Update Order Instability in Graph Dynamical Systems

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Preliminaries

Definition ([10])

A sequential dynamical system (SDS) is a triple consisting of:

- A graph $Y$ with vertex set $v[Y] = \{1, 2, \ldots, n\}$.
- For each vertex $i$ a state $y_i \in K$ (e.g. $F_2 = \{0, 1\}$) and a local function $F_i : K^n \rightarrow K^n$
  \[
  F_i(y = (y_1, y_2, \ldots, y_n)) = (y_1, \ldots, y_{i-1}, f_i(y[i]), y_{i+1}, \ldots, y_n).
  \]
- A ordering $\pi = \pi_1\pi_2\cdots\pi_n \in S_Y$ of the vertex set.

- The SDS map generated by the triple $(Y, (F_i)_1^n, \pi)$ is
  \[
  [\mathcal{Y}, \pi] = F_{\pi_n} \circ F_{\pi_{n-1}} \circ \cdots \circ F_{\pi_1}.
  \]
Functional equivalence

▶ Question: When does $[\mathfrak{Y}, \pi] = [\mathfrak{Y}, \sigma]$, for distinct update orders $\pi, \sigma \in S_Y$?

Definition. The update graph $U(Y)$ has vertex set $S_Y$. The edge $\{\pi, \sigma\}$ is present iff:

- $\pi$ and $\sigma$ differ by exactly an adjacent transposition $(i, i + 1)$,
- $\{\pi_i, \pi_{i+1}\} \notin e[Y]$.

Example. Let Circ$_4$ be the circular graph on 4 vertices.

\begin{center}
\begin{tabular}{ccccccc}
1234 & 2341 & 1243 & 1423 & 1324 & 1342 \\
3412 & 4123 & 3241 & 3421 & 3124 & 3142 \\
1432 & 2143 & 2134 & 2314 & 2413 & 2431 \\
3214 & 4321 & 4132 & 4312 & 4213 & 4231 \\
\end{tabular}
\end{center}

Figure: The update graph $U(\text{Circ}_4)$. 
Functional equivalence (cont.)

Define an equivalence relation $\sim_Y$ on $S_Y$ by $\pi \sim_Y \sigma$ if $\pi$ and $\sigma$ are on the same connected component of $U(Y)$.

**Prop.** If $\pi \sim_Y \sigma$, then $[\mathcal{S}_Y, \pi] = [\mathcal{S}_Y, \sigma]$.

- There is a bijection:
  \[ f_Y : S_Y / \sim_Y \longrightarrow \text{Acyc}(Y), \]
  thus, $\alpha(Y) := |\text{Acyc}(Y)|$ is an upper bound for the number of functionally distinct SDS maps $[\mathcal{S}_Y, \pi]$ for a fixed choice of $\mathcal{S}_Y$. This bound is known to be sharp.

- The function $\alpha$ satisfies the recurrence relation:
  \[ \alpha(Y) = \alpha(Y'_e) + \alpha(Y''_e) = T_Y(2, 0), \]
  where $Y'_e$ and $Y''_e$ are formed from $Y$ by deleting and contracting edge $e$, and $T_Y(x, y)$ is the Tutte polynomial.
Cycle equivalence

**Definition** Two finite dynamical systems $\phi, \psi : K^n \to K^n$ are *cycle equivalent* if there exists a bijection $h : \text{Per}(\phi) \to \text{Per}(\psi)$ such that

$$\psi \big|_{\text{Per}(\psi)} \circ h = h \circ \phi \big|_{\text{Per}(\phi)}.$$ 

- Let $C_n = \langle \sigma \rangle$, where $\sigma = (n, n-1, \ldots, 2, 1)$.

**Theorem ([8])**

*For any $\pi \in S_Y$, the SDS maps $[\mathfrak{S}_Y, \pi]$ and $[\mathfrak{S}_Y, \sigma(\pi)]$ are cycle equivalent.*

- On the level of acyclic orientations, $O_\pi^Y$ and $O^{\sigma(\pi)}_Y$ differ by a source-to-sink conversion.

- This puts an equivalence relation $\sim_\kappa$ on $\text{Acyc}(Y)$. 
Cycle equivalence (cont.)

- The quantity $\kappa(Y) := |\text{Acyc}(Y)/\sim_\kappa|$ is an upper-bound for the number of SDS maps up to cycle equivalence.

**Theorem ([7])**

*If e is a bridge edge of Y linking components Y_1 and Y_2, then*

$$\kappa(Y) = \kappa(Y_1)\kappa(Y_2).$$

*If e is a non-bridge edge of Y, then*

$$\kappa(Y) = \kappa(Y'_e) + \kappa(Y''_e).$$

*Thus, $\kappa(Y) = T_Y(1, 0)$.*

**Corollary ([8])**

*If Y is a tree, then for any $\pi, \sigma \in S_Y$, the SDS maps $[\mathcal{F}_Y, \pi]$ and $[\mathcal{F}_Y, \sigma]$ are cycle equivalent. Moreover, if $\mathcal{F}_Y$ is induced by the parity functions or their negations, then the phase spaces $\Gamma[\mathcal{F}_Y, \pi]$ and $\Gamma[\mathcal{F}_Y, \sigma]$ are isomorphic.*
Summary

*Question:* For a fixed choice of functions $\mathcal{F}_Y$, how many different SDS maps are there up to equivalence, obtainable through varying the update order?

- For functional equivalence, there are at most $\alpha(Y) = T_Y(2, 0)$.
- For cycle equivalence, there are at most $\kappa(Y) = T_Y(1, 0)$.

<table>
<thead>
<tr>
<th>$\alpha(Y)$</th>
<th>$\kappa(Y)$</th>
<th>$Y = \text{connected tree}$</th>
<th>$Y = \text{Circ}_n$</th>
<th>$Y = K_n$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>$2^{n-1}$</td>
<td>$2^n - 2$</td>
<td>$n!$</td>
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</tr>
<tr>
<td>$1$</td>
<td></td>
<td>$n - 1$</td>
<td>$(n - 1)!$</td>
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</tr>
</tbody>
</table>

**Conclusion.** In general, adding edges to the dependency graph of an SDS causes the dynamics to become less stable with respect to update order.
Functional Linkage Networks

► Begin with a *functional-linkage graph*:

- Corresponds to a Gene Ontology (GO) function, $f$.
- Vertices of a graph represent proteins.
- Two proteins are adjacent if we think they share the same function. The edge weight $w_{ij}$ is our level of certainty.
- Each protein is assigned a state $x_i$ from $\{+1, -1, 0\}$, depending on whether it is annotated with $f$. ($+1 = \text{yes}, -1 = \text{no}, 0 = \text{mystery}$).

**Goal**: Assign a value of $+1$ or $-1$ to all “mystery proteins.”

**Basic approach**: Given “mystery protein” $i$, is it adjacent to more $+1$ or more $-1$ proteins? i.e., compute

$$s_i = \text{sign} \left( \sum_{j \neq i \mid \{i, j\} \in E} w_{ij} x_j - \theta \right).$$

► If $s_i > \theta$, then assign $x_i = +1$. Otherwise, set $x_i = -1$.  

◮ If $s_i > \theta$, then assign $x_i = +1$. Otherwise, set $x_i = -1$. 
Functional Linkage Networks (cont.)

In [2], the proteins are update sequentially, given by an update order chosen at random. This is an SDS.

Some general questions:

▶ Does this process always converge to a fixed point? (Answer: YES)

▶ How much does the fixed point reached depend on the update order used?

▶ How quickly does it take to reach a fixed point?

▶ How reliable is this algorithm? (i.e., false negative & false positive rate)

In fact, this method has been well-received, and the reliability is superior to prior models. But as with any model, there are some “red flags” that are worth investigating.
A Mathematical Abstraction with 2-Threshold SDSs

Motivation: Let’s explore one of the “red flags” of this approach.

► Given $\mathcal{F}_Y$, define

$$\omega_{\pi}(y) = \bigcap_{n=1}^{\infty} \{[\mathcal{F}_Y, \pi]^m(y) \mid m \geq n\}.$$ 

► For $\mathcal{P} \subseteq S_Y$, define

$$\omega_{\mathcal{P}}(y) = \bigcup_{\pi \in \mathcal{P}} \omega_{\pi}(y).$$

► For a sequence of functions $\mathcal{F}_Y$, define

$$\omega(\mathcal{F}_Y) = \max \{ |\omega_{S_Y}(y)| \mid y \in K^n \}.$$ 

► Consider an SDS $[\mathcal{F}_Y, \pi]$, where $\mathcal{F}_Y = T^2_Y$, the 2-threshold local functions.

► All periodic points of a threshold SDS are fixed points.
Summary of Results

- A threshold SDS over $K_n$ can have at most $n + 1$ fixed points, and this bound is sharp.

- If $Y = K_n$ and $k \leq n$, then $\text{Fix}[T^k_Y, \pi] = \{0, 1\}$.

- If $Y$ is connected with minimal degree $d > (1 - \frac{1}{k})n$, for $k > 0$, then $\text{Fix}[T^k_Y, \pi] \subseteq \{0, 1\}$.

- If $Y$ is a tree, then $\Omega(2^n)$ fixed points can be reached by varying the update order of an SDS $[T^2_Y, \pi]$.

Theorem ([4])

Let $0 < \epsilon < 1$. Threshold systems over $G_{n,p}$, with $p = o\left(\frac{n^\epsilon}{n}\right)$, contain initial configurations from which $\Omega(2^{n^{1-\epsilon}})$ different fixed points can be reached by changing the update order, with probability $1 - o\left(\frac{1}{n^\epsilon}\right)$.

Conclusion. In general, adding edges to the dependency graph of an SDS causes the dynamics to become more stable with respect to update order.
Cellular Automata

A *cellular automaton* (CA) is a discrete dynamical system consisting of:

- A regular grid of cells
- Each cell takes on one of a finite number of states
- Each cell has a local update rule, and these are applied synchronously at each discrete time-step.

Cellular automata were invented in the 1940s at Los Alamos by Stanisław Ulam and John von Neumann, to model self-replicating systems.

They are still used in many agent-based models of biological and physical systems.
Example: Asynchronous Cellular Automata

A simple modification of an elementary CA is to allow the update rules to be applied asynchronously. This is also an SDS.

Let $Y = \text{Circ}_n$, the circular graph on $n$ vertices.

If $k = a_7a_6a_5a_4a_3a_2a_1a_0$ in binary, then Wolfram rule $k$ is defined by $\text{wolf}(k) : (y_{i-1}, y_i, y_{i+1}) \mapsto z_i$ by the following table.

<table>
<thead>
<tr>
<th>$y_{i-1}y_iy_{i+1}$</th>
<th>111</th>
<th>110</th>
<th>101</th>
<th>100</th>
<th>011</th>
<th>010</th>
<th>001</th>
<th>000</th>
</tr>
</thead>
<tbody>
<tr>
<td>$z_i$</td>
<td>$a_7$</td>
<td>$a_6$</td>
<td>$a_5$</td>
<td>$a_4$</td>
<td>$a_3$</td>
<td>$a_2$</td>
<td>$a_1$</td>
<td>$a_0$</td>
</tr>
</tbody>
</table>

Let $\text{Wolf}^{(k)} : \mathbb{F}_2^n \to \mathbb{F}_2^n$ be the corresponding local function, and $\mathcal{Wolf}^{(k)}_n = (\text{Wolf}^{(k)})$ the sequence of local functions of $\text{Circ}_n$.

The SDS map $[\mathcal{Wolf}^{(k)}_n, \pi]$, where $\pi \in S_Y$, is an asynchronous cellular automaton (ACA).
Motivation

**Question:** How does the set of periodic points of an SDS depend on the update order?

**Example.** Define the function $\text{nor}: \mathbb{F}_2^k \rightarrow \mathbb{F}_2$ by $\text{nor}(x) = \prod_{i=1}^{k} (1 + x_i)$.

Figure: Phase spaces of an SDS with different update orders.
Word-independence of SDSs

A sequence \( \mathcal{S}_Y \) is \( \pi \)-independent (\( \omega \)-independent) if \( \text{Per}[\mathcal{S}_Y, w] = \text{Per}[\mathcal{S}_Y, w'] \) for all \( w \) and \( w' \) in \( S_Y \) (fair words in \( W_Y \)).

**Proposition**

\( \mathcal{S}_Y \) is \( \pi \)-independent iff it is \( \omega \)-independent.

Since these properties are the same, we call them both word-independence.
Main theorem

**Theorem ([1])**

*Of the 16 symmetric Wolfram rules, exactly 11 are word-independent for all $n > 3$.*

**Theorem ([5])**

*Of the 256 Wolfram rules, exactly 104 are word-independent. More precisely, $\text{Wolf}^{(k)}_n$ is word-independent for all $n > 3$ iff $k \in \{0, 1, 4, 5, 8, 9, 12, 13, 28, 29, 32, 40, 51, 54, 57, 60, 64, 65, 68, 69, 70, 71, 72, 73, 76, 77, 78, 79, 92, 93, 94, 95, 96, 99, 102, 105, 108, 109, 110, 111, 124, 125, 126, 127, 128, 129, 132, 133, 136, 137, 140, 141, 147, 150, 152, 153, 156, 157, 160, 164, 168, 172, 184, 188, 192, 193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 204, 205, 206, 207, 216, 218, 220, 221, 222, 223, 224, 226, 228, 230, 232, 234, 235, 236, 237, 238, 239, 248, 249, 250, 251, 252, 253, 254, 255\}.*

These 104 rules constitute 41 distinct classes up to equivalence (inversion and reflection).
Definitions

**Proposition ([6])**

If $\mathcal{F}_Y$ is word-independent, then each $F_i$ is bijective on $P := \text{Per}(\mathcal{F}_Y)$.

Let $[\mathcal{F}_Y, \omega]^*$ denote the restriction of $[\mathcal{F}_Y, \omega]$ to the set of periodic points.

If $W' \subseteq W_Y$ then the group

$$H(\mathcal{F}_Y, W') = \langle [\mathcal{F}_Y, \omega]^*: \omega \in W' \rangle$$

is called the *dynamics group* of $\mathcal{F}_Y$ and $W'$.

- Full dynamics group: $G(\mathcal{F}_Y) := H(\mathcal{F}_Y, W_Y) = \langle F_i^*: F_i \in \mathcal{F}_Y \rangle$,
- Permutation dynamics group: $H(\mathcal{F}_Y) := H(\mathcal{F}_Y, S_Y) = \langle [\mathcal{F}_Y, \pi]^*: \pi \in S \rangle$. 
Group Computation

- The dynamics group is the homomorphic image of a Coxeter group: $|F_i| \leq 2$ and $|F_i F_j| = m_{ij}$ for $m_{ij} \in \{1, 2, 3, 4, 6, 12\}$.

**Proposition**

The dynamics group of $\mathcal{F}_Y$ is trivial iff all periodic points of $[\mathcal{F}_Y, \pi]$ are fixed points, and this is independent of $\pi \in S_Y$.

- Of the 41 non-equivalent rules, only 15 of them have a non-trivial dynamics group.

- $S_L(n)$ or $A_L(n)$: Rules 1, 9, 110, 126.
- $\mathbb{Z}_2^n$: Rules 28, 29, 51.
- $A_n$ or $A_{n-1}$: Rules 54, 57.
- $GL(n, 2)$: Rule 60.
- Not sure: Rules 73, 105, 108, 150, 156.
Flips

- For each of the 8 neighborhood state configurations \((y_{i-1}, y_i, y_{i+1})\), Wolfram rule \(k\) can be thought of as either preserving, or “flipping” the value \(y_i\).

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</table>

- All 5 word-independent rules with more than 5 flips are invertible.

- This can be extended to SDSs. Call \(0 \mapsto 1\) an *up-flip* and \(1 \mapsto 0\) a *down-flip*. Define the *signature* of \(\mathcal{F}_Y\) to be the number of up-flips minus the number of down-flips.

- The signature is an indication of stability, and a good starting point for the study of update-order stochastic SDSs.
### Table of the 104 rules

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Table: The 104 word-independent rules arranged by symmetric and asymmetric parts of their tags.
Another table of the 104 rules

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Table: The 104 Wolfram rules, and the value $m_{i,i+1}$. 
Summary

Future research directions:

- Finish analyzing the dynamics groups.
- Analyze the other 152 rules.
- Extend these ideas and techniques to general SDSs.
- Use these ideas and techniques to study stochastic systems.
- Compare to the dynamics of classical (synchronous) CAs.

The following is a reasonable measure of dynamical stability with respect to update order:

\[
0 < \frac{\text{\# of states periodic for all update orders}}{\text{\# of states periodic for some update order}} \leq 1. \]

It seems to depend more on the type of function rather than the graph topology.

This quotient is 1 for precisely the word-independent SDSs.

Conclusion. Adding edges to the dependency graph of an SDS has very little effect on the stability of the system.
Summary of Stability

We are discussing different notions of update order instability!

By update order stability, one can measure:

- How many different possible cycles structures (long term behaviors) are there...
- How many different attractor basins can be reached from a particular state ...
- Which states can arise as periodic points...

...as the update order is perturbed.

Moral: Be careful when making general statements about the update order stability of a dynamical system!

Question: These ideas have only been studied independently. Is there a way to tie them together to paint a clearer picture?
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**NDSSL:**

Web: [http://ndssl.vbi.vt.edu](http://ndssl.vbi.vt.edu)


