Boolean networks, local models, and finite polynomial dynamical systems

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Math 4500, Spring 2017

Boolean functions

Let $\mathbb{F}_2 = \{0, 1\}$. By a Boolean function, we usually mean a function $f\colon \mathbb{F}_2^n \longrightarrow \mathbb{F}_2$.

There are several standard ways to write Boolean functions:

1. As a logical expression, using $\wedge$, $\vee$, and $\neg$ (or $\overline{}$)
2. As a polynomial, using $+$, and $\cdot$
3. As a truth table.

Example

The following are three different ways to express the function that outputs 0 if $x = y = z = 1$, and 1 otherwise.

- $f(x, y, z) = \overline{x \wedge y \wedge z}$
- $f(x, y, z) = 1 + xyz$
-

x	1	1	1	1	0	0	0	0
y	1	1	0	0	1	1	0	0
z	1	0	1	0	1	0	1	0
$f(x, y, z)$	0	1	1	1	1	1	1	1

By counting the number of truth tables, there are $2^{(2^n)}$ n-variable Boolean functions.

Boolean algebra

Boolean operation	logical form	polynomial form
AND	$z = x \wedge y$	$z = xy$
OR	$z = x \vee y$	$z = x + y + xy$
NOT	$z = \overline{x}$	$z = 1 + x$

Over $\mathbb{F}_2$, we have the identity $x^2 = x$, or equivalently, $x(1+x) = 0$.

Theorem

Every Boolean function $f\colon \mathbb{F}_2^n \to \mathbb{F}_2$ is a polynomial in the quotient ring $\mathbb{F}_2[x_1, \dots, x_n]/I$, where $I = \langle x_1^2 - x_1, \dots, x_n^2 - x_n \rangle$.

Proof

Clearly, every such polynomial defines a Boolean function $f\colon \mathbb{F}_2^n \to \mathbb{F}_2$.

We want to prove the converse. It suffices to show that these sets have the same size.

There are $2^{(2^n)}$ truth tables (Boolean functions) on n variables.

Since $x_i^2 = x_i$, there are 2^n monomials in $x_1, \dots, x_n$. Every polynomial in the quotient ring is uniquely determined by a subset of these. $\square$

Easy generalization

Every function $f\colon \mathbb{F}_p^n \to \mathbb{F}_p$ is a polynomial in $\mathbb{F}_p[x_1, \dots, x_n]/\langle x_1^p - x_1, \dots, x_n^p - x_n \rangle$.

Boolean networks

Classically, a Boolean network (BN) is an n-tuple $f = (f_1, \dots, f_n)$ of Boolean functions, where $f_i \colon \mathbb{F}_2^n \to \mathbb{F}_2$. This defines a finite dynamical system (FDS) map

$$f \colon \mathbb{F}_2^n \longrightarrow \mathbb{F}_2^n, \qquad x = (x_1, \dots, x_n) \longmapsto (f_1(x), \dots, f_n(x)).$$

Any function from a finite set to itself can be described by a directed graph with every node having out-degree 1. For a BN, this graph is called the *phase space*, or *state space*.

Definition

The phase space of a BN is the digraph with vertex set $\mathbb{F}_2^n$ and edges $\big\{(x, f(x)) \mid x \in \mathbb{F}_2^n\big\}$.

Proposition

Every function $f \colon \mathbb{F}_2^n \to \mathbb{F}_2^n$ is the phase space of a Boolean network: $f = (f_1, \dots, f_n)$.

Proof

Clearly, every BN defines a function $\mathbb{F}_2^n \to \mathbb{F}_2^n$. We want to prove converse. It suffices to show that these sets have the same cardinality.

To count functions $\mathbb{F}_2^n \to \mathbb{F}_2^n$, we count phase spaces. Each of the 2^n nodes has 1 out-going edge, and 2^n destinations. Thus, there are $(2^n)^{2^n} = 2^{(n2^n)}$ phase spaces.

To count BNs: there are $2^{(2^n)}$ choices for each f_i, and so $(2^{(2^n)})^n = 2^{(n2^n)}$ possible BNs. $\square$

Local models and FDSs

Corollary

Every function $f = \mathbb{F}_2^n \to \mathbb{F}_2^n$ can be written as an n-tuple of "square-free" polynomials over $\mathbb{F}_2$. That is,

$$f = (f_1, \dots, f_n), \qquad f_i \in \mathbb{F}_2[x_1, \dots, x_n]/\langle x_1^2 - x_1, \dots, x_n^2 - x_n \rangle.$$

This all carries over to generic finite fields, but we will carefully re-define things first.

Definition

Let $\mathbb{F}$ be a finite field. A local model over $\mathbb{F}$ is an n-tuple of functions $f = (f_1, \dots, f_n)$, where each $f_i \colon \mathbb{F}^n \to \mathbb{F}$.

Definition

Every local model $f = (f_1, \dots, f_n)$ over $\mathbb{F}$ defines a finite dynamical system (FDS), by iterating the map

$$f \colon \mathbb{F}^n \longrightarrow \mathbb{F}^n, \qquad x = (x_1, \dots, x_n) \longmapsto \big(f_1(x), \dots, f_n(x)\big).$$

Remark

A classical Boolean network (BN) is just a local model over $\mathbb{F}_2$.

Local polynomial models and PDSs

Let $\mathbb{F}$ be a finite field. We slightly abuse notation and write a polynomial in the quotient ring

$$R/I = \mathbb{F}[x_1, \dots, x_n]/\langle x_1^p - x_1, \dots, x_n^p - x_n \rangle$$

as f instead of $f + I$. It is a sum of monomials with each exponent from $0, \dots, p-1$:

$$x^\alpha := x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n}, \qquad \alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{Z}_p^n.$$

Definition

An element f in $(R/I) \times \cdots \times (R/I)$ is called a local polynomial model over $\mathbb{F}$. Note that f is also a local model.

Definition

Every local polynomial model $f = (f_1, \dots, f_n)$ over $\mathbb{F}$ defines a canonical finite polynomial dynamical system (PDS), by iterating the map

$$f \colon \mathbb{F}^n \longrightarrow \mathbb{F}^n, \qquad x = (x_1, \dots, x_n) \longmapsto (f_1(x), \dots, f_n(x)).$$

Remark

Let $|\mathbb{F}| = q$. Every function $f_i \colon \mathbb{F}^n \to \mathbb{F}$ is defined by its unique truth table.

There are exactly $q^{(q^n)}$ truth tables: q^n input vectors, each having q possible outputs.

Which local models are polynomial models?

Let $\mathbb{F}$ be a finite field of order $q = p^n$.

Definition

The algebraic normal form of a polynomial $f \in R/I$ is

$$f = \sum c_\alpha x^\alpha,$$

where the sum is taken over all p^n monomials, and $c_\alpha \in \mathbb{F}$.

Proposition

There are $q^{(q^n)}$ functions $f\colon \mathbb{F}^n \to \mathbb{F}$, but only $q^{(p^n)}$ polynomials in the quotient ring

$$R/I = \mathbb{F}[x_1, \dots, x_n]/\langle x_1^p - x_1, \dots, x_n^p - x_n \rangle.$$

Proof

The number of functions $f\colon \mathbb{F}^n \to \mathbb{F}$ is just the number of truth tables: $q^{(q^n)}$.

To find $|R/I|$, we count algebraic normal forms: p^n monomials x^α, each having q possible coefficients $c_\alpha \in \mathbb{F} \Longrightarrow q^{(p^n)}$ elements of R/I. $\square$

General finite fields: local models vs. local polynomial models

Let $\mathbb{F}$ be a finite field of order $q = p^n$.

Summary

(i) There are $q^{(nq^n)}$ local models $(f_1, \dots, f_n)$ over $\mathbb{F}$.

(ii) There are $q^{(nq^n)}$ functions $\mathbb{F}^n \to \mathbb{F}^n$ (i.e., FDS maps).

(iii) There are only $q^{(np^n)}$ local polynomial models (i.e., PDS maps).

In other words, every function $\mathbb{F}^n \to \mathbb{F}^n$ is indeed the finite dynamical system (FDS) map (i.e., phase space) of a local model $(f_1, \dots, f_n)$ over $\mathbb{F}$.

However, over non-prime fields, there are FDS maps that are not PDS maps.

Said differently, over non-prime fields, there are local models that are not polynomial models

Open question

For $\mathbb{F} = \mathbb{F}_{p^n}$, characterize which functions $\mathbb{F}^n \to \mathbb{F}^n$ are PDS maps of local models.

This is likely known by someone but using completely different terminology.

Asynchronous Boolean networks

Consider a Boolean network $f=(f_1,\dots,f_n)$.

Composing the functions synchronously defines the PDS map $f\colon \mathbb{F}_2^n\to\mathbb{F}_2^n$.

We can also compose them asynchronously. For each local function f_i, define the function

$$F_i\colon \mathbb{F}_2^n \longrightarrow \mathbb{F}_2^n, \qquad x=(x_1,\dots,x_i,\dots,x_n)\longmapsto(x_1,\dots,f_i(x),\dots,x_n).$$

Definition

The asynchronous phase space of $(f_1,\dots,f_n)$ is the digraph with vertex set $\mathbb{F}_2^n$ and edges $\big\{(x,F_i(x))\mid i=1,\dots,n;\ x\in\mathbb{F}_2^n\big\}$.

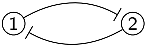
Remarks

- Clearly, this graph has $n\cdot 2^n$ edges, though self-loops are often omitted.
- Every non-loop edge connect two vertices that differ in exactly one bit. That is, all non-loops are of the form $(x,x+e_i)$, where e_i is the i^{th} standard unit basis vector.
- Unless we specifiy otherwise, the term "phase space" refers to the "synchronous phase space."
- It is elementary to extend this concept from BNs to local models over finite fields.

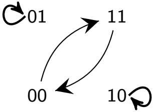
Examples: synchronous vs. asynchronous

$$\begin{cases} f_1(x_1,x_2) = \overline{x_2} \\ f_2(x_1,x_2) = \overline{x_1} \end{cases}$$

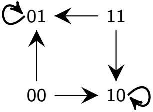
Functions



Wiring diagram



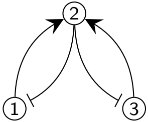
Synchronous phase space



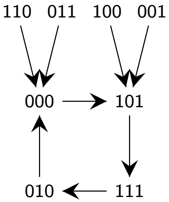
Asynchronous phase space

$$\begin{cases} f_1 = \overline{x_2} \\ f_2 = x_1 \wedge x_3 \\ f_3 = \overline{x_2} \end{cases}$$

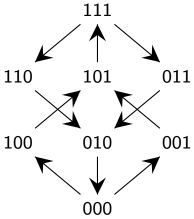
Functions



Wiring diagram



Synchronous phase space



Asynchronous phase space (self-loops omitted)

Remarks

- The 2-cycle in the 1st BN is an "artifact of synchrony."
- In the 2nd asynchronous BN, there is a directed path between any two nodes.

Asynchronous local models over finite fields

Recall: every function $\mathbb{F}^n \to \mathbb{F}^n$ can be realized as the FDS map (i.e., phase space) of a local model over $\mathbb{F}$.

Similarly, every digraph with vertex set $\mathbb{F}^n$ that "could be" the asynchronous phase space of a local model, is one.

Theorem

Let $G = (\mathbb{F}^n, E)$ be a digraph with the following local property (definition):

For every $x \in \mathbb{F}^n$ and $i = 1, \dots, n$: E contains exactly one edge of the form $(x, x + ke_i)$, where $k \in \mathbb{F}$ (possibly a self-loop)

Then G is the asynchronous phase space of some local model $(f_1, \dots, f_n)$ over $\mathbb{F}$.

Proof

It suffices to show there there are $q^{(nq^n)}$ digraphs $G = (\mathbb{F}^n, E)$ with the "local property".

Each of the q^n nodes $x \in \mathbb{F}^n$ has n out-going edges (including loops). Each edge has q possible destinations: $x + ke_i$ for $k \in \mathbb{F}$.

This gives q^n choices at each node, for all q^n nodes, for $(q^n)^{q^n} = q^{(nq^n)}$ graphs in total. $\square$

Local models over general finite fields: synchronous vs. asynchronous

Let $\mathbb{F}$ be a finite field of order $q = p^n$, and let

$$R/I = \mathbb{F}[x_1, \dots, x_n]/\langle x_1^p - x_1, \dots, x_n^p - x_n \rangle,$$

which has cardinality $q^{(p^n)}$.

Summary (updated)

There are $q^{(nq^n)}$ local models $(f_1, \dots, f_n)$ over $\mathbb{F}$.

Each local model gives rise to both a

- synchronous phase space: the FDS map $\mathbb{F}^n \to \mathbb{F}^n$;
- asynchronous phase space: a digraph $G = (\mathbb{F}^n, E)$ with the "local property".

Moreover, there are exactly $q^{(nq^n)}$ maps $\mathbb{F}^n \to \mathbb{F}^n$ and $q^{(nq^n)}$ graphs with the local property!

Of the $q^{(nq^n)}$ local models, $q^{(np^n)}$ are polynomial models. These are equal iff $\mathbb{F} = \mathbb{F}_p$.

Open questions

For $\mathbb{F} = \mathbb{F}_{p^n}$, characterize which:

- synchronous phase spaces arise from local polynomials models;
- asynchronous phase spaces arise from local polynomial models.

Phase spaces: synchronous vs. asynchronous

The synchronous phase space of a local model $f = (f_1, \ldots, f_n)$ has two types of nodes:

- *transient points*: $f^k(x) \neq x$ for all $k \geq 1$.
- *periodic points*: $f^k(x) = x$ for some $k \geq 1$. ($k = 1$: *fixed point*)

Thus, the phase space consists of periodic cycles and directed paths leading into these cycles.

The asynchronous phase space of $f = (f_1, \ldots, f_n)$ can be more complicated.

For $x, \in y \in \mathbb{F}^n$, define $x \sim y$ iff there is a directed path from x to y and from y to x.

The resulting equivalence classes are the strongly connected components (SCC) of the phase space. An SCC is terminal if it has no out-going edges from it.

A point $x \in \mathbb{F}^n$:

- *is transient* if it is not in a terminal SCC.
- *lies on a cyclic attractor* if its terminal SCC is a chordless k-cycle ($k = 1$: *fixed point*).
- *lies on a complex attractor* otherwise.

Proposition

The fixed points of a local model are the same under synchronous and asynchronous update.

Wiring diagrams

A function $f_j \colon \mathbb{F}^n \to \mathbb{F}$ is essential in x_i if for some $x \in \mathbb{F}^n$ and $k \in \mathbb{F}$,

$$f(x) \neq f(x) + ke_i,$$

where $e_i \in \mathbb{F}^n$ is the i^{th} standard unit basis vector.

Definition

The wiring diagram of a local model $(f_1, \dots, f_n)$ over $\mathbb{F}$ is a directed graph G on with vertex set $x_1, \dots, x_n$ (or just $1, \dots, n$) and a directed edge (x_i, x_j) if f_j is essential in x_i.

If $\mathbb{F} = \mathbb{F}_p$, then an edge $x_i \longrightarrow x_j$ is positive if $a \leq b$ implies

$$f_j(x_1, \dots, x_{i-1}, a, x_{i+1}, \dots, x_n) \leq f_j(x_1, \dots, x_{i-1}, b, x_{i+1}, \dots, x_n)$$

and negative if the second inequality is reversed.

Negative edges are denoted with circles or blunt arrows instead of traditional arrowheads.

Definition

A function $f_j \colon \mathbb{F}^n \to \mathbb{F}$ is unate (or monotone) if every edge in the wiring diagram is either positive or negative.

Wiring diagrams in Boolean networks

- A positive edge $x_i \longrightarrow x_j$ represents a situation where i activates j.

  Examples.
  - $f_j = x_i \wedge y$: $\quad 0 = f_j(x_i = 0, y) \leq f_j(x_i = 1, y) \leq 1.$
  - $f_j = x_i \vee y$: $\quad 0 \leq f_j(x_i = 0, y) \leq f_j(x_i = 1, y) = 1.$

- A negative edge $x_i \longrightarrow\!\!| \; x_j$ represents a situation where i inhibits j.

  Examples.
  - $f_j = \overline{x_i} \wedge y$: $\quad 1 \geq f_j(x_i = 0, y) \geq f_j(x_i = 1, y) = 0.$
  - $f_j = \overline{x_i} \vee y$: $\quad 1 = f_j(x_i = 0, y) \geq f_j(x_i = 1, y) \geq 0.$

- Occasionally, edges are neither positive nor negative:

  Example. (The logical "XOR" function):
  - $f_j = (x_i \wedge \overline{y}) \vee (\overline{x_i} \wedge y)$:
  $$\begin{aligned} 0 &= f_j(x_1 = 0, y = 0) < f_j(x_1 = 1, y = 0) = 1 \\ 1 &= f_j(x_1 = 0, y = 1) > f_j(x_1 = 1, y = 1) = 0 \end{aligned}$$

Most edges in Boolean network models are either positive or negative because most biological interactions are either simple activations or inhibitions.