Boolean Networks

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Friday 7th November, 2025

Boolean Abstraction

Boolean networks constitute a "top-down" abstraction, allowing us to model systems which are not understood in full detail.

In general, Boolean networks are well suited for modelling systems with the following properties:

- Made up of interacting entities.
- Each entity is characterised by a variable quantity.
- The events (and their mechanisms) are not directly observable, only their complete consequences.

Boolean Networks - Syntax

A Boolean network f of dimension $n \in \mathbb{N}$ (on n variables) is a collection of n-ary Boolean functions f_1, \ldots, f_n :

$$f=(f_1,\ldots,f_n)$$

For each $i \in \{1, ..., n\}$, $f_i : \mathbb{B}^n \to \mathbb{B}$ is the **local function** of the *i*-th variable.

The Boolean network itself can be understood as a Boolean vector function $f: \mathbb{B}^n \to \mathbb{B}^n$, defined as $f(\mathbf{x}) = (f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_n(\mathbf{x}))$.

Example:

$$f_1(\mathbf{x}) = \mathbf{x}_3 \wedge (\neg \mathbf{x}_1 \vee \neg \mathbf{x}_2)$$

 $f_2(\mathbf{x}) = \mathbf{x}_1 \wedge \mathbf{x}_3$
 $f_3(\mathbf{x}) = \mathbf{x}_1 \vee \mathbf{x}_2 \vee \mathbf{x}_3$

Boolean Networks - Semantics

A Boolean network defines a finite dynamical system with discrete states (**transition system**). A transition system (S, \rightarrow) is composed of:

- A finite set of states *S*;
- An irreflexive transition relation $\rightarrow \subseteq S \times S$;

We use the natural infix notation for the transition relation, $\mathbf{x} \to \mathbf{y}$ instead of $(\mathbf{x}, \mathbf{y}) \in \to$.

For a Boolean network of dimension n, the set of states is the set of all Boolean vectors of length n, $S = \mathbb{B}^n$.

EXAMPLE:

For dimension n = 3, $S = \{000, 001, 010, 100, 011, 101, 110, 111\}$.

The exact shape of the transition relation is determined by the chosen **update mode**.

Multiple different update modes are commonly employed.

Update Modes

Given a configuration $\mathbf{x} \in \mathbb{B}^n$, then for each variable $i \in \{1, ..., n\}$, $f_i(\mathbf{x})$ is the "next value" of the *i*-th variable.

In particular a variable such that $\mathbf{x}_i \neq f_i(\mathbf{x})$ is called **frustrated** (in the configuration \mathbf{x}).

There are multiple ways of upgrading configurations:

- All variables update value simultaneously;
- Variables update value sequentially;
- Variables are split into blocks and each block updates values simultaneously;
- ...each block updates values sequentially;
- Internal clocks;
- ...

Update Functions

Update functions are a family of functions which are restating the local functions f_1, \ldots, f_n as direct modification of the configurations, $\Phi \colon \mathbb{B}^n \to \mathbb{B}^n$.

For any subset of variables $W \subseteq \{1, ..., n\}$, the update function $\Phi_W \colon \mathbb{B}^n \to \mathbb{B}^n$ is defined as $\Phi_W \colon \mathbf{x} \mapsto \mathbf{y}$ where for each $i \in \{1, ..., n\}$:

$$\mathbf{y}_i \stackrel{\triangle}{=} \begin{cases} f_i(\mathbf{x}) & \text{if } i \in W \\ \mathbf{x}_i & \text{if } i \notin W \end{cases}$$

EXAMPLES:

$$\Phi_{\emptyset} = id : \mathbf{x} \mapsto \mathbf{x}
\Phi_{\{1,\dots,n\}} : \mathbf{x} \mapsto (f_1(\mathbf{x}), f_2(\mathbf{x}), \dots, f_n(\mathbf{x}))
\forall i \in \{1,\dots,n\}, \Phi_{\{i\}} = \Phi_i : \mathbf{x} \mapsto (\mathbf{x}_1,\dots,\mathbf{x}_{i-1}, f_i(\mathbf{x}), \mathbf{x}_{i+1},\dots,\mathbf{x}_n)$$

A transition of the form $\mathbf{x} \to \Phi_W(\mathbf{x})$ for some $W \subseteq \{1, \dots, n\}$ is called **elementary**.

Boolean Networks in Systems Life Sciences

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"All variables have their value updated simultaneously."

Synchronous semantics only uses one update function, $\Phi_{\{1,\ldots,n\}}$: $\mathbf{x} \mapsto (f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_n(\mathbf{x}))$. Formally:

$$\forall \mathbf{x} \neq \mathbf{y} \in \mathbb{B}^n, \mathbf{x} \stackrel{sync}{\longrightarrow} \mathbf{y} \stackrel{\Delta}{\Longleftrightarrow} \mathbf{y} = \Phi_{\{1,\dots,n\}}(\mathbf{x})$$

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Deterministic – Each configuration has at most one successor.

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$$f_{1}(\mathbf{x}) = \mathbf{x}_{3} \wedge (\neg \mathbf{x}_{1} \vee \neg \mathbf{x}_{2}) \qquad 001 \xrightarrow{sync} 101$$

$$f_{2}(\mathbf{x}) = \mathbf{x}_{1} \wedge \mathbf{x}_{3} \qquad 100 \xrightarrow{sync} 001 \qquad 101 \xrightarrow{sync} 111$$

$$f_{3}(\mathbf{x}) = \mathbf{x}_{1} \vee \mathbf{x}_{2} \vee \mathbf{x}_{3} \qquad 010 \xrightarrow{sync} 001 \qquad 011 \xrightarrow{sync} 101$$

$$110 \xrightarrow{sync} 001 \qquad 111 \xrightarrow{sync} 011$$

Fully Asynchronous Semantics

"Only one variable updates value in each transition."

Fully asynchronous semantics use all singleton update functions, $\Phi_i : \mathbf{x} \mapsto (\mathbf{x}_1, \dots, \mathbf{x}_{i-1}, f_i(\mathbf{x}), \mathbf{x}_{i+1}, \dots, \mathbf{x}_n), i \in \{1, \dots, n\}$. Formally:

$$\forall \mathbf{x} \neq \mathbf{y} \in \mathbb{B}^n, \mathbf{x} \stackrel{async}{\longrightarrow} \mathbf{y} \stackrel{\Delta}{\Longleftrightarrow} \exists i \in \{1, \dots, n\}, \mathbf{y} = \Phi_i(\mathbf{x})$$

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$$110 \xrightarrow{async} 100 \qquad 101 \xrightarrow{async} 111$$

$$110 \xrightarrow{async} 111 \qquad 011 \xrightarrow{async} 111$$

$$111 \xrightarrow{async} 011 \qquad 011 \xrightarrow{async} 001$$

"Any subset of variables has their values updated simultaneously."

Generalised asynchronous semantics use all update functions, Φ_W for $W \subseteq \{1, \dots, n\}$. Formally:

$$\forall \mathbf{x} \neq \mathbf{y} \in \mathbb{B}^n, \mathbf{x} \xrightarrow{gen} \mathbf{y} \stackrel{\Delta}{\Longleftrightarrow} \exists W \subseteq \{1, \dots, n\}, \mathbf{y} = \Phi_W(\mathbf{x})$$

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$$\overset{\textit{sync}}{\longrightarrow} \subseteq \overset{\textit{gen}}{\longrightarrow} \text{ and } \overset{\textit{async}}{\longrightarrow} \subseteq \overset{\textit{gen}}{\longrightarrow}.$$

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$$\stackrel{sync}{\Longrightarrow} \stackrel{gen}{\Longrightarrow} \text{ and } \stackrel{async}{\Longrightarrow} \stackrel{gen}{\Longrightarrow}$$

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$$010 \xrightarrow{gen} 001 \qquad 110 \xrightarrow{gen} 111 \qquad 011 \xrightarrow{gen} 111$$

$$010 \xrightarrow{gen} 000 \qquad 110 \xrightarrow{gen} 000 \qquad 011 \xrightarrow{gen} 001$$

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 $110 \xrightarrow{gen} 101$

A maximum value for each variable, $m_1, \ldots, m_n \ge 1$, giving us the following state space $S = \{0, \ldots, m_1\} \times \{0, \ldots, m_2\} \times \cdots \times \{0, \ldots, m_n\}$.

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THOMAS NETWORKS (Discrete multivalued networks with thresholds)

The network definition remains unchanged $f = (f_1, \dots, f_n) : \mathbb{B}^n \to \mathbb{B}^n$, but additionally an $n \times n$ matrix T of thresholds has to be specified.

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$$f_1(\mathbf{x}) = \delta_1(\mathbf{x})_3 \wedge (\neg \delta_1(\mathbf{x})_1 \vee \neg \delta_1(\mathbf{x})_2)$$

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$$f_3(\mathbf{x}) = \delta_3(\mathbf{x})_1 \vee \delta_3(\mathbf{x})_2 \vee \delta_3(\mathbf{x})_3$$

Where:

$$\delta_i(\mathbf{x}) = (T_{1,i} \leq \mathbf{x}_1, \dots, T_{n,i} \leq \mathbf{x}_n)$$

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$$W \subseteq \{1, \dots, n\}$$

$$\Phi_{W} : S \to S$$

$$\Phi_{W} : \mathbf{x} \mapsto \mathbf{y} \text{ where for } i \in \{1, \dots, n\}:$$

$$f_{2}(\mathbf{x}) = \delta_{2}(\mathbf{x})_{1} \wedge \delta_{2}(\mathbf{x})_{3}$$

$$f_{3}(\mathbf{x}) = \delta_{3}(\mathbf{x})_{1} \vee \delta_{3}(\mathbf{x})_{2} \vee \delta_{3}(\mathbf{x})_{3}$$

$$Where:$$

$$\delta_{i}(\mathbf{x}) = (T_{1,i} \leq \mathbf{x}_{1}, \dots, T_{n,i} \leq \mathbf{x}_{n})$$

$$\mathbf{y}_{i} \triangleq \begin{cases} max(0, \mathbf{x}_{i} - 1) & \text{if } i \in W \\ & \text{and } f_{i}(\mathbf{x}) = 0 \\ & \text{win}(m_{i}, \mathbf{x}_{i} + 1) & \text{if } i \in W \\ & \text{and } f_{i}(\mathbf{x}) = 1 \\ \mathbf{x}_{i} & \text{if } i \notin W \end{cases}$$