean networks. Other terms are also used in the literature: dynamic-algebraic networks, difference-algebraic networks, singular networks, degenerate networks. Chinese scientists [5–14], using the semi-tensor product method [15] as their primary research tool, actively study various properties of singular Boolean networks. The paper [16] notes the usefulness of this method in the theoretical study of the dynamic properties of Boolean networks and also points out its main drawback, which is the need to operate with $2^n \times 2^n$ dimension matrices when using this method (n is the Boolean system state dimension).

A new method developed by authors for the qualitative analysis of the dynamic properties of BDS (the Boolean constraints method) and its application to autonomous systems is considered in [17]. Let us list the main provisions of this method:

- The formalization of definitions of dynamic properties in the language of predicate logic. The use of bounded quantifiers of existence and universality. The use of bounded quantifiers provides a dynamical property specification language familiar to the dynamics specialist.
- The conversion of the logical formula of the dynamical property to a form that takes into account the equations of the BDS dynamics.
- The elimination of bounded quantifiers and obtaining a property formula in the applied predicate logic with unbounded quantifiers.

As the result of the sequential execution of these three stages, we get a model of the dynamical property as a Boolean constraint (Boolean equation or quantified Boolean formula). Verifying the satisfiability of a BDS property is reduced to the problem of feasibility of a Boolean constraint using modern SAT [18] and QSAT [19] solvers. Since there is a significant increase in the performance of specialized algorithms for solving SAT and QSAT problems now (due to the usage of efficient heuristics and deep parallelization of the computational process), the total variables count in the dynamical property model can be measured in thousands.

The Boolean constraint method is a sufficiently general method for the qualitative analysis of BDS in a finite time interval. It applies not only to autonomous systems but also to various other classes of binary dynamic models. The objective of this work is to use this method for a qualitative study of the trajectories behaviour of singular BDS.

The presentation of the research materials is organized as follows. Section 1 presents a mathematical model of a singular Boolean network, gives a typification of its states, gives a definition of a solution to a singular network for a given initial state, presents a condition for the absence of deadlocks in the form of a quantified Boolean formula, writes out equivalent Boolean network equations for one-step and multi-step transitions. Section 2 is devoted to the study of local dynamic properties. Section 3 discusses the periodicity property of trajectories. Section 4 investigates the reachability property of the target set of states from the set of initial ones. The implementation of the proposed method is described in Section 5. In Section 6, the technology of qualitative analysis of singular Boolean networks using the Boolean constraints method is demonstrated in examples. In the conclusion section, we summarize the study results, and directions of its further development are indicated concerning the problems of singular networks control.

1. Mathematical model of a singular BDS

Let us consider a Boolean network whose dynamics are described by the following system of equations:

$$\mathbf{x}^{t+1} = \mathbf{F}(\mathbf{x}^t, \mathbf{z}^t), \tag{1}$$

$$\mathbf{H}(\mathbf{x}^t, \mathbf{z}^t) = 0, \tag{2}$$

where $t \in T = \{0, 1, 2, \ldots, k\}$ is discrete time, $\mathbf{x} \in B^n$ is the state vector, $B = \{0, 1\}$, $\mathbf{z} \in B^l$ is the vector of auxiliary variables, $\mathbf{F}(\mathbf{x}, \mathbf{z})$, $\mathbf{H}(\mathbf{x}, \mathbf{z})$ are the vector functions of the Boolean algebra, called the transition function and the constraint function, respectively ($\mathbf{F} : B^n \times B^l \to B^n$, $\mathbf{H} : B^n \times B^l \to B$). Equation (1) specifies the dynamics of BDS transitions from one state to another. Equation (2) defines the constraints on such transitions. Let $\mathbf{x}^* \in B^n$ be some BDS state. Depending on the number of solutions to the equation

$$\mathbf{H}(\mathbf{x}^*, \mathbf{z}) = 0 \tag{3}$$

concerning the unknown vector of auxiliary variables $\mathbf{z}$, three different situations are possible with the state $\mathbf{x}^*$:

- If Eq. (3) has a unique solution, the state $\mathbf{x}^*$ is called deterministic (the state $\mathbf{x}^*$ has one successor).
- If Eq. (3) has several solutions, the state $\mathbf{x}^*$ is called a branching state (the state $\mathbf{x}^*$ has several successors; their number is equal to the number of solutions to Eq. (3)).
- If Eq. (3) has no solutions, the state $\mathbf{x}^*$ is called a deadlock (state $\mathbf{x}^*$ has no successors).

Let $\mathbf{x}^0 = \mathbf{x}(t)|_{t=0}$ be some given initial state of the Eq. (1). Let us denote $\mathbf{x}(t, \mathbf{x}^0)$ through a sequence of states $(\mathbf{x}^0, \mathbf{x}^1, \ldots, \mathbf{x}^k)$. Such a sequence is called a solution to system (1), (2) on the time interval T, if for any $\mathbf{x}^t$ there is a value $\mathbf{z}^t$, such that each pair of adjacent states $\mathbf{x}^t, \mathbf{x}^{t+1}$ $(t = 0, 1, 2, \cdots, k+1)$ satisfies the Eq. (1). The solution $\mathbf{x}(t, \mathbf{x}^0)$ determines a path of length k in the transition graph of the system (1), (2). Such a path is called a trajectory in the state space B^n.

As follows from the definition of a solution to system (1), (2), the trajectory $\mathbf{x}(t, x^0)$ does not contain deadlock states. If the system (1), (2) has branching states, then its behaviour for the general case is non-deterministic. So to some initial states $\mathbf{x}^0 \in B^n$, a set of solutions $X(t, \mathbf{x}^0)$ called a funnel of trajectories can correspond. Thus, in contrast to the classical Boolean network, the solution $\mathbf{x}(t, \mathbf{x}^0)$ may not be unique. This fact must be taken into account for the formulation of dynamical properties of a singular Boolean network using the Boolean constraints method, which we use for qualitative analysis of such networks.

The condition for the presence of deadlock states in the system (1), (2) is written in the form of the following quantified Boolean formula (QBF):

$$(\exists \mathbf{x} \in B^n)(\forall \mathbf{z} \in B^l)\mathbf{H}(\mathbf{x}, \mathbf{z}). \tag{4}$$

If the Boolean formula (4) is true, then at least one deadlock state $\mathbf{x}^*$ exists. Otherwise, there are no deadlock states. For small-scale problems, verification of the truth of the formula (4) is performed using the QSAT solver DepQBF [20] with the "issue a certificate" option set [21]. The certificate, in our case, is the deadlock state $\mathbf{x}^*$. For calculating the next deadlock state (if it exists), a clause $\bigvee\limits_{i=1}^{n} \bar{\mathbf{x}}_i^*$ is added to the final formula $\mathbf{H}(\mathbf{x}, \mathbf{z})$. This clause corresponds to the constraint that excludes the repeated finding of the deadlock state $\mathbf{x}^*$. The DepQBF solver is launched with updated final formula. For problems of large dimensions, a similar parallel solver Hpc2qall-v2 has been developed, with the help of which, if the formula is TRUE, a constructive solution is also found. This solver is a modified version of the previously developed solver Hpcqsat [22].

According to the Boolean constraints method [17], we represent the system (1), (2) as one equivalent Boolean equation. For $k = 0$ (only one-step transitions are considered), this equation has the form:

$$L(\mathbf{x}^0, \mathbf{x}^1, \mathbf{z}^0) = \bigvee_{i=1}^{n} (\mathbf{x}_i^1 \oplus \mathbf{F}_i(\mathbf{x}^0, \mathbf{z}^0)) \vee \mathbf{H}(\mathbf{x}^0, \mathbf{z}^0) = 0, \tag{5}$$

where $\mathbf{x}_i^1$ is i-th component of vector $\mathbf{x}^1$, $\oplus$ is the modulo-2 addition operation, $\mathbf{F}^i$ is i-th component of vector $\mathbf{F}$. The solutions of this equation define a loaded directed graph (phase portrait) consisting of 2^n vertices corresponding to the states of the set B^n. The vertices $\mathbf{x}^0$ and $\mathbf{x}^1$ of the graph are connected by an arc labelled by the value of the vector $\mathbf{z} \subset B^l$ and directed from the state $\mathbf{x}^0$ to the state $\mathbf{x}^1$. Let us call the state $\mathbf{x}^1$ the successor of the state $\mathbf{x}^0$, and $\mathbf{x}^0$ — the predecessor of the state $\mathbf{x}^1$.

For k-step transitions ($k \geq 1$) the Eq. (5) has the following form:

$$\Phi_k(\mathbf{x}^0, \mathbf{x}^1, \ldots, \mathbf{x}^k, \mathbf{z}^0, \mathbf{z}^1, \ldots, \mathbf{z}^{k-1}) = \bigvee_{t=1}^{k} L(\mathbf{x}^{t-1}, \mathbf{x}^t, \mathbf{z}^{t-1}) = 0. \tag{6}$$

Solutions of Eq. (6) determine the entire set of trajectories of length k in the phase space of the system (1), (2).

2. Local dynamical properties

Equation (5) allows studying the local dynamic properties of each state from B^n, such as the presence of immediate predecessors and successors of the state, the presence of equilibrium states, and the possibility of transition from one state to another in one step. All these properties are determined by setting constraints on the initial state $\mathbf{x}^0$ and the following state $\mathbf{x}^1$ in the Boolean Eq. (5). When solving these problems, the vector of auxiliary variables $\mathbf{z}$ is assumed unknown and is determined based on the imposed restrictions on $\mathbf{x}^0$ and $\mathbf{x}^1$. All immediate predecessors $\mathbf{x}^0$ of the state $\mathbf{x}^1 = \mathbf{c}$ are found by solving the Boolean equation

$$L(\mathbf{x}^0, \mathbf{x}^1, \mathbf{z}^0)|_{\mathbf{x}^1=\mathbf{c}} = 0 \tag{7}$$

and all immediate successors $\mathbf{x}^1$ of any state $\mathbf{x}^0 = \mathbf{c}$ are found by solving the Boolean equation

$$L(\mathbf{x}^0, \mathbf{x}^1, \mathbf{z}^0)|_{\mathbf{x}^0=\mathbf{c}} = 0. \tag{8}$$

The state $\mathbf{x}^0$ is called an equilibrium state if the condition $\mathbf{x}^1 = \mathbf{x}^0$. All equilibrium states (if they exist) are determined by solutions of the Boolean equation

$$L(\mathbf{x}^0, \mathbf{x}^1, \mathbf{z}^0)|_{\mathbf{x}^1=\mathbf{x}^0} = 0. \tag{9}$$

concerning unknown variables $\mathbf{x}^0$, $\mathbf{z}^0$. To study the equilibrium state isolation, equations (7), (8) should be used.

Eq. (5) allows determining the possibility of a one-step transition from the state $\mathbf{x}^0 = \mathbf{c}^0$ to the state $\mathbf{x}^1 = \mathbf{c}^1$ by solving the Boolean equation

$$L(\mathbf{x}^0, \mathbf{x}^1, \mathbf{z}^0)|_{\substack{\mathbf{x}^0=\mathbf{c}^0\\ \mathbf{x}^1=\mathbf{c}^1}} = 0. \tag{10}$$

concerning the unknown vector of auxiliary variables $\mathbf{z}^0$.

It should be noted that the calculated value of the vector $\mathbf{z}^0$ in equations (7)–(10) is the condition for the solvability of these equations concerning the corresponding state vectors.

Eq (6) allows studying the following properties of multistep trajectories of length k ($k > 1$):

- The periodicity of trajectories.
- Various properties of the reachability type of the target set $X^* \subset B^n$ by trajectories with initial states from the set $X^0 \subset B^n$ on the time interval T.

3. Periodicity property of trajectories

The trajectory $\mathbf{x}^0$, $\mathbf{x}^1$, $\ldots$, $\mathbf{x}^k$ ($k \geq 2$) is called a periodic trajectory of length k (or a cycle of length k) if the states $\mathbf{x}^0$, $\mathbf{x}^1$, $\ldots$, $\mathbf{x}^{k-1}$ are different from each other and $\mathbf{x}^k = \mathbf{x}^0$. In a singular Boolean network, cyclic sequences of length k (if they exist) are solutions of the Boolean equation

$$\Phi_k(\mathbf{x}^0, \mathbf{x}^1, \ldots, \mathbf{x}^k, \mathbf{z}^0, \mathbf{z}^1, \ldots, \mathbf{z}^{k-1})\Big|_{\mathbf{x}^k=\mathbf{x}^0} \vee R(\mathbf{x}^0, \mathbf{x}^1, \ldots, \mathbf{x}^{k-1}) = 0, \tag{11}$$

where

$$R(\mathbf{x}^0, \mathbf{x}^1, \ldots, \mathbf{x}^{k-1}) = \bigvee_{\substack{1\leq q\leq k-1\\ k \mod q=0}} \bigwedge_{i=1}^{n} y_i^{0q} = 0 \quad (y_i^{0q} = \mathbf{x}_i^0 \wedge \mathbf{x}_i^q \vee \bar{\mathbf{x}}_i^0 \wedge \bar{\mathbf{x}}_i^q)$$

is the condition for a pairwise distinction of the set of states C of a cycle of length k. In Eq. (11), in contrast to the usual (classical) network, the vector of auxiliary variables $\mathbf{z}$ participates in the formation of the cycle, the value of which depends on the current state of this cycle. Thereby, the definition and conditions for the isolation of the cycle are changed as follows. The cycle is called isolated if none of its states has predecessors and successors belonging to set C. For the classic network, no successors are required. Let the states of set C be determined by the solutions of the Boolean equation $G^c(\mathbf{s}) = 0$. Then it is not difficult to show that the condition for the isolation of the cycle of a singular network is the absence of solutions for the following Boolean equations

$$G^C(\mathbf{s}) \vee L(\mathbf{x}^0, \mathbf{x}^1, \mathbf{z}^0)|_{\mathbf{x}^1=\mathbf{s}} \vee \bar{G}^c(\mathbf{x}^0) = 0, \quad G^C(\mathbf{s}) \vee L(\mathbf{x}^0, \mathbf{x}^1, \mathbf{z}^0)|_{\mathbf{x}^0=\mathbf{s}} \vee \bar{G}^c(\mathbf{x}^1) = 0. \tag{12}$$

Solutions to Eq. (12) (if they exist) define cycle states that have predecessors or successors that do not belong to the set C.

4. Reachability property

An important property that is usually of interest to a specialist in automatic dynamics is the reachability property and its several variations [17]. Let X^0 and X^* be the sets of initial and target states determined using Boolean equations $G^0(\mathbf{x}) = 0$ and $G^*(\mathbf{x}) = 0$ ($\mathbf{x} \in B^n$).

The main property of reachability of the set X^* from the set X^0 is formulated as follows. For any $\mathbf{x}^0 \in X^0$, there is at least one trajectory $\mathbf{x}(t, \mathbf{x}^0)$ from the funnel of trajectories that reaches the target set X^*. This definition of the reachability property differs from the corresponding definition for classic networks [17], and this difference consists in taking into account the non-uniqueness of the solution $\mathbf{x}(t, \mathbf{x}^0)$.

With the use of bounded quantifiers of existence and universality, the logical formula for the reachability property of a singular network is:

$$(\forall \mathbf{x}^0 \in X^0)(\exists t \in T)(\exists \mathbf{x}(t, \mathbf{x}^0))(\mathbf{x}(t, \mathbf{x}^0) \in X^*). \tag{13}$$

Taking into account the equation of dynamics (6), we write formula (13) in the form

$$\left(\forall \mathbf{x}^0, \mathbf{x}^1, \ldots, \mathbf{x}^k, \mathbf{z}^0, \mathbf{z}^1, \ldots, \mathbf{z}^{k-1} : \overline{G^0(\mathbf{x}^0) \vee \Phi_k(\mathbf{x}^0, \mathbf{x}^1, \ldots, \mathbf{x}^k, \mathbf{z}^0, \mathbf{z}^1, \ldots, \mathbf{z}^{k-1})}\right) \left(\bigvee_{t=1}^{k} \bar{G}^*(\mathbf{x}^t)\right) = 0. \tag{14}$$

Similarly to [17], the truth of logical formula (14) is equivalent to the absence of zeros for the following Boolean equation

$$\left(G^0(\mathbf{x}^0) \vee \Phi_k(\mathbf{x}^0, \mathbf{x}^1, \ldots, \mathbf{x}^k, \mathbf{z}^0, \mathbf{z}^1, \ldots, \mathbf{z}^{k-1})\right) \vee \left(\bigvee_{t=1}^{k} \bar{G}^*(\mathbf{x}^t)\right) = 0. \tag{15}$$

If the Eq. (15) has at least one solution, the reachability property does not hold. This solution provides a counterexample for the tested property and can help identify the cause of this situation.

The definitions of other properties of the reachability type and their qualitative analysis using the Boolean constraints method can be found in [17].

5. Method implementation

The proposed method is implemented based on the previously developed Applied Microservices Package (AMP) [23]. The composition of AMP complexes for constructing a Boolean model and solving problems of qualitative analysis of controlled BDS is extended with the corresponding microservices for the qualitative analysis of singular Boolean networks. AMP functionality, access to AMP, and data management are described in detail in [24–26], respectively.

A fragment of a computational model for qualitative analysis of singular networks is shown in Fig. 1. This model is used for verifying the satisfiability of the considered dynamic properties using the method of Boolean constraints.

The computational model (knowledge base, KB) is presented as a set of parameters of the subject domain and functional relations between them. Each functional relation is implemented by a software module that calculates the values of the output parameters of the module using the given values of the input parameters. Applied software modules are implemented in the form of computational microservices installed in the nodes of a distributed computational environment. The microservice developer delegates rights on the microservice launch to the AMP agent installed on the same node. The AMP agent performs the

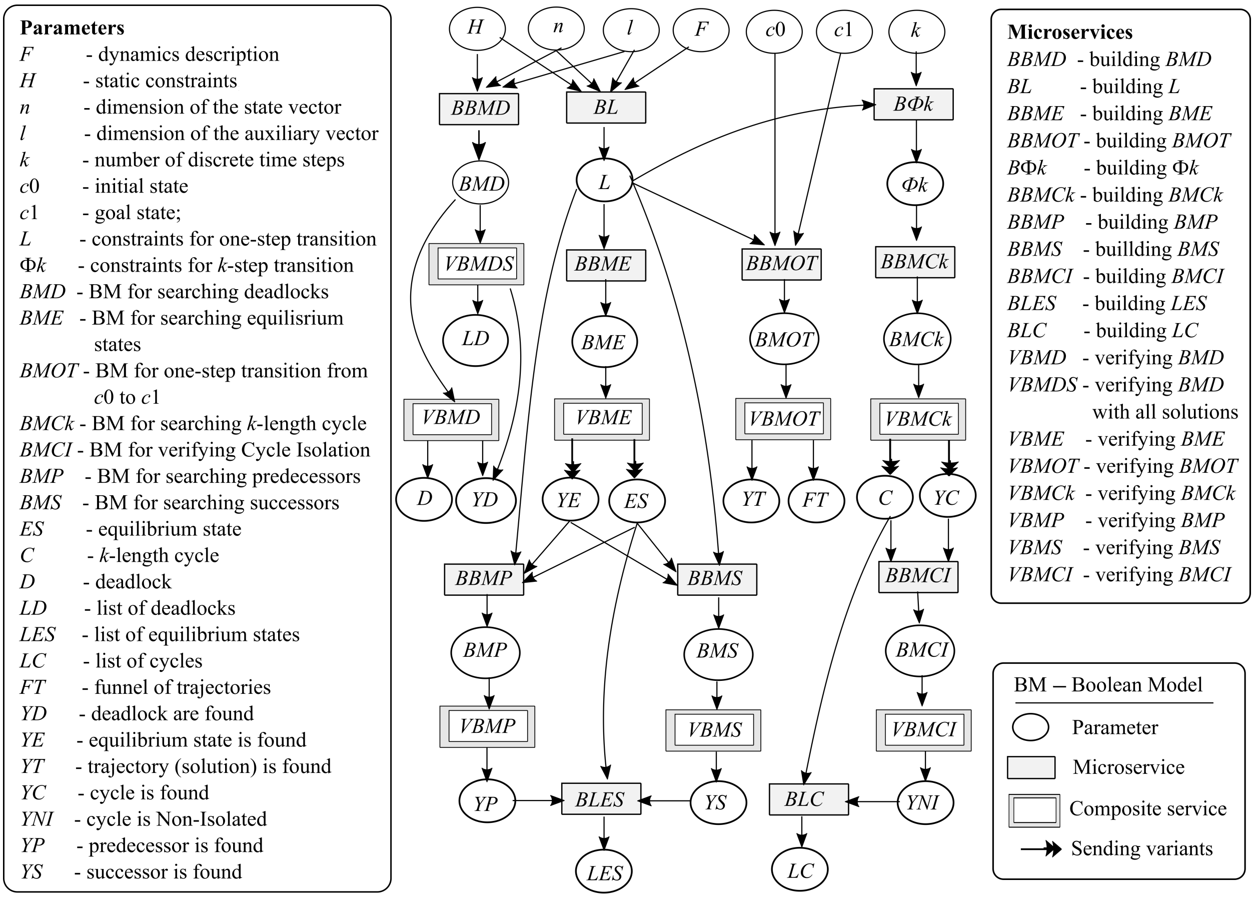

Fig. 1. Fragment of the computational model

launch of the microservice required for solving problem P on the model KB. The use of a microservice-based approach provides independence, reproducibility, autonomy, scalability of the modules of the developed application and their interaction using a lightweight messaging mechanism and better isolation of failures. Thus, this approach creates independently deployable microservice [27]. As noted in [28], decentralized control and data management allow microservices to be independent and avoid standardizing an application based on a single technology. In the case of decentralized control, solving problem P includes the following stages:

- Forming an active group of agents if the problem P is solvable on the KB.
- Excluding redundant parameters from the set A_0 unrequired for calculating parameters from the set B_0.
- Joint acting of the active group of agents for solving problem P by launching the necessary computational microservices.

Interactions of agents are coordinated by the event control (by input data readiness) in all stages of solving problem P.

The computational model allows formulating a problem from a given class by fixing the known A_0 and required B_0 model parameters. A pair of sets $P = (A_0, B_0)$ is called a non-procedural problem statement (NPS) (meaningful request) on the KB model. There are following examples of the formulation of problems on the KB fragment (Fig. 1) for qualitative analysis of singular Boolean networks:

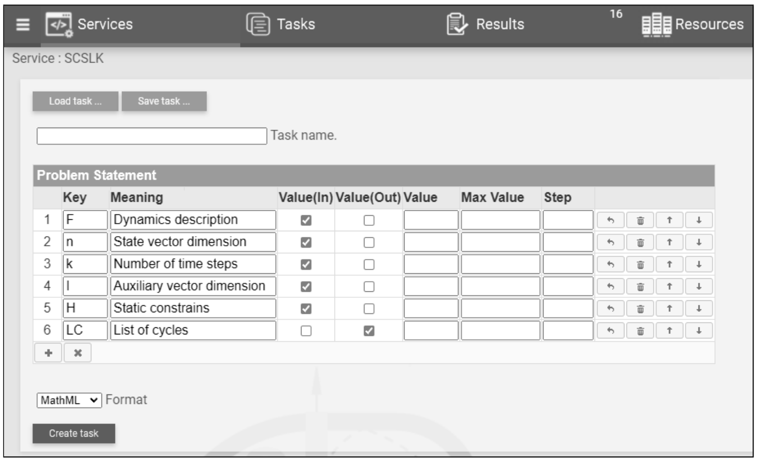

Fig. 2. Forming the NPS P_2 in the web interface of the user agent

- Searching for equilibrium states: $P_1 = (A_0 = \{F, H, n, l\}, B_0 = \{LES\})$.
- Searching for cycles of the length k: $P_2 = (A_0 = \{F, H, n, l, k\}, B_0 = \{LC\})$.
- Searching for deadlocks: $P_3 = (A_0 = \{H, n, l\}, B_0 = \{YD, D\})$.

The NPS is formed in the web interface of the AMP manager-agent (Fig. 2).

For verifying the feasibility of Boolean models, composite services [29] are used (Fig. 1). In these services, depending on the dimension of the model, sequential or parallel solvers are launched. A parallel 2QBF solver Hpc2qall-v2 has been developed to check the truth of 2QBF. This MPI-solver is focused on verifying the truth of the 2QBF of the form $\exists\, \mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n \,\forall\, \mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_l \varphi(\mathbf{x}, \mathbf{z})$, where $\varphi(\mathbf{x}, \mathbf{z})$ is in conjunctive normal form. Unlike the existing parallel 2QBF solvers, the Hpc2qall-v2 gives both the verifying result and all sets of variables under the existential quantifier, leading to the SAT result (the formula value is TRUE). The DepQBF solver is used as the base solver in child threads.

6. Examples

As an illustration of the proposed approach, let us consider four simple singular Boolean networks, the dynamics of which are described by the following equations with the corresponding Boolean constraints L for a one-step transition:

- Example 1

$$
\begin{gathered}
\mathbf{x}_1^{t+1} = \bar{\mathbf{x}}_2^t, \\
\mathbf{x}_2^{t+1} = \mathbf{x}_1^t \wedge \mathbf{z}_1^t, \\
(\mathbf{x}_2^t \vee \mathbf{z}_1^t) \wedge \bar{\mathbf{x}}_1^t = 0, \\
L(\mathbf{x}^0, \mathbf{x}^1, \mathbf{z}^0) = \bar{\mathbf{x}}_1^1 \wedge \bar{\mathbf{x}}_2^0 \vee \mathbf{x}_1^1 \wedge \mathbf{x}_2^0 \vee \bar{\mathbf{x}}_2^1 \wedge \mathbf{x}_1^0 \wedge \mathbf{z}_1^0 \vee \mathbf{x}_2^1 \wedge \bar{\mathbf{x}}_1^0 \vee \\
\vee \mathbf{x}_2^1 \wedge \bar{\mathbf{z}}_1^0 \vee \mathbf{x}_2^0 \wedge \bar{\mathbf{x}}_1^0 \vee \bar{\mathbf{x}}_1^0 \wedge \mathbf{z}_1^0 = 0.
\end{gathered}
$$

- Example 2

$$
\begin{gathered}
\mathbf{x}_1^{t+1} = \mathbf{x}_2^t \wedge \mathbf{z}_1^t, \\
\mathbf{x}_2^{t+1} = \bar{\mathbf{x}}_1^t \vee \mathbf{z}_1^t, \\
\mathbf{z}_1^t \wedge \mathbf{x}_1^t \wedge \mathbf{x}_2^t \vee \bar{\mathbf{z}}_1^t \wedge \bar{\mathbf{x}}_1^t \vee \bar{\mathbf{z}}_1^t \wedge \bar{\mathbf{x}}_2^t = 0, \\
L(\mathbf{x}^0, \mathbf{x}^1, \mathbf{z}^0) = \bar{\mathbf{x}}_1^1 \wedge \mathbf{x}_2^0 \wedge \mathbf{z}_1^0 \vee \mathbf{x}_1^1 \wedge \bar{\mathbf{x}}_2^0 \vee \mathbf{x}_1^1 \wedge \bar{\mathbf{z}}_1^0 \vee \bar{\mathbf{x}}_2^1 \wedge \bar{\mathbf{x}}_1^0 \vee \bar{\mathbf{x}}_2^1 \wedge \mathbf{z}_1^0 \vee \bar{\mathbf{x}}_2^1 \wedge \bar{\mathbf{x}}_1^0 \wedge \mathbf{z}_1^0 \vee \\
\vee \mathbf{z}_1^0 \wedge \mathbf{x}_1^0 \wedge \mathbf{x}_2^0 \vee \bar{\mathbf{z}}_1^0 \wedge \bar{\mathbf{x}}_1^0 \vee \bar{\mathbf{z}}_1^0 \wedge \bar{\mathbf{x}}_2^0 = 0.
\end{gathered}
$$

- Example 3

$$\mathbf{x}_1^{t+1} = \mathbf{x}_2^t,$$
$$\mathbf{x}_2^{t+1} = (\mathbf{x}_1^t \vee \mathbf{x}_2^t) \wedge \mathbf{z}_1^t,$$
$$(\bar{\mathbf{x}}_1^t \vee \bar{\mathbf{x}}_2^t \vee \bar{\mathbf{z}}_1^t) \wedge (\mathbf{x}_2^t \vee \mathbf{z}_1^t) = 0,$$
$$L(\mathbf{x}^0, \mathbf{x}^1, \mathbf{z}^0) = \bar{\mathbf{x}}_1^1 \wedge \mathbf{x}_2^0 \vee \mathbf{x}_1^1 \wedge \bar{\mathbf{x}}_2^0 \vee \bar{\mathbf{x}}_2^1 \wedge \mathbf{x}_1^0 \wedge \mathbf{z}_1^0 \vee \bar{\mathbf{x}}_2^1 \wedge \mathbf{x}_2^0 \wedge \mathbf{z}_1^0 \vee \mathbf{x}_2^1 \wedge \bar{\mathbf{x}}_2^0 \wedge \bar{\mathbf{x}}_1^0 \vee$$
$$\vee \mathbf{x}_2^1 \wedge \bar{\mathbf{z}}_1^0 \vee \bar{\mathbf{x}}_1^0 \wedge \mathbf{x}_2^0 \vee \mathbf{x}_2^0 \wedge \bar{\mathbf{z}}_1^0 \vee \bar{\mathbf{x}}_1^0 \wedge \mathbf{z}_1^0 \vee \bar{\mathbf{x}}_2^0 \wedge \mathbf{z}_1^0 = 0.$$

- Example 4

$$\mathbf{x}_1^{t+1} = \mathbf{x}_2^t,$$
$$\mathbf{x}_2^{t+1} = (\mathbf{x}_1^t \vee \mathbf{x}_2^t) \wedge \mathbf{z}_1^t,$$
$$(\bar{\mathbf{x}}_1^t \vee \bar{\mathbf{z}}_1^t) \wedge (\mathbf{x}_1^t \vee \mathbf{z}_1^t) \vee \mathbf{x}_2^t = 0,$$
$$L(\mathbf{x}^0, \mathbf{x}^1, \mathbf{z}^0) = \bar{\mathbf{x}}_1^1 \wedge \mathbf{x}_2^0 \vee \mathbf{x}_1^1 \wedge \bar{\mathbf{x}}_2^0 \vee \bar{\mathbf{x}}_2^1 \wedge \mathbf{x}_1^0 \wedge \mathbf{z}_1^0 \vee \bar{\mathbf{x}}_2^1 \wedge \mathbf{x}_2^0 \wedge \mathbf{z}_1^0 \vee \mathbf{x}_2^1 \wedge \bar{\mathbf{x}}_2^0 \wedge \bar{\mathbf{x}}_1^0 \vee$$
$$\vee \mathbf{x}_2^1 \wedge \bar{\mathbf{z}}_1^0 \vee \mathbf{x}_1^0 \wedge \mathbf{x}_2^0 \wedge \bar{\mathbf{z}}_1^0 \vee \bar{\mathbf{x}}_1^0 \wedge \mathbf{x}_2^0 \wedge \mathbf{z}_1^0 = 0.$$

For these examples, phase portraits (transition diagrams) are shown in Fig. 3. In this figure, circles indicate the states of the dynamic part of the system (1). The arcs are marked with the value of the variable $\mathbf{z}_1$, at which the corresponding transition is possible.

For each of the examples, when verifying QBF (4), a deadlock state (01) is found in the first and third examples.

By solving Boolean equations (7)–(9), the following is established:

- In example 1, there are two branching states (10), (11), and one equilibrium state (10), which remains at the value $\mathbf{z}_1 = 0$.
- Example 2 belongs to the class of conventional classical networks.
- In example 3, there are two equilibrium states — (00) for the value $\mathbf{z}_1 = 0$ and (11) for the value $\mathbf{z}_1 = 1$. The state (1,1) is isolated.
- In example 4, there is one branching state (10) and two equilibrium states — an isolated state (11) for the value $\mathbf{z}_1 = 1$ and a non-isolated state (00) for values $\mathbf{z}_1 = 0$, $\mathbf{z}_1 = 1$.

By solving Eq. (10), the possibility of transition in one step from the state (10) to state (00) is shown for $\mathbf{z}_1 = 0$ in example 4.

By solving equations (11), (12), a single non-isolated cycle of length $k = 3$ is detected: (00/0) → (10/1) → (11/0) → (00/0) in example 1 and (00/1) → (01/1) → (11/0) → (00/0) in example 2. The non-isolated cycle (01/0) → (10/1) → (01/0) of length $k = 2$ is detected in example 4. The value of $\mathbf{z}_1$ required for the transition to the next state is given after the symbol “/”.

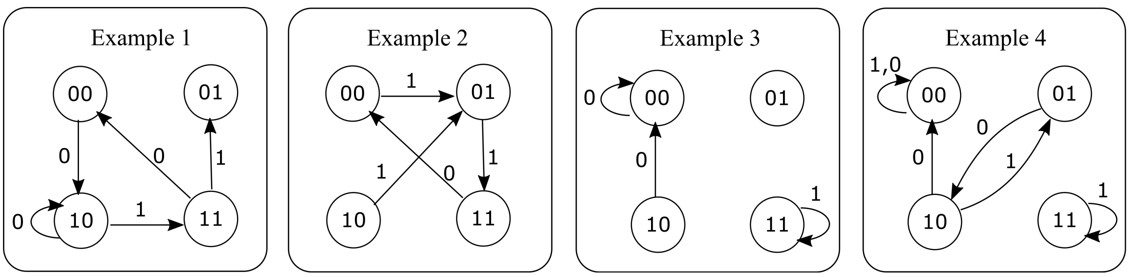

Fig. 3. Phase portraits for examples 1–4

By solving the Eq. (6) for $k = 3$ and the initial state $\mathbf{c} = (01)$, the following funnel of trajectories is found in example 4:

$$
\begin{gathered}
(01/0) \to (10/1) \to (01/0) \to (10),\\
(01/0) \to (10/0) \to (00/0) \to (00),\\
(01/0) \to (10/0) \to (00/1) \to (00).
\end{gathered}
$$

Verifying the truth of the logical formula (14) showed that in example 4, for $k = 2$, the state (00) is reachable from the state (01) (Eq. (15) has no solutions).

Conclusion

Based on the Boolean constraints method developed by the authors, a constructive solution to the problems of a qualitative study of the dynamics of the trajectories behaviour of singular Boolean networks on a finite time interval is obtained. Dynamical properties models of these networks attract considerable attention in computational biology when analyzing the behaviour of social and cellular networks. Taking into account algebraic constraints leads (in comparison with classical networks) to a significant modification of the definitions of dynamic properties, which are interesting for a specialist in the qualitative analysis of binary dynamic models. Based on the logical properties specification and equations of the system dynamics, the models of local dynamical properties, the periodicity properties of trajectories, and properties of the reachability type are obtained in the form of Boolean constraints. Depending on the property, the verification of Boolean models is reduced to the Boolean satisfiability problem or the problem of verifying the truth of a quantified Boolean formula. An advantage of the developed tools for the qualitative analysis of singular binary dynamical systems is their orientation towards systems with a high dimension of the state vector and a large interval of discrete time variation. The method implementation allows data parallelism and provides high scalability with an increase in the number of variables in the Boolean constraint.

Another important direction of application of the method of Boolean constraints to singular networks is associated with the solution of the following problems: a qualitative study of the properties of controllability and observability, as well as synthesis of feedback (static or dynamic, by state or by output), which provides the satisfiability of the required dynamical property in a closed system.

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ВЫЧИСЛИТЕЛЬНЫЕ ТЕХНОЛОГИИ

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Применение метода булевых ограничений для качественного анализа динамических свойств сингулярных булевых сетей

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Аннотация

С использованием метода булевых ограничений решены задачи качественного исследования динамики поведения траекторий на конечном интервале времени сингулярных булевых сетей. Получены в виде булевых ограничений модели локальных динамических свойств, свойства периодичности траекторий и свойства достижимости целевого множества состояний из множества начальных состояний. В зависимости от свойств проверка булевых ограничений сводится к задаче булевой выполнимости или задаче проверки истинности квантифицированной булевой формулы. Приведен ряд примеров, на которых продемонстрирована технология качественного исследования динамических свойств в микросервисной гетерогенной вычислительной среде. Прикладные программные модули для построения булевой модели динамического свойства сингулярной булевой сети и проверки выполнимости модели реализованы в виде вычислительных микросервисов. Применение такого подхода обеспечивает независимость, воспроизводимость, автономность и масштабируемость модулей. Разработанные микросервисы расширили репозиторий пакета прикладных микросервисов для качественного исследования двоичных динамических систем. Права на запуск микросервисов делегированы управляющим агентам этого пакета, установленным в узлах распределенной среды. Разработанные средства автоматизации позволяют специалисту по автоматной динамике формулировать постановку задач на вычислительной модели предметной области в содержательных терминах.

Ключевые слова: сингулярные булевы сети, качественный анализ, булевы ограничения, сервис-ориентированный решатель.

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