Emergent Criticality Through Adaptive Information Processing in Boolean Networks

by

Alireza Goudarzi, Natali Gulbahce, Thimo Rohlf, and Christof Teuscher

Preprint no.: 17 2011
Emergent Criticality Through Adaptive Information Processing in Boolean Networks

Alireza Goudarzi\textsuperscript{1}, Christof Teuscher\textsuperscript{1}, Natali Gulbahce\textsuperscript{2} and Thimo Rohlf\textsuperscript{3,4,5}

\textsuperscript{1}Portland State University, 1900 SW 4th Ave, Portland, OR 97206 USA
\textsuperscript{2}University of California, San Francisco, 1700 4th, San Francisco, CA 94158 USA
\textsuperscript{3}Interdisciplinary Center for Biomathematics, University Leipzig, Haertelstr. 16-18, D-04107 Leipzig, Germany
\textsuperscript{4}Epigenomics Project, iSSB, Genopole Campus 1, 5 Rue Henri Desbrueres, F-91034 Evry, France
\textsuperscript{5}Max-Planck-Institute for Mathematics in the Sciences, Inselstr. 22, D-04103 Leipzig, Germany.

(Dated: April 26, 2011)

We study information processing in populations of Boolean networks with evolving connectivity and systematically explore the interplay between the learning capability, robustness, the network topology, and the task complexity. We solve a long-standing open question and find computational limits that, for large system sizes \(N\), adaptive information processing drives the networks to a critical connectivity \(K_c = 2\). For finite size networks, the connectivity approaches the critical value with a power-law of the system size \(N\). We show that network learning and generalization are optimized near criticality, given task complexity and the amount of information provided surpass threshold values. Both random and evolved networks exhibit maximal topological diversity near \(K_c\). We hypothesize that this diversity supports efficient exploration and robustness of solutions, also reflected in our observation that the variance of the fitness values is maximal in critical network populations. Finally, we discuss implications of our results for determining the optimal topology of adaptive dynamical networks that solve computational tasks.

PACS numbers: 89.75.Hc, 05.45.-a, 05.65.+b, 89.75.-k

In 1948, Alan Turing proposed several unorganized machines made up from randomly interconnected two-input NAND logic gates [1] as a biologically plausible model for computing. He also proposed to train such networks by means of a “genetical or evolutionary search.” Much later, random Boolean networks (RBN) were introduced as simplified models of gene regulation [2, 3], focusing on a system-wide perspective rather than on the often unknown details of regulatory interactions [4]. In the thermodynamic limit, these disordered dynamical systems exhibit a dynamical order-disorder transition at a sparse critical connectivity \(K_c\) [5]. For a finite system size \(N\), the dynamics of RBNs converge to periodic attractors after a finite number of updates. At \(K_c\), the phase space structure in terms of attractor periods [6], the number of different attractors [7] and the distribution of basins of attraction [8] is complex, showing many properties reminiscent of biological networks [3].

In [9–12] simulated annealing (SA) and genetic algorithms (GAs) were used to train feedforward RBNs and to study the thermodynamics of learning. For a given task with predefined input-output mappings, only a fraction of the input space is required for training to obtain networks that generalize perfectly on all input patterns. This fraction depends on the network size and the task complexity. Moreover, the more inputs a task has, the smaller the training set needs to be to obtain full generalization. In this context, learning refers to correctly solving the task for the training samples while generalization refers to correctly solving the task for novel inputs. We use adaptation to refer to the phase where networks have to adapt to ongoing mutations (i.e., noise and fluctuations), but have already learned the input-output mapping. In this Letter, we study adaptive information processing in populations of Boolean networks with an evolving topology. Rewiring of connections and mutations of the functions occur at random, without bias toward particular topologies (e.g., feedforward). We systematically explore the interplay between the learning capability, the network topology, the system size \(N\), the training sample \(T\), and the complexity of the computational task.

First, let us define the dynamics of RBNs. A RBN is a discrete dynamical system composed of \(N\) automata. Each automaton is a Boolean variable with two possible states: \(\{0, 1\}\), and the dynamics is such that \(\mathbf{F} : \{0, 1\}^N \rightarrow \{0, 1\}^N\), where \(\mathbf{F} = (f_1, ..., f_i, ..., f_N)\), and each \(f_i\) is represented by a look-up table of \(K_i\) inputs randomly chosen from the set of \(N\) automata. Initially, \(K_i\) neighbors and a look-table is assigned to each automaton at random. For practical reasons we restrict the maximum \(K_i\) to 8. An automaton state \(\sigma_i^t \in \{0, 1\}\) is updated using its corresponding Boolean function, \(\sigma_i^{t+1} = f_i(x_{i_1}^t, x_{i_2}^t, ..., x_{i_K}^t)\).

The automata are updated synchronously using their
corresponding Boolean functions. For the purpose of solving computational tasks, we define $I$ inputs and $O$ outputs. The inputs of the computational task are randomly connected to an arbitrary number of automata. The connections from the inputs to the automata are subject to rewiring and are counted to determine the average network connectivity $\langle K \rangle$. The outputs are read from a randomly chosen but fixed set of $O$ automata. All automata states are initialized to 0 before each experiment.

Methodology.— We evolve the networks by means of a traditional genetic algorithm (GA) to solve three computational tasks of varying difficulty, each of which defined on a 3-bit input: full-adder (FA), even-odd (EO), and the cellular automata rule 85 (R85) [13]. The FA task receives two binary inputs $A$, $B$, an input carry bit $C_{in}$, and outputs the binary sum of the three inputs $S = A + B + C_{in}$ on the 2-bit output and the carry bit $C_{out}$. The EO task outputs a 1 if there is an odd number of 1s in the input (independent of the order), a 0 otherwise. R85 is defined for three binary inputs $A$, $B$, and $C$, and outputs the negation of $C$. The output for that task therefore only depends on one input bit. The FA represents the most difficult task, followed by the EO and R85 task.

The genetic algorithm we use is mutation-based only, i.e., no cross-over operation is applied. For all experiments we ran a population of 30 networks with a mutation rate of 0.8. Each mutation is decomposed into $1 + \alpha$ steps repeated with probability $p(\alpha) = (0.5^\alpha)/2$, where $\alpha \geq 0$. Each step involves flipping a random location of the look-up table of a random automata combined with adding or deleting one link. Each population is run for 30,000 generations. We repeat each experiment 30 times and average the results. In each generation and for each tested input configuration, the RBN dynamics are run for $T$ updates, after which the network output (i.e., the state of the output nodes) is determined.

An experiment consists of choosing a different training sample size $T \in \{1, 2, ..., 8\}$ at the beginning of each generation. The training sample set $M$ is randomly chosen without replacement from the $2^3$ possible input patterns. During each generation, the fitness of each individual is determined by $f = 1 - E_M$, where $E_M$ is the normalized average error over the $T$ random training samples: $E_M = \frac{1}{2} \sum_{i \in M} \sum_{j \in O} (o_{ij} - a_{ij})^2$. $a_{ij}$ is the value of the output automata $j$ for the input pattern $i$, and $o_{ij}$ is the correct value of the same bit for the corresponding task. The generalization score is calculated using the same equation with $M$ including all $2^3$ inputs rather than a random sample. Finally, selection is applied to the population as a deterministic tournament. Two individuals are picked randomly from the old population and their fitness values are compared. The better individual is mutated and inserted into the new population, the worse individual is discarded. We repeat the process repeats until we have 30 new individuals in the new population.

Results.— We observe a convergence of $\langle K \rangle$ close to the critical value $K_c = 2$ for large system sizes $N$ and training sample sizes larger or equal to $T = 4$. For $T = 8$, populations always evolve close to criticality for moderate $N$ already. For smaller $T$, the average over all evolutionary runs is found at slightly higher values of $\langle K \rangle$ (Fig. 1). If the average is taken only over the best individuals, however, $\langle K \rangle$ values close to $K_c$ are recovered. This observation can be explained from the fact that for $T < 8$, due to the limited information provided for learning, some populations cannot escape local optima, and hence do not reach maximum fitness. Sub-optimal network populations show a large scatter in $\langle K \rangle$ values in the evolutionary steady state, while those with high fitness scores cluster around $K_c = 2$ (Fig. 1, inset). For the simple R85 task we do not observe any convergence to $K_c = 2$, independent of the training samples. For the other tasks, the finite size scaling of $\langle K \rangle$ (Fig. 2) exhibits convergence towards $K_c$ with a power-law as a function of the system size $N$. For $T = 8$, the exponent $b$ of the power-law for the three tasks EO, FA, and R85 is $-1.63$, $-1.11$, and $-0.30$ respectively (Fig. 2). Altogether, these results suggest that the amount of information provided by the input training sample helps to drive the network to a critical connectivity.

Let us now discuss the evolutionary dynamics from a population perspective. Fisher’s fundamental theory of natural selection states that “[t]he rate of increase in the mean fitness of any organism at any time ascribable to [natural selection] acting through changes in gene frequencies is exactly equal to its genetic variance in fitness at that time” [14]. This very general statement also applies to GAs, where evolution favors populations with maximum diversity (entropy) [15] because more configurations of the search space are available to find optimal solutions [9–11].
FIG. 2. Finite size scaling of $\langle K \rangle$ as a function of $N$ for the three tasks, EO (black), FA (blue), R85 (red), and the training sample size $T = 4$ (a) and $T = 8$ (b). Points represent the data of the evolved networks, lines represent the fits. The finite size scaling for $\langle K \rangle$ shows that it scales with a power-law as a function of the system size $N$. The dashed lines represent the power-law fit of the form $a \cdot x^b + c$. We favor the data for larger $N$ by weighting the data according to $N/N_{\max}$, where $N_{\max} = 500$.

Hence, we expect that “successful” populations clustered near $K_c$ should exhibit the largest diversity in the fitness distributions. Indeed, we find that the standard deviation of the fitness values in the populations has a local maximum in this range (Fig. 4, inset), with a sharp decay toward larger $\langle K \rangle$. Evidently, this diversity helps to maintain a high fitness population in the face of continuous mutations with a fairly high rate (0.8 in our study). While the average fitness can be lower (and often is), compared to less diverse populations, the probability to find and maintain high fitness solutions is strongly increased. Indeed, we find that populations where the best mutant has maximum fitness ($f = 1$) sharply peak near $K_c$ (Fig. 4), as well as populations where the best mutant reaches perfect generalization. To find a possible source of fitness diversity, we determined several topological measures of the networks [16]: the eccentricity, $e$, the betweenness, $b$, and the characteristic path length, for Erőss-Rényi (ER), exponential Random Graphs (XRG), as well as the evolved networks (Fig. 3). In fact, we find that the graph-theoretical measures have maximal variance near $K_c = 2$. Similarly, other authors have shown that dynamical diversity is maximized near $K_c$, too [17]. Our results suggest that evolving RBN can indeed exploit this diversity to optimize learning.

In addition, we find that during the learning process of the networks, the in-degree distribution changes from a Poissonian to an exponential distribution. In particular, we observe that the topological properties of the networks reach a compromise between ER graphs and the XRG. The same observation was made in input- and outputless RBNs that were driven to criticality by using a local rewiring rule [19]. This significant topology change is related to diversity (entropy) maximization during the learning phase [18]. However, this is beyond the scope of this paper and will be discussed in a separate publication.

Finally, we measured damage propagation in the evolved RBNs [5] from random initial states differing in one bit, in order to provide evidence for dynamical criticality of the networks. Fig. 5 shows a sharp peak in the damage distribution of evolved networks around an average damage $d = 1$ for $T = 1$, $T = 4$ and $T = 8$, indicating marginal damage spreading in the majority of evolved RBNs as a consequence of ongoing learning. For $T = 1$ (all tasks) and the R85 task, no peak was found. This again supports our conclusion that efficient exploitation of criticality for complex computation occurs only above certain thresholds both with respect to task complexity and the amount of information provided for learning.

Discussion.— We investigated the learning and generalization capabilities in RBNs and showed that they evolve toward a critical connectivity of $K_c \approx 2$ for large networks and large input sample sizes. For finite size networks, the connectivity approaches the critical value with a power-law of the system size $N$. We showed that network learning and generalization are optimized near criticality, given task complexity and the amount of information provided surpass threshold values. Furthermore, critical RBN populations exhibit the largest diversity (variance) in fitness values, which supports learning and robustness of solutions under continuous mutations. By considering graph-theoretical measures, we determined that $K_c$ corresponds to a region in network ensemble space where the topological diversity is maximized, which may explain the observed diversity in crit-
FIG. 4. The conditional probability that evolving populations, where the best mutant reaches maximum fitness (i.e., \( f_{\text{best}} = f_{\text{max}} = 1 \)), have average connectivity \( \langle K \rangle \) shows a sharp peak near \( K_c \) (red curve), the same is found for maximum generalization (green). Inset: diversity of evolving populations, quantified in terms of the standard deviation \( \sigma(f) \) of fitness distributions, has a maximum near \( K_c = 2 \). All data sampled over the best 22 out of 30 populations for full-adder task with \( T = 4 \) and \( N = 100 \).

FIG. 5. The average damage \( \bar{d} \) of \( N = 100 \) networks with a generalization score of \( G \geq 0.8 \) for \( T = 1 \) (a), \( T = 4 \) (b), and \( T = 8 \) (c). The sharp peak for \( T = 8 \) (c) implies the provided information in the input patterns is sufficient to evolve the networks toward criticality. For \( T = 1 \) (a), almost no networks are able to successfully compute the FA and the EO task [12].

high-diversity populations are maintained and on-going adaptation and robustness are optimized. Our study may have important implications for determining the optimal topology of a much larger class of complex dynamical networks where adaptive information processing needs to be achieved efficiently, robustly, and with limited connectivity (i.e., resources). This has applications, e.g., in the area of neural networks, complex networks, and more specifically in the area of emerging molecular and nanoscale networks and computing devices, which are expected to be built in a bottom-up way from vast numbers of simple, densely arranged components that exhibit high failure rates, are relatively slow, and connected in an unstructured way.

Acknowledgements. This work was partly funded by NSF grant # 1028120. The first author is grateful for the fruitful discussions with Guy Feldman and Lukas Svec.