Characterizing short-term stability for Boolean networks over any distribution of transfer functions

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We present a characterization of short-term stability of Kauffman's N-K (random) Boolean networks under arbitrary distributions of transfer functions. Given such a Boolean network where each transfer function is drawn from the same distribution, we present a formula that determines whether short-term chaos (damage spreading) will happen. Our main technical tool which enables the formal proof of this formula is the Fourier analysis of Boolean functions, which describes such functions as multilinear polynomials over the inputs. Numerical simulations on mixtures of threshold functions and nested canalyzing functions demonstrate the formula's correctness. To the best of our knowledge, previous formal characterizations only worked for special cases of "balanced" families.

INTRODUCTION

Living systems composed of a wide variety of cells, genes, or organs operate with uncanny synchrony and stability, as do numerous engineered and social systems. In a series of seminal papers, Kauffman introduced *Boolean networks* to study systems composed of interdependent components that function as one unit. This abstraction involves a network representing connectivity, and a family of Boolean functions determining states of network nodes to model dynamic behavior [1, 2]. Boolean networks have been used to model numerous dynamical systems, including genetic regulatory networks [1] and political systems [3], and have received much theoretical attention [4–12].

A Boolean network has a set of n nodes linked to each other by a directed graph G. Each node i has a Boolean state in $\{-1, +1\}$, an in-degree K, and an associated Boolean function $f_i : \{-1, +1\}^K \to \{-1, +1\}$, termed *transfer function*. If the state of node i at time t is $x_i(t)$, its state at time $t+1$ is described by $x_i(t+1) = f_i(x_{i_1}(t), \dots, x_{i_K}(t))$. For the sake of analysis, it is common to study a randomized ensemble of Boolean networks. The graph G is a directed Kauffman N-K network, where each each vertex i chooses K in-neighbors uniformly at random. There is an underlying distribution (or family) of Boolean transfer functions $\mathcal{F}$. Each vertex i independently chooses the transfer function f_i from $\mathcal{F}$.

A key parameter of interest is the *short-term stability* of the Boolean network. Specifically, if a single node has its state flipped, does the effect of this perturbation die out (quiescence), exponentially cascade over time (chaos), or is the system right in between (criticality)? There have been numerous empirical and mathematical observations about the characteristics of critical transition points in classes of Boolean networks [4–9, 11, 12, 15–17], These results require $\mathcal{F}$ to have specific properties, for example, that each truth table entry is i.i.d., or that functions are *balanced* (number of $+1$ and -1 outcomes is the same) on average.

Various natural classes of functions do not satisfy this condition. For example, Kauffman proposed a family of *canalyzing functions*, which tries to model real genetic regulatory systems [2, 4, 8, 18]. A canalyzing function has at least one input, and one value of that input, that fully determines the output of the function. Previous formal analyses do not yield characterizations of short-term stability for such families. *Threshold functions* is another important class of transfer function families, which are often used in modeling processes such as influence cascades on social and biological networks [19–25]. A threshold function is of the form $f(x_1, x_2, \dots, x_K) = \mathrm{sign}(\sum_i c_i x_i - \Theta)$, where c_is and Θ are constants. Commonly, there is a bias towards a particular state (for example, representing inertia or non-activation), and previous characterizations fail to predict the critical threshold in such imbalanced families of threshold functions [11]. Previous work on the asymmetry between the on/off states also emphasizes how this bias is a significant aspect of the dynamics [14], but only studies a special subclass of threshold functions with $\Theta = 0$ and binary weights c_i.

Our main insight is to use the Fourier decomposition of the transfer functions to give an exact formula for predicting the short-term dynamics of Boolean networks, for any fixed distribution of transfer functions. The Fourier decomposition represents a Boolean function (which is a discrete object) as a multilinear polynomial over its inputs. This method was first used in [26] to analyze the *E. Coli* regulatory network. They argue that the Mutual Information of a subset of nodes relates to their importance in determining the states of other nodes. Our analysis, however, is significantly broader and more powerful.

We represent the asymmetry between states as a technical quantity called the "imbalance", and prove that it evolves as a polynomial recurrence. Using this recurrence, our main result gives a formula that determines if a single-bit perturbation spreads through the Boolean network. We assume that the topology of the network is fixed (after it is drawn). All we need from the topology is a local tree-structure (as first shown in [27], and extensively used in later results), which is guaranteed with high probability for Kauffman N-K random graph distributions. We assume that each node receives a transfer function from a fixed distribution. Using this formula, we can compute critical points for families of distributions by solving degree K polynomials (thus, it is independent of n).

While no previous result provides such a formula, our work is closely related to the following. Mozeika and Saad [10, 16, 17] give a powerful generating function framework for analysis of Boolean networks, but do not characterize short-term stability. Kahn et al. [28] introduced the notion of *influence* $\mathrm{I}(\mathcal{F})$ on Boolean functions; an analogous notion was proposed by Shmulevich and Kaufmann [5] in the context of Boolean networks. Seshadhri et al. [11] show that the influence characterizes the short-term behavior for a highly restricted class of *balanced* families $\mathcal{F}$: on average, functions in $\mathcal{F}$ are equally likely to output $+1$ and -1. Interestingly, they give examples where the influence does not characterize stability/chaos, thereby showing the limitation of influence for this purpose.

Squires et al. [13] study the correlations between topology and transfer function and give a computational approach to study short-term dynamics. In contrast to almost all previous work (including this result), they allow the transfer function to depend on the node. This is much richer and arguably more realistic, but previous techniques fail to work for this setting. In our result, by assuming the same distribution $\mathcal{F}$ for all nodes, we have uncorrelated topology from the transfer functions.

PRELIMINARIES

We are interested in the sensitivity of a Boolean network state $x(t) = \{x_1(t) \dots, x_n(t)\}$ to a small initial perturbation. Formally, consider the following experiment. Suppose that a Boolean network starts from state x, and after t steps reaches a state $F_t(x)$. Now, consider another initial state, $x^{(i)}$ which only differs from x in the ith bit. Let H_t be the expected Hamming distance between $F_t(x)$ and $F_t(x^{(i)})$, where x is drawn from some specified (typically uniform) distribution. If H_t can be expressed as $e^{\lambda t}$, then λ is the Lyapunov exponent. If $\lambda < 0$, the Boolean network is quiescent; if $\lambda > 0$, the network is chaotic.

We use tools from *harmonic analysis of Boolean functions*, pioneered by Kahn, Kalai, and Linial [28]. The convention in this field is that -1 denotes TRUE and $+1$ is FALSE (so multiplication in $\{-1, +1\}$ maps to XOR of $\{0, 1\}$ bits). Consider $f : \{-1, +1\}^K \to \{-1, +1\}$, where we think of f as one of the transfer functions. The standard representation is as a truth table, with 2^K entries in $\{-1, +1\}$. An alternative representation is as a linear combination of *basis functions*. In the following, we use $y \in \{-1, +1\}^K$ to denote an input to the transfer function. We use $[K]$ for set $\{1, 2, \dots, K\}$, which denotes the input coordinates. Refer to [29] for details on the following.

- **Biased distributions:** We use $\mathcal{D}_\rho$ to denote the distribution over $\{-1, +1\}$ where the probability of 1 is $(1 + \rho)/2$. We choose this notation because the expected value is exactly ρ, the bias. Abusing notation, for $y \in \{-1, +1\}^K$, we say $y \sim \mathcal{D}_\rho$ when each coordinate of y is chosen i.i.d. from $\mathcal{D}_\rho$.
- **Imbalance:** The *imbalance* of the Boolean network at time t, denoted by δ_t, is $\sum_{i=1}^n x_i(t)/n$. Informally, this measures the difference between the $+1$s and -1s in the network. Observe that if the starting state $x(0)$ is chosen from $\mathcal{D}_\rho$, then $\delta_0 = \rho$.
- **Parity functions:** For any subset S of coordinates in $[K]$, $\prod_{i \in S} y_i$ is the *parity* on S. (For $S = \emptyset$, we set the parity to be 1.)
- **Fourier representation:** Any Boolean function f can be expressed as $f(y) = \sum_{S \subseteq [K]} \widehat{f}(S) \prod_{i \in S} y_i$, where $\widehat{f}(S)$ are called Fourier coefficients. This expansion represents f as a multilinear polynomial over the Boolean variables $y_1, \dots, y_K$. It can be shown that $\widehat{f}(S) = 2^{-K} \sum_y f(y) \prod_{i \in S} y_i$, the correlation between f and the parity on S. (The Fourier coefficients are the Walsh-Hadamard transform of the truth table.) There are exactly 2^K Fourier coefficients, one for each subset of the K inputs. For example, consider $K = 2$, and the AND function. A calculation yields $AND(y_1, y_2) = 1/2 + y_1/2 + y_2/2 - y_1 y_2/2$.
- **Level sets of coefficients, σ_r:** Of special interest is $\sigma_r(f) = \sum_{C:|C|=r} \widehat{f}(C)$, where $0 \le r \le K$. This is simply the sum of coefficients corresponding to sets of size r. Note that $\sigma_0(f) = \widehat{f}(\emptyset) = \sum_y f(y)$. This is exactly the imbalance in the truth table of f.
- **Influence:** For any function f, the influence of the ith variable is denoted $\mathrm{Inf}_i(f) = \Pr_y[f(y) \neq f(y^{(i)})]$ (where the probability is over the uniform distribution and $y^{(i)}$ is obtained by flipping y at the ith bit), and the total influence is $\mathrm{I}(f) = \sum_i \mathrm{Inf}_i(f)$. We will define a biased version of this quantity, $\mathrm{Inf}_i(f; \rho) = \Pr_{y \in \mathcal{D}_\rho}[f(y) \neq f(y^{(i)})]$, and analogously $\mathrm{I}(f; \rho) = \sum_i \mathrm{Inf}_i(f; \rho)$.

When taking expectations $\mathbf{E}[\dots]$, we usually provide a subscript clarifying the randomness over which expectations are taken. Thus, $\mathbf{E}_{y \sim \mathcal{D}}[\dots]$ means we are taking expectations over y distributed according to $\mathcal{D}$.

We prove a standard proposition relating the influence to the Fourier coefficients.

Proposition 1 *The value of* $\mathrm{Inf}_i(f; \rho)$ *is equal to the following two expressions.*

- $(1/4)\mathbf{E}_{y \sim \mathcal{D}_\rho}[(f(y) - f(y^{(i)}))^2]$

- $\mathbf{E}_{y\sim\mathcal{D}_\rho}\left[\left(\sum_{S\ni i}\widehat{f}(S)\prod_{j\in S\setminus i}(y_j)\right)^2\right]$

Proof: Since the probability distribution is always $\mathcal{D}_\rho$, we drop the subscript $y \sim \mathcal{D}_\rho$. We have $\mathrm{Inf}_i(f;\rho) = \Pr[f(y) \neq f(y^{(i)})]$. Observe that $(f(y) - f(y^{(i)}))^2 = 4$ if $f(y) \neq f(y^{(i)})$ and zero otherwise. Hence, $4 \cdot \mathrm{Inf}_i(f;\rho) = \mathbf{E}[(f(y) - f(y^{(i)}))^2]$. We expand this expression:

$$
\begin{aligned}
4 \cdot \mathrm{Inf}_i(f;\rho) &= \mathbf{E}[(f(y) - f(y^{(i)}))^2] \\
&= \mathbf{E}\left[\Big(\sum_S \widehat{f}(S)(\prod_{j\in S} y_j - \prod_{j\in S} y_j^{(i)})\Big)^2\right] \\
&= \mathbf{E}\left[\Big(\sum_{S\ni i} \widehat{f}(S)(y_i - y_i^{(i)}) \prod_{j\in S\setminus i} y_j\Big)^2\right] \\
&= 4\mathbf{E}\left[\Big(\sum_{S\ni i} \widehat{f}(S) \prod_{j\in S\setminus i} y_j\Big)^2\right],
\end{aligned}
$$

where the penultimate step follows since for $j \neq i$, $y_j = y_j^{(i)}$, and the final step is because $|y_i - y_i^{(i)}| = 2$.

MATHEMATICAL RESULTS

We can derive closed form expressions for the evolution of δ_t (the expected imbalance at time t) and H_t (the expected Hamming distance at time t after a single bit perturbation).

The evolution of δ_t ($t > 0$) is determined by the level sets of coefficients of the transfer functions. We use $\sigma_r(\mathcal{F}) = \mathbf{E}_{f\sim\mathcal{F}}[\sigma_r(f)]$ and $\mathrm{I}(\mathcal{F};\delta) = \mathbf{E}_{f\sim\mathcal{F}}[\mathrm{I}(f;\delta)]$.

Theorem 2 *Let the initial state $x(0)$ be chosen from $\mathcal{D}_\rho$ (so $\delta_0 = \rho$). Then δ_t evolves according to the polynomial recurrence $\delta_{t+1} = \sum_{r\geq 0}\sigma_r(\mathcal{F})\delta_t^r$.*

An equivalent formulation of this recurrence has been derived by the generating function method in Mozeika and Saad [10], though their approach is completely different (they do not show a connection to Fourier coefficients). Our approach offers a clean description of this recurrence, since $\sigma_r(\mathcal{F})$ can be easily computed from $\mathcal{F}$.

Our main theorem shows how the damage caused by a bit perturbation spreads.

Theorem 3 *Let $\delta_0, \delta_1, \ldots$ be as given by Theorem 2. For $t \leq (\log n)/K$, $H_t = \prod_{0\leq h<t}\mathrm{I}(\mathcal{F};\delta_h)$.*

In many situations, δ_t converges to some δ^*. By Theorem 2, this convergence is independent of n, the size of the Boolean network. Thus we can apply Theorem 3, deriving $H_t \approx [\mathrm{I}(\mathcal{F};\delta^*)]^t$. The Lyapunov exponent is $\log \mathrm{I}(\mathcal{F};\delta^*)$, so we get a critical point at $\mathrm{I}(\mathcal{F};\delta^*) = 1$. Our formula gives a provable characterization of short-term stability, for *any* transfer function family $\mathcal{F}$.

Balanced families: We derive previous results that only held for balanced families $\mathcal{F}$. In such families, the expected difference (over $\mathcal{F}$) between $+1$'s and -1's in the transfer functions is exactly zero. This contains the classic random families of Kauffman. For such a family, $\sigma_0(\mathcal{F}) = \mathbf{E}_{f\sim\mathcal{F}}[\sigma_0(f)] = 0$. The starting distribution is given by $\mathcal{D}_0$, so $\delta_0 = 0$. Regardless of the values of $\sigma_r(\mathcal{F})$ (for $r > 0$), by Theorem 2, $\delta_t = 0$ for all t. Hence, $H_t = [\mathrm{I}(\mathcal{F};0)]^t$, and $\mathrm{I}(\mathcal{F};0) = 1$ is the critical threshold. This is exactly the main result of [11].

We provide formal proofs for our theorems in the next section.

How Harmonic Analysis Helps

The Boolean network problem is fundamentally discrete, and the questions are about iterating the discrete function that the Boolean network represents. Harmonic analysis allows us to represent the discrete transfer functions as multilinear polynomials over the inputs (which are still discrete). To understand the evolution of imbalance, we take expectations over the distribution of inputs. An application of the linearity of expectation implies that the imbalance evolves as an iterated polynomial. This is the gist of the proof of Theorem 2. We stress that the polynomial representation of the transfer functions is crucial for this insight.

Additionally, damage spreading is related to changes in the function represented by the Boolean network on flipping some bits. The Fourier representation essentially represents the function in terms of how it changes when specific subsets of its inputs change. Thus, it helps in rigorous analysis of damage spreading in Boolean networks.

For Theorem 3, we use the standard observation that the local neighborhood of a Kauffman N-K network is a tree. For a timescale of less than $\log n$, we can imagine that the Boolean network (from the perspective of a single node) is just a tree. This allows for the calculations to be performed independently over subtrees. Since we represent transfer functions as polynomials, we can express the state of a node as a polynomial over the states of the leaves. We can then perform an analysis of perturbations to prove Theorem 3.

PROOFS

Recall that for $\rho \in [-1,1]$, we define a biased distribution $\mathcal{D}_\rho$ on $\{-1,+1\}$ as follows. The probability of $+1$ is $(1+\rho)/2$ and that of -1 is $(1-\rho)/2$. Note that expectation is exactly ρ. We sometimes abuse notation and use $\mathcal{D}_\rho$ to denote the product distribution over n bits. The uniform distribution is given by $\mathcal{D}_0$.

For a Boolean network $\mathcal{N}$, we use $f_t(x)$ to denote the total state after t steps starting with an initial state x. We use $f_{v,t}(x)$ to denote the (Boolean) state at the vertex v. Our aim is to understand $H_t = (1/n)\sum_{i=1}^{n} \mathbf{E}_{x\sim\mathcal{D}_\rho}[f_t(x) - f_t(x^{(i)})]$. That is, we calculate the expected Hamming distance over the starting state x for a random bit flip. As proven in previous work, this is the same as $\frac{1}{n}\sum_{1\leq u,v\leq n} \mathrm{Inf}_u(f_{v,t};\rho)$. This is the average value (over all vertices v) of $\sum_u \mathrm{Inf}_u(f_{v,t};\rho)$. Since the construction of Boolean networks is random where all vertices are symmetric, in expectation, all these influence sums are the same. Hence, we will fix a single vertex and focus on this sum.

Fix a vertex v. Let us consider the function $f_{v,t}$ for small $t \ll \log n$. Previous work tells us that we can assume (asymptotically) this is a rooted tree [27]. Note that this assumption also holds for sparse configuration models, such as Erdős-Rényi random graphs, but we focus on models where the degree, K, is fixed. We define a distribution $\mathcal{B}_t$ on Boolean networks that runs for t steps on rooted trees with height t. We take a K-ary directed tree rooted at v of depth t , with edges pointing towards the root v. For every internal node u, we choose a transfer function ϕ_u distributed according to $\mathcal{F}$. The leaves of the tree are the input nodes, collectively denoted as x. We will set the state at leaf nodes from the distribution $\mathcal{D}_\rho$. So $\delta_0 = \rho$ is the initial imbalance.

The Boolean network runs for t steps to yield the state at the root. We will use $v_1, v_2, \ldots$ to denote the children of v. The Fourier expansion yields the following proposition.

Proposition 4 $f_{v,t} = \sum_{A\subseteq[K]} \widehat{\phi_v}(A)\prod_{i\in A} f_{v_i,t-1}$

Proof: Suppose the state at v_i is y_i. The state at v is determined by applying the transfer function ϕ_v on the states $(y_1, y_2, \ldots, y_K)$. Using the Fourier expansion of ϕ_v, we get the state at v is $\sum_{A\subseteq[K]} \widehat{\phi_v}(A)\prod_{i\in A} y_i$. The state y_i is given by the function $f_{v_i,t-1}$, and the state at v is $f_{v,t}$. □

We take expectations of the formula in Prop. 4, noting that $\delta_t = \mathbf{E}_{\mathcal{B}_t}[\mathbf{E}_{x\sim\mathcal{D}_\rho}[f_{v,t}(y)]]$. (Verbal explanation follows.)

$$
\begin{aligned}
\delta_t = \mathbf{E}_{x,\mathcal{B}_t}[f_{v,t}(y)] &= \mathbf{E}_{x,\mathcal{B}_t}[\sum_{A\subseteq[K]} \widehat{\phi_v}(A)\prod_{i\in A} f_{v_i,t-1}(y)] \\
&= \sum_{A\subseteq[K]} \mathbf{E}_{x,\mathcal{B}_t}\Big[\widehat{\phi_v}(A)\prod_{i\in A} f_{v_i,t-1}(y)\Big] \\
&= \sum_{A\subseteq[K]} \mathbf{E}_{\mathcal{F}}[\widehat{\phi}(A)]\prod_{i\in A} \mathbf{E}_{x,\mathcal{B}_{t-1}}[f_{v_i,t-1}(y)]
\end{aligned}
$$

The second line is just linearity of expectation. The final line is obtained through independence. Note that ϕ_v is independent of the Boolean networks rooted at the v_is. These Boolean networks are also independent of each other. Hence, the expectation of the product is the product of expectations. The function ϕ_v is a random function ϕ chosen from $\mathcal{F}$. Because of the recursive construction, the distribution of $\mathcal{B}_t$ rooted at v induces the distribution of $\mathcal{B}_{t-1}$ rooted at the v_is. Now, observe that $\mathbf{E}_{x,\mathcal{B}_{t-1}}[f_{v_i,t-1}(y)] = \delta_{t-1}$.

Plugging this in and collecting all terms corresponding to sets of the same size (recall $\sigma_r = \mathbf{E}_{\phi\sim\mathcal{F}}[\sum_{C:|C|=r}\widehat{\phi}(C)]$),

$$
\begin{aligned}
\delta_t &= \sum_{A\subseteq[K]} \delta_{t-1}^{|A|}\mathbf{E}_{\mathcal{F}}[\widehat{\phi}(A)] \\
&= \sum_{r\geq 0}\delta_{t-1}^r \sum_{A:|A|=r}\mathbf{E}_{\mathcal{F}}[\widehat{\phi}(A)] = \sum_{r\geq 0}\sigma_r\delta_{t-1}^r \qquad (1)
\end{aligned}
$$

This proves Theorem 2.

For the spreading of perturbations, we focus on $\mathrm{I}_t(\rho_0)$. This is the expected average (over all nodes) influence of a node at t-steps, when the initial distribution is $\mathcal{D}_{\rho_0}$. We can express $\mathrm{I}_t(\rho_0)$ as follows. By the tree approximation, $H_t = \mathbf{E}_{\mathcal{B}_t}[\sum_\ell \mathrm{Inf}_\ell(f_{v,t});\rho]$ (where ℓ is over all leaves). In words, we look at the ρ-biased influence summed over all leaves. For convenience, we will drop the time/height subscript and simply write f_u instead of $f_{u,h}$.

Partition the leaves into subsets $S_1, S_2, \ldots, S_K$, where S_i contains all leaves that are descendants of v_i. Focus on a leaf $\ell \in S_1$. The first equality below is a technical statement proven earlier as Prop. 1. Applying Prop. 4,

$$
\begin{aligned}
&\mathbf{E}_{\mathcal{B}_t}[\mathrm{Inf}_\ell(f_v;\rho)] \\
&= (1/4)\mathbf{E}_{\mathcal{B}_t,x\sim\mathcal{D}_\rho}[(f_v(y) - f_v(y^{(\ell)}))^2] \\
&= (1/4)\mathbf{E}_{\mathcal{B}_t,x\sim\mathcal{D}_\rho}\left[\Big\{\sum_A \widehat{\phi}_v(A)(\prod_{i\in A} f_{v_i}(y) - \prod_{i\in A} f_{v_i}(y^{(\ell)}))\Big\}^2\right]
\end{aligned}
$$

Observe that for $i \neq 1$, $f_{v_i}(y) = f_{v_i}(y^{(\ell)})$. (This is because ℓ is not in the subtree of v_i.) In the summation above, only the terms corresponding to $A \ni 1$ are nonzero. Expanding further,

$$
\begin{aligned}
&\left\{\sum_{A\ni 1}\widehat{\phi}_v(A)(\prod_{i\in A} f_{v_i}(y) - \prod_{i\in A} f_{v_i}(y^{(\ell)}))\right\}^2 \\
&= \left\{\sum_{A\ni 1}\widehat{\phi}_v(A)\big(\prod_{\substack{i\in A\\ i\neq 1}} f_{v_i}(y)\big)(f_{v_1}(y) - f_{v_1}(y^{(\ell)}))\right\}^2 \\
&= \big(f_{v_1}(y) - f_{v_1}(y^{(\ell)})\big)^2\left\{\sum_{A\ni 1}\widehat{\phi}_v(A)\prod_{\substack{i\in A\\ i\neq 1}} f_{v_i}(y)\right\}^2 \qquad (2)
\end{aligned}
$$

Each f_{v_i} is defined over disjoint parts of the underlying tree with disjoint inputs. Hence, when we take the expectation $\mathbf{E}_{\mathcal{B}_t,x}$ over the product, we get the product of expectations. Thus,

$$\begin{aligned}
&\mathbf{E}_{\mathcal{B}_t}[\mathrm{Inf}_\ell(f_v;\rho)] \\
&= (1/4)\mathbf{E}_{\mathcal{B}_t,x\sim\mathcal{D}_\rho}[\big(f_{v_1}(y)-f_{v_1}(y^{(\ell)})\big)^2]\times \\
&\quad \mathbf{E}_{\mathcal{B}_t,x\sim\mathcal{D}_\rho}\left[\Big\{\sum_{A\ni 1}\widehat{\phi}_v(A)\prod_{\substack{i\in A\\ i\neq 1}} f_{v_i}(y)\Big\}^2\right] \qquad (3)
\end{aligned}$$

The first term, $(1/4)\mathbf{E}_{\mathcal{B}_t,x\sim\mathcal{D}_\rho}[\big(f_{v_1}(y)-f_{v_1}(y^{(\ell)})\big)^2]$, is exactly $\mathbf{E}_{\mathcal{B}_{t-1}}[\mathrm{Inf}_\ell(f_{v_1};\rho)]$.

We deal with the second term. The random variable $f_{v_i}(x)$ is in $\{-1,+1\}$ and $\mathbf{E}_{\mathcal{B}_{t-1},x\sim\mathcal{D}_\rho}[f_{v_i}(y)] = \delta_{t-1}$. Hence, it is distributed as $\mathcal{D}_{\delta_{t-1}}$. Taking expectations over $\mathcal{B}_{t-1}, x$, setting $y_i = f_{v_i}(y)$ and Prop. 1,

$$\begin{aligned}
&\mathbf{E}_{\mathcal{B}_t,x\sim\mathcal{D}_\rho}\left[\Big\{\sum_{A\ni 1}\widehat{\phi}_v(A)\prod_{\substack{i\in A\\ i\neq 1}} f_{v_i}(y)\Big\}^2\right] \\
&= \mathbf{E}_{\phi\sim\mathcal{F},y\sim\mathcal{D}_{\delta_{t-1}}}\left[\Big\{\sum_{A\ni 1}\widehat{\phi}_v(A)\prod_{i\in A\setminus 1} y_i\Big\}^2\right] \\
&= \mathbf{E}_{\phi\sim\mathcal{F}}[\mathrm{Inf}_1(\phi;\delta_{t-1})] \qquad (4)
\end{aligned}$$

The final equality uses Prop. 1 to show that that the term in the expectation above is exactly $\mathrm{Inf}_1(\phi;\delta_{t-1})$.) Thus, for $\ell\in S_i$, we get $\mathbf{E}_{\mathcal{B}_t}[\mathrm{Inf}_\ell(f_v;\rho)] = \mathbf{E}_{\mathcal{F}}[\mathrm{Inf}_i(\phi;\delta_{t-1})]\mathbf{E}_{\mathcal{B}_{t-1}}[\mathrm{Inf}_\ell(f_{v_i};\rho)]$. We combine all our observations.

$$\begin{aligned}
H_t &= \sum_\ell \mathbf{E}_{\mathcal{B}_t}[\mathrm{Inf}_\ell(f_{v,t};\rho)] \\
&= \sum_{i=1}^K\sum_{\ell\in S_i}\mathbf{E}_{\mathcal{B}_t}[\mathrm{Inf}_\ell(f_{v,t})] \\
&= \sum_{i=1}^K \mathbf{E}_{\mathcal{F}}[\mathrm{Inf}_i(\phi;\delta_{t-1})]\sum_{\ell\in S_i}\mathbf{E}_{\mathcal{B}_{t-1}}[\mathrm{Inf}_\ell(f_{v_i};\rho)] \\
&= \sum_{i=1}^K \mathbf{E}_{\mathcal{F}}[\mathrm{Inf}_i(\phi;\delta_{t-1})]\mathbf{E}_{\mathcal{B}_{t-1}}[\sum_{\ell\in S_i}\mathrm{Inf}_\ell(f_{v_i};\rho)] \\
&= H_{t-1}\sum_{i=1}^K \mathbf{E}_{\mathcal{F}}[\mathrm{Inf}_i(\phi;\delta_{t-1})] \\
&= H_{t-1}\cdot \mathrm{I}(\mathcal{F};\delta_{t-1}) \qquad (5)
\end{aligned}$$

Uncoiling the recurrence yields the Theorem 3.

APPLICATIONS

Mixtures of threshold function families: convergence of opinion

Threshold functions are commonly used to understand the spread of new ideas/viral propogations in social networks, inspired by pioneering work in sociology [19–21]. Consider two types of people (vertices) in a network. Some simply side with the majority of their neighbors. Others are more resistant to change, and only take up a new belief if all their neighbors believe it. We will first demonstrate our theorem on a synthetic distribution inspired by this application. For simplicity of analysis, set $K = 3$. The majority function, MAJ, is $M(y) = \mathrm{sign}(\sum_i y_i)$ and the AND function $\Lambda(y) = \mathrm{sign}(\sum_i y_i + 2.5)$ (this is -1 iff all inputs are -1). Our distribution $\mathcal{F}$ picks MAJ with probability β and AND with probability $1-\beta$. We can use our harmonic analysis method to characterize how much of the initial network needs to have a new belief for it to propagate through the network, and how sensitive this belief is to perturbations in the initial state. Formally, we calculate the dynamics for the initial distribution $\mathcal{D}_\rho$. Note that a vertex state is -1 (TRUE) if that vertex currently believes the new idea.

We start with the Fourier expansions of MAJ and AND.

$$\begin{aligned}
M(y) &= \sum_i y_i/2 - y_1y_2y_3/2 \\
\Lambda(y) &= 3/4 + \sum_i y_i/4 - \sum_{i\neq j} y_iy_j/4 + y_1y_2y_3/4
\end{aligned}$$

We compute $\sigma_0(\mathcal{F}) = 3(1-\beta)/4$, $\sigma_1(\mathcal{F}) = 3\beta/2 + 3(1-\beta)/4 = 3(1+\beta)/4$, $\sigma_2(\mathcal{F}) = 3(\beta-1)/4$, and $\sigma_3(\mathcal{F}) = -\beta/2 + (1-\beta)/4 = (1-3\beta)/4$. From Theorem 2,

$$\begin{aligned}
\delta_{t+1} = (1-3\beta)\delta_t^3/4 + 3(\beta-1)\delta_t^2/4 \\
+ 3(1+\beta)\delta_t/4 + 3(1-\beta)/4 \qquad (6)
\end{aligned}$$

Any fixed point is a root of the following polynomial $p(\delta)$. Note that when $p(\delta_t) > 0$, then $\delta_{t+1} > \delta_t$ (and vice versa).

$$\begin{aligned}
p(\delta) &= [(1-3\beta)\delta^3 + 3(\beta-1)\delta^2 + (3\beta-1)\delta + 3(1-\beta)]/4 \\
&= (\delta-1)(\delta+1)[(1-3\beta)\delta - 3(1-\beta)]/4 \qquad (7)
\end{aligned}$$

This characterizes the limits of δ_t as $t\to\infty$ (assuming convergence). The first two are trivial roots, since the all -1s and all $+1$s states are fixed points imbalances for the Boolean network. The third root $3(1-\beta)/(1-3\beta)$ is a new valid imbalance (in the range $(-1,1)$) only when $\beta > 2/3$.

Now, we can explain the dynamics. (We ignore the trivial cases $\rho = -1, +1$.)

- $\beta \leq 2/3$: The polynomial $p(z) > 0$ for any $z \in (-1,1)$. Hence, for any non-trivial starting distribution $\mathcal{D}_\rho$, the Boolean network converges to the all $+1$s state. So the new belief will always die out.
- $\beta > 2/3$: There exists a new unstable fixed point for the imbalance at $\delta^* = 3(1-\beta)/(1-3\beta)$. We have

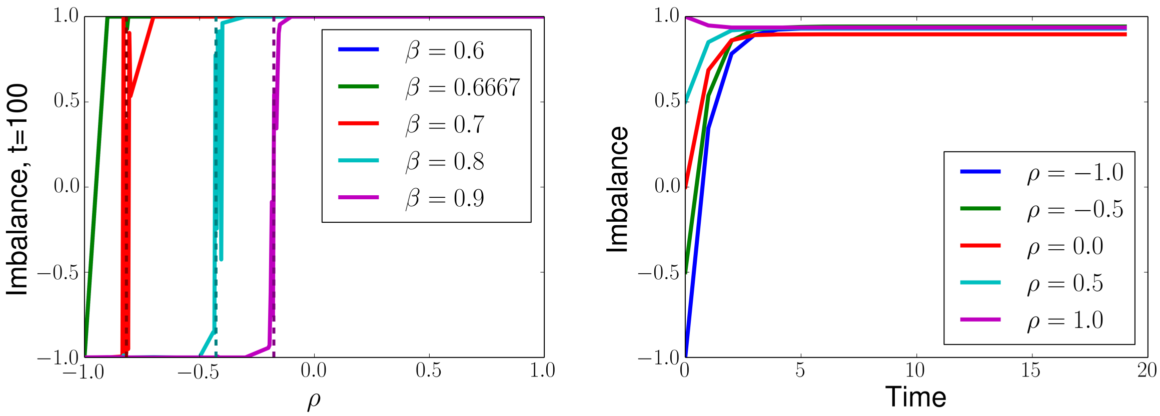

FIG. 1: Experimental results (color online). (Left figure (a)) This is for the threshold function distribution. Each line plots (for a fixed β; β increases from left to right within the plot) the limiting imbalance as a function of the initial input imbalance ρ. We observe a sharp threshold in each case coinciding with the prediction shown as a dotted line. (Right figure (b)) This is for the nested canalyzing distribution. Each line plots the imbalance over time for different input imbalances ρ (where the value of ρ increases from bottom to top within the plot). Observe it always converges to the same value.

$p(z) > 0$ if $z > \delta^*$ and $p(z) < 0$ if $z < \delta^*$. If $\rho > \delta^*$, the eventual state is all +1s. If $\rho < \delta^*$, the eventual state is all −1s.

To understand the sensitivity to bit flips, it is quite natural that for situations where δ_t converges to −1 or +1, the network is insensitive to perturbations. Calculations yield that $\mathrm{Inf}(\mathcal{F}; -1)$ and $\mathrm{Inf}(\mathcal{F}; +1)$ are < 1. By Theorem 3, the networks are quiescent. At $\rho = \delta^*$, $\mathrm{I}(\mathcal{F}; \delta^*) = 3\beta(1-(\delta^*)^2)/2 + 3(1-\beta)(1-\delta^*)^2/4$. By some elementary algebra, $\mathrm{I}(\mathcal{F}; \delta^*) > 1$ when $\beta > 2/3$. Hence, for $\rho = \delta^*$, the dynamics are chaotic (again, this is expected).

We performed simulations on Boolean networks with 10^4 nodes. For a given β, we vary the starting distribution ρ and measure the imbalances at $t = 100$. We average over 1000 runs for each experiment, sampling network configuration and initial condition ,from the distributions specified, for each instance. The results are in Figure 1a, where each line denotes a different choice of β, increasing from left to right. The predicted transition of $\delta^* = 3(1-\beta)/(1-3\beta)$ is denoted by the dashed line, coinciding nicely with the numerical transition point. As expected, we see some fluctuations (due to chaotic behavior at δ^*) at the transition point.

Mixtures of threshold functions: examples of criticality

In the previous section, we considered settings where the entire network eventually converges to the same state. We now consider two functions that have *opposing* actions: namely, the negated majority (NMAJ) and the AND function. The NMAJ, denoted by N, is just the negation of the MAJ function, and thus, this gives the opposite state of the majority of its neighborhood. The Fourier expansion is given by $N(y) = -\sum_i y_i/2 + y_1y_2y_3/2$.

The distribution $\mathcal{F}_\beta$ is obtained by choosing NMAJ with probability β and AND with probability $1-\beta$. We compute $\sigma_0(\mathcal{F}) = 3(1-\beta)/4$, $\sigma_1(\mathcal{F}) = -3\beta/2 + 3(1-\beta)/4 = 3(1-3\beta)/4$, $\sigma_2(\mathcal{F}) = 3(\beta-1)/4$, and $\sigma_3(\mathcal{F}) = \beta/2 + (1-\beta)/4 = (1+\beta)/4$. From Theorem 2,

$$\begin{aligned}\delta_{t+1} &= (1+\beta)\delta_t^3/4 + 3(\beta-1)\delta_t^2/4 \\ &\quad + 3(1-3\beta)\delta_t/4 + 3(1-\beta)/4 \qquad (8)\\ p_\beta(\delta) &= \big[(1+\beta)\delta^3 + 3(\beta-1)\delta^2 \\ &\quad -(1+9\beta)\delta + 3(1-\beta)\big]/4 \qquad (9)\end{aligned}$$

As before, roots of $p(\delta)$ in $[-1, 1]$ are fixed points. When $\beta = 0$ (all AND), there is a stable fixed point at $\delta = 1$, corresponding all nodes at +1. When $\beta = 1$ (all NMAJ), the stable fixed point is at $\delta = 0$, corresponding to half the nodes at +1. By varying β, we can move the stable fixed point in the range $[0, 1]$. Let us denote this root by δ^*_β, which is the limit of the imbalance for the distribution $\mathcal{F}_\beta$.

The expressions for $\mathrm{I}(\Lambda; \delta)$ and $\mathrm{I}(N; \delta)$ are polynomials in δ. (These are obtained by looking at which bit flips change values of AND and NMAJ respectively.)

$$\mathrm{I}(\Lambda; \delta) = 3\delta^2/4 - 3\delta/2 + 3/4 \qquad (10)$$

$$\mathrm{I}(N; \delta) = -3\rho^2/2 + 3/2 \qquad (11)$$

Thus, $\mathrm{I}(\mathcal{F}_\beta; \delta) = \beta \cdot \mathrm{I}(N; \delta) + (1-\beta) \cdot \mathrm{I}(\Lambda; \delta)$.

$$\mathrm{I}(\mathcal{F}_\beta; \delta) = (-9\beta/4 + 3/4)\delta^2 + (3\beta/2 - 3/2)\delta + (3\beta/4 + 3/4) \qquad (12)$$

To understand the short-term dynamics for any β, as per Theorem 3, we compute $\mathrm{I}(\mathcal{F}_\beta; \delta^*_\beta)$. We plot this quantity as a function of β in Figure 2a. The horizontal dashed line corresponds to $\mathrm{I}(\mathcal{F}_\beta; \delta^*_\beta) = 1$. By Theorem 3, the vertical dashed line shows the critical point. This reveals an interesting phase transition in the short term dynamics. When $\mathrm{I}(\mathcal{F}_\beta; \delta^*_\beta)$ is less than 1, the dynamics is quiescent (bit flips die out). When it is greater than 1, the dynamics is chaotic. The critical point is at $\beta = 0.5552\ldots$, when the limiting influence is exactly 1.

This is validated by our empirical simulations, shown in Figure 2b. We begin with a value of β. We generate a random Boolean network with 10^4 nodes with transfer functions drawn from $\mathcal{F}_\beta$, and run it from a uniform random input (so $\delta_0 = 0$) for 20 timesteps. We then flip a random bit in the same input, run it again, and track the Hamming distances between the states at each timestep. We repeat this entire process 10^3 times, and plot the average Hamming distance as a function of the timestep. As shown in Figure 2b, we perform this simulation for $\beta = 0.4, 0.5$ (below the critical point), $\beta = 0.5552\ldots$ (the critical point, denoted as β^*), and $\beta = 0.6, 0.7$ (above the critical point). Note that the average Hamming distance is in logscale, so we expect the plots to be roughly linear (except when the distance is comparable to 10^4), by Theorem 3. In accordance with the analysis presented above, the Hamming distance drops below 1 for $\beta < \beta^*$, and increases exponentially for $\beta > \beta^*$.

Nested canalyzing functions

For another application, we consider the nested canalyzing functions of [18]. Fix positive integer α and a series of canalyzing input values $c_1, c_2, \ldots, c_K$ and $d_1, d_2, \ldots, d_K, d_{def}$ (where each of these is in $\{-1, +1\}$). The function is defined as follows:

$$f(x) = \begin{cases} d_1 & \text{if } y_1 = c_1 \\ d_2 & \text{if } y_1 \neq c_1 \text{and } y_2 = c_2 \\ \vdots & \\ sd_K & \text{if } y_1 \neq c_1, \ldots, y_{K-1} \neq c_{K-1} \text{and } y_K = c_k \\ d_{def} & \text{otherwise} \end{cases}$$

For any parameter $\alpha > 0$, the distribution is given by $\Pr[c_i = -1] = \Pr[d_i = -1] = \exp(-\alpha/2^i)/(1 + \exp(-\alpha/2^i))$. Kauffman et al [18] suggest that $\alpha = 7$ is reflective of real biological networks, and corresponding Boolean networks are quiescent.

We can use our theorems to validate the quiescence. Let us the consider the polynomial $\delta_{t+1} - \delta_t$. For example at $K = 5$, a technical calculation yields $p(\delta) = -0.001\delta^4 + 0.016\delta^3 - 0.11\delta^2 - 0.69\delta + 0.71$. For $K = 10$, $p(\delta) = -0.007\delta^4 + 0.012\delta^2 - 0.099\delta^2 - 0.7\delta + 0.71$. These polynomials have a single stable root $\delta^* \approx 0.9$ in $[-1, +1]$. Even as K varies, the root is quite stable, so that fixed point imbalance is at least 0.9 when $K \geq 2$.

We perform experiments for varying degree distributions with 10^4 nodes, and varying starting state distributions $\mathcal{D}_\rho$. (We show only the results for $K = 5$ for space reasons.) In Figure 1b, we plot the imbalance as a function of time for varying ρ, with ρ increasing from bottom to top. Observe that the imbalance *always* rapidly converges to around 0.9. *This means that roughly 90% of the nodes converge to the* $+1$ *(FALSE) state.* The influence $\mathrm{I}(\mathcal{F}; \delta^*)$ is roughly 0.3, so the network is quiescent. In our experiments, we observe that the Hamming distance rapidly decays to 0, validating our influence calculation.

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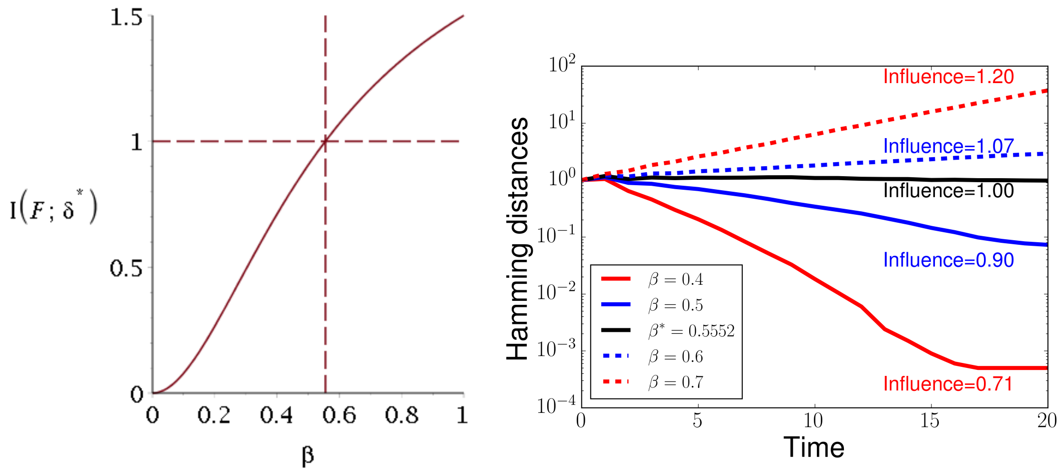

FIG. 2: Experimental results (color online): (Left figure (a)) This plots the value of $\mathrm{I}(\mathcal{F};\delta^*_\beta)$ as a function of β. (Right figure (b)) This plots the average Hamming distance as a function of time for different values of β, with β increasing from bottom to top within the plot. The middle line (influence equal to 1.0) shows the critical point. The dotted lines are above the critical point, and show chaotic behavior.

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