Discrete Algebraic Models in Systems Biology

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"To understand biology at the system level, we must examine the structure and dynamics of cellular and organismal function, rather than the characteristics of isolated parts of a cell or organism. Properties of systems, such as robustness, emerge as central issues, and understanding these properties may have an impact on the future of medicine. . . ."

H. Kitano, Science 295, March 2002
To understand biology at the system level, we must examine the structure and dynamics of cellular and organismal function, rather than the characteristics of isolated parts of a cell or organism. Properties of systems, such as robustness, emerge as central issues, and understanding these properties may have an impact on the future of medicine. 

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That is, we need to focus on

- the wiring diagram,
- the local functions of each unit,
- the global dynamics of the system.
Gene Regulatory Networks

"The transcriptional control of a gene can be described by a discrete-valued function of several discrete-valued variables."

"A regulatory network, consisting of many interacting genes and transcription factors, can be described as a collection of interrelated discrete functions and depicted by a wiring diagram similar to the diagram of a digital logic circuit."

R. Karp, Notices of AMS, 2002
Example
Example

The wiring diagram:
Example

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Let $f_1 = \neg x_2$, $f_2 = x_4 \lor (x_1 \land x_3)$, $f_3 = x_4 \land x_2$, $f_4 = x_2 \lor x_3$. 
Example

The wiring diagram:

Let $f_1 = \neg x_2$, $f_2 = x_4 \lor (x_1 \land x_3)$, $f_3 = x_4 \land x_2$, $f_4 = x_2 \lor x_3$.

The phase space of $f$:
Finite Dynamical Systems.

Let \( x_1, \ldots, x_n \) be variables which take values in a finite set \( X \). Let \( f_1, \ldots, f_n \) be functions such that \( f_i : X^n \rightarrow X \) determines the state of variable \( x_i \) (local update function). Then we get

\[
f : (f_1, \ldots, f_n) : X^n \rightarrow X^n
\]

The function \( f \) is called a finite dynamical system (FDS).
Polynomial Dynamical Systems.

Let $X = \mathbb{K}$ be a finite field. Then each function

$$f_i : \mathbb{K}^n \rightarrow \mathbb{K}$$

can be expressed uniquely as a polynomial in $\mathbb{K}[x_1, \ldots, x_n]$: 
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can be expressed uniquely as a polynomial in $\mathbb{K}[x_1, \ldots, x_n]$:

Suppose $|\mathbb{K}| = q$. Then

$$f_i(x_1, \ldots, x_n) = \sum_{(c_1, \ldots, c_n) \in \mathbb{K}^n} [f_i(c_1, \ldots, c_n) \prod_{i=1}^{n}(1 - (x_i - c_i)^{q-1})]$$
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The FDS $f = (f_1, \ldots, f_n)$ is called a Polynomial dynamical system (PDS).
Polynomial Dynamical Systems.

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The FDS $f = (f_1, \ldots, f_n)$ is called a Polynomial dynamical system (PDS).

Cellular automata and Boolean networks are classes of PDS.
Inference Problem

Let $\mathbb{K}$ be a finite field, $x_1, \ldots, x_n$ variables with values in $\mathbb{K}$. Let $(s_1, r_1), \ldots, (s_t, r_t)$ be state transition observations, where $s_j, r_j \in \mathbb{K}^n$.

- Find the "most-likely" wiring diagram.
- Find the "most-likely" function $f : \mathbb{K}^n \rightarrow \mathbb{K}^n$, such that $f(s_i) = r_i$, for all $i$. 
Inference of Polynomial Networks

Given \((s_1, r_1), \ldots, (s_t, r_t)\); state transition observations, where \(s_j, r_j \in \mathbb{F}_q^n\)

- Find all possible static networks (dependency graphs, interaction networks, wiring diagram)
- Using available biological information, identify a static network \(Y\),
- Find all PDS \(f\) such that \(f\) fits the data: \(f : K^n \rightarrow K^n\) with \(f(s_j) = r_j\),
- Select a "biologically relevant" model \(f\),
- Study the dynamics of \(f\).
All Dynamic Models - Laubenbacher & Stigler
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For each coordinate \(i\), find all possible functions (polynomials) \(f_i : \mathbb{K}^n \rightarrow \mathbb{K}\) such that \(f_i(s_j) = r_{j,i}\).
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Find one particular function. For example,

\[
g_i(x_1, \ldots, x_n) = \sum_{j=1}^{t} r_{j,i} \prod_{e=1}^{n} (1 - (x_e - s_{j,e})^{q-1})
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Find the set \(I\) of all functions \(h\) such that \(h(s_j) = 0\) for all \(1 \leq j \leq r\).
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The set of all functions \(f_i\) such that \(f_i(s_j) = r_{j,i}\) is the set \(g_i + I := \{g_i + h \mid h \in I\}\).
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The model space is \(g + I := \{(g_1 + h_1, \ldots, g_n + h_n) : h_1, \ldots, h_n \in I\}\).
$g + I$ is huge!

Three possible ways to proceed:
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Pick some minimal functions with respect to some term orders and analyze their dynamics.
\[ g + I \text{ is huge!} \]

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Build a probabilistic model from ALL minimal functions using the Gröbner fan of the ideal \( I \).
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Pick some minimal functions with respect to some term orders and analyze their dynamics.

Build a probabilistic model from ALL minimal functions using the Gröbner fan of the ideal $I$.

Restrict the model space $g + I$ to ONLY biologically relevant models.
Probabilistic Polynomial Model

- The Gröbner fan of $I$ has finitely many cones.
- Any two term orders in the same cone give the same minimal (normal form) of $g_i$, for all $i$.
- For each $i$, Let $h_{i1}, \ldots, h_{ij}$ be the set of all minimal forms of $g_i$.
- For each $h_{ik}$, assign a probability $p_{ik}$ based on the size and number of cones which gives $h_{ik}$ as the minimal form.
Biologically Relevant Functions
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Out of the model space $g + I$, identify a biologically relevant function?
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Different classes of functions have been proposed: Chain functions, Stabilizing functions, biologically meaningful functions, (nested) canalyzing functions,...
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Different classes of functions have been proposed: Chain functions, Stabilizing functions, biologically meaningful functions, (nested) canalyzing functions,....

“canalisation” introduced by the geneticist Waddington (1942) to represent the ability of a genotype to produce the same phenotype regardless of environmental variability.
Canalyzing Functions
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Let $f$ be a Boolean function on the variables $x_1, \ldots, x_n$. That is, for $1 \leq i \leq n$, there exists $(a_1, \ldots, a_n) \in \mathbb{F}_2^n$ such that

$$f(a_1, \ldots, a_{i-1}, a_i, a_{i+1}, \ldots, a_n) \neq f(a_1, \ldots, a_{i-1}, 1 + a_i, a_{i+1}, \ldots, a_n).$$
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**Definition.** $f$ is canalyzing if there exists $i$ and $a$ such that

$$f(x_1, \ldots, x_{i-1}, a, x_{i+1}, \ldots, x_n) = b$$

is constant.
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is constant.

**Example.** $AND(x, y) = x \land y$ is a canalyzing function in the variable $x$ with input 0 and output 0.

$XOR(x, y) := (x \lor y) \land (\overline{x} \land y)$ is not canalyzing in either variable.
Nested Canalyzing Functions
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**Definition.** $f$ is a *nested canalyzing function* (NCF) in the variable order $x_1, x_2, \ldots, x_n$ with canalyzing input values $a_1, \ldots, a_n$ and canalyzed output values $b_1, \ldots, b_n$, respectively, if

$$f(x) = \begin{cases} 
  b_1 & \text{if } x_1 = a_1, \\
  b_2 & \text{if } x_1 \neq a_1 \text{ and } x_2 = a_2, \\
  b_3 & \text{if } x_1 \neq a_1 \text{ and } x_2 \neq a_2 \text{ and } x_3 = a_3, \\
  \vdots & \vdots \\
  b_n & \text{if } x_1 \neq a_1 \text{ and } \cdots \text{ and } x_{n-1} \neq a_{n-1} \text{ and } x_n = a_n, \\
  b_n + 1 & \text{if } x_1 \neq a_1 \text{ and } \cdots \text{ and } x_n \neq a_n.
\end{cases}$$
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  \vdots & \vdots \\
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  b_n + 1 & \text{if } x_1 \neq a_1 \text{ and } \cdots \text{ and } x_n \neq a_n.
\end{cases}
\]

**Example.** \( f(x, y, z) = x(y - 1)z \) is NSF. While \( g(x, y, z, w) = x(y + z) \) is NOT NCF.
Nested Canalyzing in any variable order
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Let $\sigma$ be a permutation on $[n]$. A function $f = \sum_{S \subseteq [n]} c_S \prod_{i \in S} x_i$ is a nested canalyzing function in the variable order $x_{\sigma(1)}, \ldots, x_{\sigma(n)}$ if and only if $(c_\emptyset, \ldots, c_{[n]}) \in V_{\sigma}^{ncf}$, where

$$V_{\sigma} = \{(a_\emptyset, \ldots, a_{[n]}) \in \mathbb{F}_2^{2^n} : a_{[n]} = 1, \ a_S = a_{[r_\sigma S]} \prod_{w \in [r_\sigma S] \setminus S} a_{[n]\{w\}}, \ S \subseteq [n]\}.$$
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\]

The set of all nested canalyzing functions in any variable order is

\[
V = \bigcup_\sigma V_\sigma.
\]
All NCF in $g_i + I$
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Recall that $g_i(x_1, \ldots, x_n) = \sum_{j=1}^{t} r_{j,i} \prod_{e=1}^{n} (1 - (x_e - s_{j,e}))$ and $I = \langle \prod_{j=1}^{t} (1 - \prod_{e=1}^{n} (1 - (x_e - s_{j,e}))) \rangle$. 
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$f_i \in g_i + I$ if and only if $f_i = g_i + h(x_1, \ldots, x_n) \prod_{j=1}^{t}(1 - \prod_{e=1}^{n}(1 - (x_e - s_{j,e})))$, for some polynomial $h$, say $h = \sum_{H \subseteq [n]} b_H \prod_{i \in H} x_i$. 
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Expand the right hand side and collect terms,

$f_i = \sum_{S \subseteq [n]} W_S(b_H, r_i, s_j) \prod_{i \in S} x_i$. 
All NCF in $g_i + I$

Recall that $g_i(x_1, \ldots, x_n) = \sum_{j=1}^{t} r_{j,i} \prod_{e=1}^{n}(1 - (x_e - s_{j,e}))$ and $I = \langle \prod_{j=1}^{t}(1 - \prod_{e=1}^{n}(1 - (x_e - s_{j,e}))) \rangle$.

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Expand the right hand side and collect terms,
$f_i = \sum_{S\subseteq[n]} W_S(b_H, r_i, s_j) \prod_{i\in S} x_i$.

Let $J$ be the ideal generated by $\{c_S - W_S(b_H, r_i, s_j) : S \subseteq [n] \}$. Then $I(V) + J \cap \mathbb{F}_2[c_S, r_i, s_j]$ is the ideal of all NCFs in the model space.
Other classes of Functions?

- Define (nested) canalyzing over arbitrary finite field. Parameterize this set of functions and identify them from the model space.

- Parameterize the class of logical functions and identify them from the model space.
Static Network from Data
Static Network from Data

Given \((s_1, r_1), \ldots, (s_t, r_t)\); state transition observations, where \(s_j, r_j \in \mathbb{K}^n\). Find all possible static networks that govern these data.
Static Network from Data

Given \((s_1, r_1), \ldots, (s_t, r_t)\); state transition observations, where \(s_j, r_j \in \mathbb{K}^n\). Find all possible static networks that govern these data.

For each transition,

\[
\begin{align*}
    s_j &= (s_{j,1}, \ldots, s_{j,n}) \\
    r_j &= (r_{j,1}, \ldots, r_{j,n})
\end{align*}
\]
Static Network from Data

Given \((s_1, r_1), \ldots, (s_t, r_t)\); state transition observations, where \(s_j, r_j \in \mathbb{K}^n\). Find all possible static networks that govern these data.

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For a fixed coordinate \(i\), find all possible (minimal) subsets \(\{y_1, \ldots, y_v\} \subseteq \{x_1, \ldots, x_n\}\) such that there a function \(f_i \in \mathbb{K}[y_1, \ldots, y_v]\) and \(f_i(s_j) = r_{j,i}\).
Static Network from Data (cont.)
Static Network from Data (cont.)

For each fixed coordinate $i$, let $T_0, T_1, \ldots, T_{q-1} \subset \mathbb{K}^n$ where

$$T_a = \{ s_j \mid r_{j,i} = a \} \text{ for all } a \in \mathbb{K}. $$
Static Network from Data (cont.)

For each fixed coordinate $i$, let $T_0, T_1, \ldots, T_{q-1} \subset K^n$ where

$$T_a = \{ s_j \mid r_{j,i} = a \} \text{ for all } a \in K.$$

Let

$$Y = \{ g \in K[x_1, \ldots, x_n] \mid g(b) = a, \text{ for all } b \in T_a \text{ and all } a \in K \}.$$
Static Network from Data (cont.)

For each fixed coordinate $i$, let $T_0, T_1, \ldots, T_{q-1} \subset K^n$ where

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Let

$$Y = \{ g \in K[x_1, \ldots, x_n] \mid g(b) = a, \text{ for all } b \in T_a \text{ and all } a \in K \}.$$ 

We are interested in the elements of $Y$ which involve only a small number of the variables.
Static Network from Data (cont.)
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**definition.** Let $M_T \subset K[x_1, \ldots, x_n]$ be the square-free monomial ideal generated by

$$\{m(p, q) \mid p \in T_a, q \in T_b, \text{ and } 0 \leq a < b < q\},$$

where, for $p, q \in K^n$,

$$m(p, q) := \prod_{p_\alpha \neq q_\alpha} x_\alpha.$$
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**Theorem** For any subset $F \subset [n], K[x_i \mid i \in F] \cap Y \neq \emptyset$ if and only if $M_T \subset \langle x_i \mid i \in F \rangle$. 
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Static Network from Data (cont.)

**Theorem** For any subset $F \subset [n]$, $\mathbb{K}[x_i \mid i \in F] \cap Y \neq \emptyset$ if and only if $M_T \subset \langle x_i \mid i \in F \rangle$.

**Proof.** $M_T \subset \langle x_i \mid i \in F \rangle \iff \prod_{p \neq q} x_{\alpha} \in \langle x_i \mid i \in F \rangle$ for all $p \in T_a, q \in T_b$, and $0 \leq a < b < q \iff$ For $p \in T_a, q \in T_b$, and $0 \leq a < b < q$, there exists $\alpha \in F$ such that $p_{\alpha} \neq q_{\alpha} \iff$ there exists $g \in \mathbb{K}[x_i \mid i \in F]$ such that $g(p) \neq g(q)$ for all $p \in T_a, q \in T_b$, and $0 \leq a < b < q \iff \mathbb{K}[x_i \mid i \in F] \cap Y \neq \emptyset$
Static Network from Data (cont.)

**Theorem** For any subset $F \subset [n]$, $\mathbb{K}[x_i \mid i \in F] \cap Y \neq \emptyset$ if and only if $M_T \subset \langle x_i \mid i \in F \rangle$.

**Proof.** $M_T \subset \langle x_i \mid i \in F \rangle \iff \prod_{p_\alpha \neq q_\alpha} x_\alpha \in \langle x_i \mid i \in F \rangle$ for all $p \in T_a, q \in T_b$, and $0 \leq a < b < q \iff$ For $p \in T_a, q \in T_b$, and $0 \leq a < b < q$, there exists $\alpha \in F$ such that $p_\alpha \neq q_\alpha \iff$ there exists $g \in \mathbb{K}[x_i \mid i \in F]$ such that $g(p) \neq g(q)$ for all $p \in T_a, q \in T_b$, and $0 \leq a < b < q \iff \mathbb{K}[x_i \mid i \in F] \cap Y \neq \emptyset$.

**Compute the primary decomposition of** $M_T$.
References:


Thank You