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Heterogeneity and its impact on Thermal Robustness and Attractor Density

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Abstract

There is considerable research relating the structure of Boolean networks to their state space dynamics. In this paper, we extend the standard model to include the effects of thermal noise, which has the potential to deflect the trajectory of a dynamical system within its state space, sending it from one stable attractor to another. We introduce a new "thermal robustness" measure, which quantifies a Boolean network's resilience to such deflections. In particular, we investigate the impact of structural homogeneity on two dynamical properties: thermal robustness and attractor density. Through computational experiments on cyclic Boolean networks, we ascertain that as a homogeneous Boolean network grows in size, it tends to underperform most of its heterogeneous counterparts with respect to at least one of these two dynamical properties. These results strongly suggest that during an organism's growth and morphogenesis, cellular differentiation is required if the organism seeks to exhibit *both* an increasing number of attractors *and* resilience to thermal noise.

Keywords:
boolean networks, cellular automata, dynamical systems, noise, robustness.

1. Introduction

Since the seminal work of Von Neumann [1], the subject of cellular automata has received considerable and continued attention (see [2, 3] for brief surveys). Understanding how the structure of a cellular network impacts its behavior as a dynamical system is crucial to determining how networks should be built, how they evolve over time, and how they can be made to grow while still exhibiting desired dynamical properties.

Biological networks (e.g. neural networks) are typically subject to a Darwinian preferential selection process, and are seen to exhibit evolution over long time scales. It is reasonable to expect that this selection process would be based not only on the structural properties [4] of networks, but on their dynamical properties as well [5]. Previous researchers have considered measures such as landscape ruggedness [6, 7] and redundancy [8] in evaluating dynamical systems. In this work, the dynamical property we consider is the robustness of a dynamical system's attractors against thermal noise from the environment. We refer to this property, formally defined in Section 3, as *thermal robustness*.

Thermal or Johnson-Nyquist noise manifests as non-deterministic point mutations in the state of individual cells of the organism. Such noise effectively deflects the trajectory of the system within its phase space, and can cause it to leave a stable orbit of one attractor by throwing it instead into the basin of a different attractor.

In addition to evolution over long time scales, biological networks also exhibit cellular differentiation over short time scales, particularly during morphogenesis, when changes in the cellular structure frequently arise from symmetry breaking during growth. One striking example of this occurs in the inner cell mass of a blastocyst, which goes on to form the diverse and specialized tissues of the human body. In this work, we explore the impact of cell differentiation on the thermal robustness of a network.

In our investigations we shall consider Boolean networks comprised of cells whose instantaneous state is either 0 or 1. Such networks have been the subject of considerable research since their introduction by Kauffman [9] as plausible models of genetic regulatory networks. Although Boolean networks are typically considered in terms of the well-charted class of potentially dense random Boolean "NK" networks [10], here we consider the more restricted class of linear cyclic networks. Such one dimensional automata have received considerable attention themselves [11], and are already known to exhibit a significant range of the phenomena observed in their more general NK counterparts [12]. We assume that the dynamic evolution in our networks is given by synchronous deterministic rules; it is well-known that asynchronous behavior with small temporal tolerances can be transformed into synchronous behavior [13]. Our approach is computational, based on simulations grounded in a formal mathematical model that builds upon existing research in the area of synchronous Boolean networks and cellular automata. Determining network dynamics is a computationally intensive endeavor, and data collected from the somewhat more accessible class of synchronous, cyclic, Boolean networks is used here to draw conclusions about the general relationship between structural homogeneity, attractor density, and robustness to thermal noise.

2. Mathematical Preliminaries

Structure. We consider organisms whose cellular structure may be modeled as an undirected cyclic graph $C = (V, E)$ of size n, whose vertices are considered "cells", and are enumerated $V = \{v_0, \ldots, v_{n-1}\}$. Each cell v_i in V is connected in cyclic order to two neighbors, so that $E = \{(v_i, v_{i+1 \,(\mathrm{mod}\, n)}) \mid i = 0, \ldots, n-1\}$. Microscopic cellular behavior within an organism is modeled by fixing a function $f : V \to \mathcal{F}$ that assigns to each cell $v \in V$, a function $f(v)$ from $\mathcal{F} = \{g : \{0,1\} \times \{0,1\} \to \{0,1\}\}$, the set of all binary Boolean functions; note that $|\mathcal{F}| = 2^{2 \cdot 2} = 16$. The action of f at a vertex v_i can be thought of as a truth table mapping v_i's left and right neighbors' current state, to v_i's state at the next time step.

$s(v_{i-1}, t)$	$s(v_i, t)$	$s(v_{i+1}, t)$	$s(v_i, t+1)$
0	$*$	0	b_0
0	$*$	1	b_1
1	$*$	0	b_2
1	$*$	1	b_3

Since each of the bits b_0, b_1, b_2, b_3 must be either 0 or 1, in what follows, we will frequently use the 4-bit binary string $b_0b_1b_2b_3$ to name the function f. Together, the pair (C, f) define the microscopic *structure* of the organism. An organism is said to be **homogeneous** if $|Im(f)| = 1$; otherwise it is said to be **heterogeneous**.

State. Since at each instant, a cell can have a value of either 0 or 1, the instantaneous *state* of the organism is specifiable as a function $V \to \{0,1\}$. The state of the organism over (discrete) time may then be represented by a function $s : V \times \mathbb{N} \to \{0,1\}$ where $s(v_i, t)$ is the state of cell $v_i \in V$ at time t. Since cell v_i behaves (across all time) according to function $f(v_i)$, and all cells are assumed to operate synchronously, the state of the organism evolves over time according to the following law:

$$s(v_i, t+1) = f(v_i)\left(s(v_{i-1\,(\mathrm{mod}\, n)}, t),\ s(v_{i+1\,(\mathrm{mod}\, n)}, t)\right)$$

for each $i = 0, \ldots n-1$ and $t \geqslant 0$. Informally, the state of the organism's constituent cells evolves according to the rule specified by Boolean function operating at that cell, together with the current state of its two adjacent cellular neighbors. We denote the subset of cells whose state is "on" (i.e. 1) at time t as $s^+(t) = \{v \in V \mid s(v, t) = 1\}$. Note

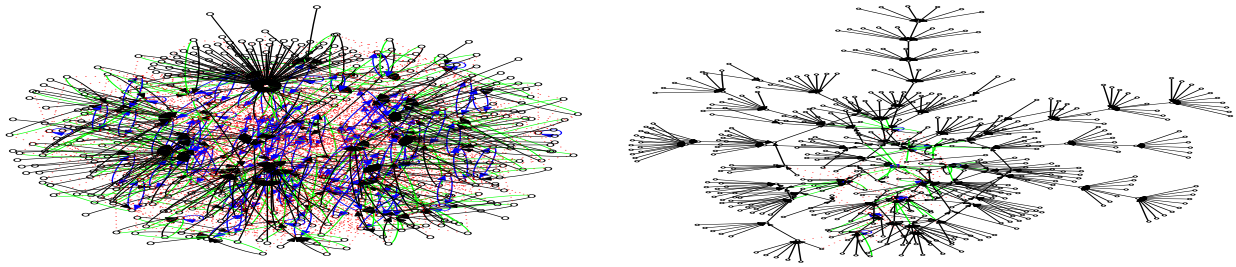

Figure 1. The phase space of a homogeneous network (left) and a heterogeneous one (right).

that to identify the system's state it suffices to know $s^+(t)$, since we can infer that the remaining cells are in state 0. In what follows, we will frequently identify the state of the organism at time t with the subset $s^+(t) \subset V$.

Dynamics. The macroscopic dynamics of the organism are represented as a directed graph $\mathcal{S} = (2^V, D)$ whose vertex set consists of all possible states of the organism (i.e. the power set of V), and whose edge set D includes every ordered pair (X, Y) for which $s^+(t) = X \implies s^+(t+1) = Y$. Informally, $\mathcal{S}$ is a directed graph representing the organism's phase space, in which (X, Y) is an edge if it can be said that whenever the organism is in state X at time t, it is necessarily (absent noise) in state Y at time $t + 1$.

For any pair of states $X, Z \subset V$, we say that $X \rightsquigarrow Z$ if there exists $k \geqslant 1$ and a sequence of states $Y_0, Y_1, \ldots, Y_k \subset V$ satisfying $Y_0 = X$, $Y_k = Z$, and $(Y_i, Y_{i+1}) \in D$ for $i = 0, \ldots, k-1$. Informally, $X \rightsquigarrow Y$ means there is a path from X to Y in the graph $\mathcal{S}$. We define $X \approx_R Y$ whenever both $X \rightsquigarrow Y$ and $Y \rightsquigarrow X$. To say that $X \approx_R Y$ means that in $\mathcal{S}$ there is both a path from X to Y, and a path from Y to X; this implies that X and Y are part of the same attractor cycle.

A state $X \subset V$ is said to be "on an attractor" if $X \rightsquigarrow X$. Let $A \subset 2^V$ be the set of all states that are on an attractor. Since $\approx_R$ defines an equivalence relation on A, it is possible to consider the quotient set $[A] = A/R$, wherein each $c \in [A]$ represents an attractor whose constituent states are given by cR. Conversely, given a state $X \subset V$, if $X \in A$, we denote the corresponding attractor as $[X]$. Thus A is simply the subset of the organism's phase space that constitutes attractor cycles, and the remaining states in $2^V \backslash A$ constitute tributaries which form the basins of attraction. If $X \in A$, then $[X]$ denotes the attractor that X lies in. The number of attractors in the dynamics of the organism is denoted

$$\alpha = |[A]|$$

3. Models of Thermal Noise and Thermal Robustness

Thermal Noise. We encode the effects of environmental thermal noise on an organism's dynamics using an undirected graph $\mathcal{N} = (2^V, M)$ whose vertex set consists of all possible states, and whose edge set M is defined in terms of single bit mutations in state: $(X, Y) \in M \iff |(X \cup Y) \backslash (X \cap Y)| = 1$. Informally, a mutation is an edge which connects from two states that differ only by 1 bit. For example, a 3-celled organism whose state is $0, 0, 1$ has three possible mutations edges that connect to states $1, 0, 1$, and $0, 1, 1$, and $0, 0, 0$. A mutation represents a non-deterministic state transition that occurs when thermal noise induces one of the organism's cells to "flip" state from 0 to 1 or from 1 to 0. The graph $\mathcal{N}$ is thus easily seen to be isomorphic to a $|V|$-dimensional hypercube.

Thermal robustness. Given an attractor $c \in [A]$, we consider $m(c) = \{(X, Y) \in M \mid X \in cR, (X, Y) \in M\}$ to be the possible mutations of c. We focus on mutations out of attractors (and disregard mutations out of basins of attraction), because over long time scales and in the absence of thermal noise, an organism spends almost all of its time spinning in its attractors. Out of the set of mutations $m(c)$, the subset that returns to cR is denoted $r(c) = \{(X, Y) \in m(c) \mid Y \rightsquigarrow X\} \subseteq m(c)$.

We define the *thermal robustness* of attractor c to be $\rho(c) = |r(c)|/|m(c)|$. This quantity, being equal to the fraction of mutation edges leaving c that return back to c, is an estimate of the probability that a random mutation will throw the organism out of attractor c. We define the *mean thermal robustness of the organism* as

$$\rho = \frac{1}{\alpha} \sum_{c \in [A]} \rho(c).$$

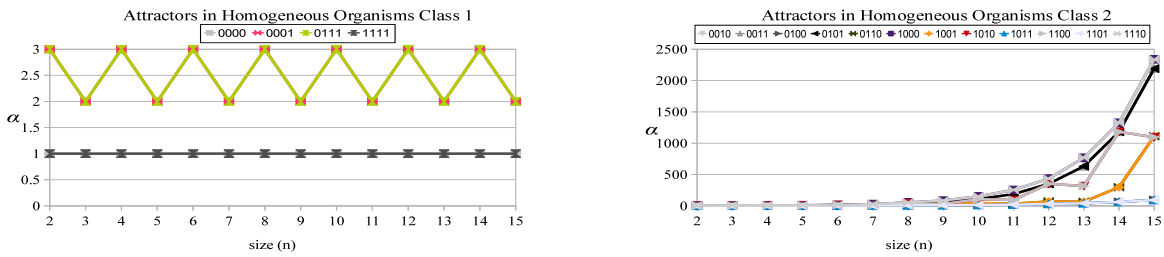

Figure 2. Homogeneous organisms with bounded (left) and unbounded (right) numbers of attractors.

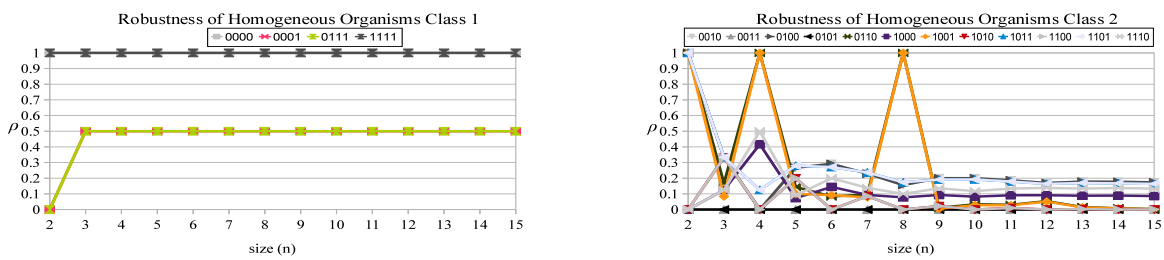

Figure 3. Robustness of homogeneous organisms of class 1 (left) and 2 (right).

Informally, this quantity captures the organism's resilience to noise-induced deflections in its state space trajectory that cause it to leave an otherwise stable attractor. In Figure 1 we see examples of what the phase space of two organisms looks like at size $n = 9$. Blue edges are used for attractor cycles, while black edges denote tributaries; mutations $r(c)$ that return to the same attractor are in green, while those in $m(c)\backslash r(c)$ causing deflections to a different attractor are in red.

4. Results

In what follows, we shall examine how the homogeneity (or heterogeneity) of an organism's structure (C, f) *impacts its dynamics, both in terms of its (expected) number of attractors* α*, and its thermal robustness* ρ*.*

4.1. Homogenous Networks

The two graphs of Figure 2 describe the number of attractors α in homogeneous cyclic networks of increasing size. Note that since $|\mathcal{F}| = 16$, for each size n there are only 16 possible distinct types homogeneous organisms. The 16 curves corresponding to these 16 types have been segregated into two graphs: The graph on the left shows homogeneous organisms whose structure is defined by $f(V)$ in $\{0000, 0001, 0111, 1111\}$. In these 4 organisms we see that α remains bounded as the organisms grow in size–that is, it is either a constant 1, or it oscillates between 2 and 3. In contrast, the graph on the right shows how the number of attractors α changes for homogeneous organisms whose structure is defined by $f(V)$ in $\{0010, 0011, 0100, 0101, 0110, 1000, 1001, 1010, 1011, 1100, 1101, 1110\}$. For these 12 organisms, we see that the number of attractors α grows unboundedly as these organisms become larger.

Based on the results of these simulations we found it useful to define two classes of homogeneous organisms. A homogeneous organism (C_n, f) will be said to be of *Class 1* if its number of attractors α remains uniformly bounded by some constant b as it grows $n \to \infty$. Alternately, an organism will be said to be of *Class 2* if for all constants b, there exists a size n_b at which the number of attractors α exceeds b. Informally, homogeneous organisms designated as Class 1 if they exhibit a bounded number of attractors, and are designated Class 2 otherwise. A growing organism might seek an increasing number of attractors as it grows, since attractors represent distinct dynamic equilibria for the system.

Having partitioned homogenous organisms on the basis of attractor density in this manner, we now turn to the question of thermal robustness. Figure 3 displays thermal robustness ρ for growing homogeneous Class 1 organisms.

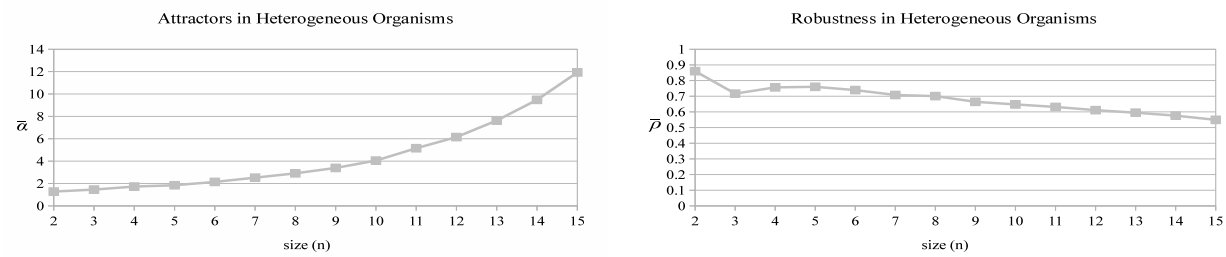

Figure 4. Attractors and robustness in heterogeneous organisms.

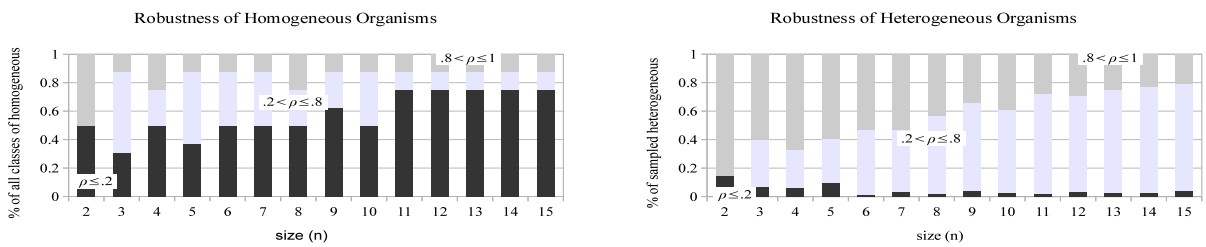

Figure 5. Exploring the relative benefits of heterogeneity on robustness.

The graph shows a constant $\rho = 1$ corresponding to the organisms which exhibiting $\alpha = 1$ attractor; this is expected, since having just one attractor implies that thermal noise can pose no threat to the organism's dynamic behavior at the level of attractors. In contrast, we see that, when sufficiently large, homogeneous Class 1 organisms whose number of attractors α is bounded between between 2 and 3, have $\rho = 0.5$. The graphs show that during growth, the 4 homogeneous Class 1 organisms maintain relatively high thermal robustness.

By comparison, Class 2 homogeneous organisms exhibit decreasing thermal robustness, with $\liminf \rho$ tending to a value < 0.2 (the exceptions which prevent this from being a uniform limit are two functions who for size 2^i spike to $\rho = 1$ but $\alpha = 1$). The graphs of Figure 3 thus show that while growing, the 12 homogeneous Class 2 organisms are unable to consistently maintain high thermal robustness, since this dynamical property is seen to tend to a value < 0.2.

4.2. Heterogenous Networks

Given the dichotomous choice faced by homogeneous organisms with respect to numbers of attractors α and thermal robustness ρ, here we examine whether a departure from the homogeneity condition can serve to relieve the organism from this bind. Unfortunately, the number of distinct heterogeneous organisms is $|\mathcal{F}|^{|V|} = 16^n$, which is too large to explore exhaustively for all but small values of n. Therefore, in order to estimate expected α and ρ for heterogeneous organisms of size n, we sample the space of heterogeneous organisms of size n by constructing random functions $f : V \to \mathcal{F}$. To select 1,000 random heterogeneous organisms, for example, we choose 1,000 random functions $f_1, \ldots, f_{1000}$. Each f_k assigns to cell $v \in V$ a randomly chosen binary Boolean function from the 16 choices available in $\mathcal{F}$. In effect, each cell in the organism is operating a randomly generated truth table. The likelihood that this sampling procedure will generate a homogeneous organism is 16^{-n+1}, which tends to 0 for large n.

In Figure 4 we see the mean number of attractors $\bar{\alpha}$ and the mean thermal robustness $\bar{\rho}$ for 1,000 randomly selected heterogeneous organisms of each size. The graph on the left shows that the expected number of attractors $\bar{\alpha}$ increases unboundedly with increasing size, in contrast to the limitations exhibited by Class 1 homogeneous organisms. The graph on the right shows that the expected robustness $\bar{\rho}$ approaches 0.5, a value that is superior to the < 0.2 limiting experienced by Class 2 organisms, and comparable to the high robustness exhibited by Class 1 organisms.

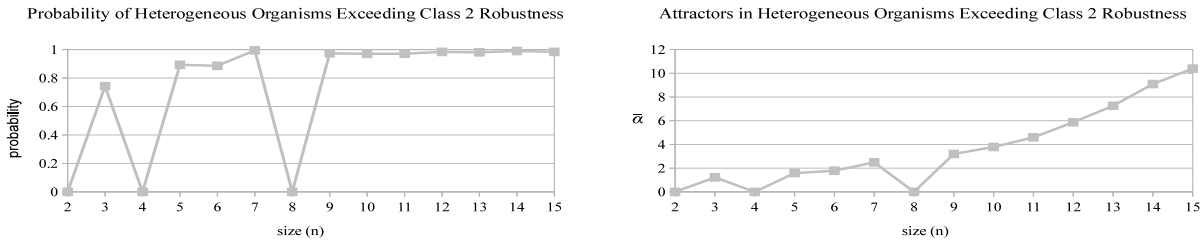

Figure 6. Heterogeneity makes it easy for a growing organism to achieve good robustness and increasing numbers of attractors.

4.3. Further Comparisons

In the previous section we considered the expected number of attractors and expected robustness of heterogeneous organisms. It is problematic, however, to argue on the basis of expected values alone, that a departure from homogeneity is in the interests of a growing organism. We interpret "interests" to mean growth in number of cellular units and number of attractors, without significant decline in thermal robustness. Here we consider the distribution of the random variables α and ρ more carefully, to determine if this is in fact the case.

In Figure 5 the chart on the left shows the proportion of homogeneous organisms (both Class 1 and Class 2) whose thermal robustness lies in each of the three bands: the low band: $0.0 \leq \rho \leq 0.2$, the middle band: $0.2 < \rho \leq 0.8$, and the high band: $0.8 < \rho \leq 1$. The analogous breakdown for heterogeneous organisms is shown in the chart on the right. Here we see that only the four Class 1 homogeneous organisms maintain uniform $\rho > 0.2$; the rest suffer from poor robustness as they grow. In contrast, the chart on the right shows that even though the expected thermal robustness $\overline{\rho}$ of heterogeneous organisms decreases as their size increases, the relative proportion of heterogeneous organisms for which robustness is very poor $\rho \leq 0.2$ is insignificant.

In Figure 6 the chart on the left estimates the probability that the robustness ρ of a randomly chosen heterogeneous organism (of a given size) will be greater than the robustness achieved by all Class 2 organisms (of corresponding size). What we see is that except for sizes of the form 2^i (a set of measure 0), this probability tends to 1. The chart on the right side of the figure shows the expected number of cycles $\overline{\alpha}$, for *just* those heterogeneous organisms whose robustness ρ outperforms the robustness of all Class 2 organisms of the corresponding size. Disregarding organisms of size 2^i (a set of measure 0), the expected number of attractors exhibited by these robustness-favored heterogenous organisms is seen to grow unboundedly.

5. Conclusion

In Part 4.1 of this investigation we saw that as an organism grows, it faces only two possible options if it remains homogeneous. If it chooses to be a Class 1 organism, then it will enjoy high thermal robustness ρ but suffer from bounded numbers of attractors α. On the other hand, if it opts to be a Class 2 organism, then it can enjoy unbounded numbers of attractors α, but will suffer from low thermal robustness ρ.

In Part 4.2 of this investigation we saw that as heterogeneous organisms grow in size, the expected number of attractors α is unbounded, and expected thermal robustness ρ is high. Thus heterogenous organisms are, on average, able to have their cake and eat it too. They circumvent the dilemma of the homogeneous organisms which we found were unable to grow and exhibit both increasing numbers of attractors α and high thermal robustness.

In Part 4.3 of this investigation we saw that a randomly chosen heterogeneous organism is very likely to outperform its homogenous Class 2 counterparts of equivalent size with respect to robustness. Moreover, such robustness-favored heterogenous organisms typically enjoy increasing numbers of attractors as they grow. Therefore, if an organism requires an increasing number of attractors as it grows, and high thermal robustness is naturally preferred, then heterogeneous organisms will be selected.

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