

Maximum Power Efficiency and Criticality in Random Boolean Networks

Hilary A. Carteret,¹ Kelly John Rose,^{1,2} and Stuart A. Kauffman¹

¹*Institute for Biocomplexity and Informatics, Biosciences,
University of Calgary, Calgary, Alberta, T2N 1N4, Canada.**

²*Department of Mathematics and Statistics,
University of Calgary, Calgary, Alberta, T2N 1N4, Canada.†*

(Dated: October 3, 2008)

Random Boolean networks are models of disordered causal systems that can occur in cells and the biosphere. These are open thermodynamic systems exhibiting a flow of energy that is dissipated at a finite rate. Life does work to acquire more energy, then uses the available energy it has gained to perform more work. It is plausible that natural selection has optimized many biological systems for *power* efficiency: useful power generated per unit fuel. In this letter we begin to investigate these questions for random Boolean networks using Landauer’s erasure principle, which defines a minimum entropy cost for bit erasure. We show that critical Boolean networks maximize available power efficiency, which requires that the system have a finite displacement from equilibrium. Our initial results may extend to more realistic models for cells and ecosystems.

PACS numbers: 89.75.Fb, 87.10.-e, 05.45.-a

Introduction: Random Boolean networks (RBNs) are a powerful class of models for complex causal systems [1, 2]. However, a thermodynamics for such networks has not yet been developed. In this paper we define a minimum rate of energy flow for general RBNs and show that dynamically critical RBNs maximize *power* efficiency.

A Boolean network (BN) consists of n nodes that output one bit each per time-step. Each node i receives inputs from k_i nodes and uses a Boolean function f_i that can be defined thus:

$$f_i : \{0, 1\}^{k_i} \mapsto \{0, 1\} \quad (1)$$

to compute its output. A BN model is logically equivalent to the system it is simulating. Random BNs are used to make statistical statements about systems whose logical structure is unknown (or incompletely known). The number of connections between the nodes of an RBN can come from any desired distribution. The Boolean functions are assigned to the nodes randomly from a uniform distribution over the possible Boolean functions, and all the nodes’ outputs update synchronously. A state of a Boolean network is the current outputs of the n nodes; the system traces out a trajectory of state transitions until it reaches a state-cycle attractor.

There exist a variety of metrics which can be used to characterize the behavior of Boolean nets. One of these is the Hamming metric, which is the number of bits by which two states differ. For any of these metrics, there exists an ordered regime, where nearby states lie on trajectories that converge on average in state space, and a chaotic regime where nearby states have divergent trajectories [2]. These two regimes are separated by a critical surface (i.e. a phase transition) on which such trajectories stay the same average Hamming distance apart. (See [3] for an example of this effect in another metric.)

One way to derive thermodynamics starts from the definition of the Carnot cycle, which gives a criterion for

maximizing *energy* efficiency: the most energy efficient machine for performing work is a reversible one, i.e. that a machine must be at least as energy-inefficient as it is irreversible [4]. We show that by using a minimal notion of reversibility and hence an entropy production rate for RBNs, it is possible to define such a thermodynamics in terms of a *specific dissipation rate* [5, 6].

In the next two sections we outline some of the concepts we use in the paper and develop them into formal definitions in the following section. Using Landauer’s erasure principle [7] we derive expressions for the minimum (intrinsic) entropy production rate and hence the maximum possible *power* efficiency for RBNs and demonstrate that the power efficiency of RBNs is maximized when the network is critical. We finish by proposing a “maximum power principle” for RBNs and discuss some possible further developments of this work.

Logically reversible computation and Landauer’s principle A reversible Turing machine [8, 9] is similar to a conventional Turing machine (TM); both of them have a *tape* that consists of a string of “cells”, each of which can contain only one bit. The tape is used as a memory and initially may contain input data (if used) that is accessed by a read-write *head*, which can move left or right and passes information to and from the processor, which consists of a *transition function* (or *table*) that is a finite set of instructions (the program) together with the *state register* that stores the state of the processor, thus enabling the TM to keep track of where it is in its table. Unlike a conventional TM, a reversible TM is also required to be able to run backwards, i.e., at every step of the computation, the immediately preceding state must be uniquely defined. If we think of the TM as tracing out paths in a space of possible states, this requirement means that whenever two paths in this state-space merge, the TM must somehow keep track of which path it followed to

reach that point. This information is called the *history* of the computation and can be thought of as being written on a second tape. (One tape is sufficient, but two are often used for pedagogical purposes.)

The only logically irreversible step in a computation is the erasure of information. Landauer’s erasure principle [7] is a corollary of Boltzmann’s definition for the entropy, $S = k_B \ln \Omega$, and states that a logically irreversible erasure is also thermodynamically irreversible. Thus the irreversible erasure of a completely random, unknown, binary bit of information must generate an amount of entropy not less than $k_B \ln 2$.

The definition of an irreversible erasure for a logical bit is subtle, not least because there may be multiple, redundant copies of each bit in the machine’s memory. In order for a bit to survive a computational step, we must be able to find a copy of it after the step in a specified location that only depends on the program being executed, but not on the values of the other variables. If the information in the bit ends up in different places depending on some other variables, it cannot be retrieved in this way [10]. The ability to retrieve the logical bit at a later time is essential; even with a complete description of a given TM, this entire-machine erasure rate is an uncomputable function, even for computations that halt [11].

After the machine has completed its calculation and copied its result, it must somehow return to its initial state in order to close the work-cycle. However, it cannot simply reset its memory, as this would require logically irreversible erasures (i.e., dissipation). The only way the machine can clean up its memory without erasing anything is to “uncompute” the calculation it has just performed and run backwards to its initial state.

A minimal thermodynamics for RBNs: The original motivation for reversible computation theory was to determine if computation required a non-zero rate of energy dissipation. The fact that it doesn’t led Bennett to compare a reversible computation to a Carnot cycle [9, 12].

Bennett’s results were obtained for Turing machines; strictly speaking, a Boolean network is not a Turing machine. However, a BN can be described as a network of finite TM nodes operating in parallel with each node computing the value of its Boolean logic function. The nodes can output at most one bit at each computing cycle, though they are permitted to make copies of that bit and distribute them along the edges of their network digraph to some number of other nodes. The TM at each node has a k -bit memory (part of its tape) for the values on the input edges to that node, and it only needs a finite size working space on its tape (as any Boolean function on k inputs can always be implemented by something no bigger than a finite-size look-up table, thus needs only a finite memory). Thus we need only consider a finite-size, k -bit input TM at each node; the asymptotic limit in our analysis is the limit when the number of nodes tends to infinity, not when k tends to infinity. This is fortunate,

because if each node was a full-size TM, the erasure rate at each node would also be an uncomputable function (by Zurek’s argument in [11]) as well as the erasure rate for the infinite BN as a whole.

For a Boolean function with a probability p of outputting a 1 (called the “bias” of the function) erasure produces a change in entropy ΔS of at least $-k_B S(p)$, where $S(p)$ is the Shannon entropy [13] of the bit. As long as the values of the nodes continue to change, the BN has not halted, even after it has entered a limit cycle. The BN will continue to erase bits every time it passes through a point in state space where a trajectory joins that limit cycle, because the system cannot remember what its precursor state was without storing at least one history bit [14]. Thus these history bits must be either stored or erased whenever a tributary trajectory joins the limit cycle. Landauer’s principle dictates that erasing these history bits must cause dissipation.

Furthermore, reversible TMs can only achieve computation without dissipation if proceeding at zero speed [9, 12]. Fortunately, Bennett extended his rules to finite-speed computation [9, 10, 12, 14, 15]. As soon as the computation leaves this adiabatic limit, the laws governing the entropy generation rate change: computation at finite speed requires dissipation, just as the ideal energy efficiency for any work-cycle can only be achieved in the adiabatic limit, when it is performed quasi-statically.

If our BN is to run at a non-zero speed for a useful length of time, we must supply power to drive it. For example, consider a BN implemented as a set of coupled chemical reactions: the concentrations of the reagents will only fluctuate around their equilibrium values unless active steps are taken to drive the system away from equilibrium. For a reversible TM to be r times more likely to move forwards as backwards requires $k_B T \ln r$ energy to be dissipated per computational step [12, 14]. The need to drive the BN with some (generalized) force is a general fact about reversible computation at finite speed and is completely independent of its implementation; it holds whether the BN is a genetic network or something else. Only the dimensionless expression for r will depend on these details. This implies an energy cost for copying; while logically reversible, it can only be done for free if performed infinitely slowly [9, 12]. The faster the copies are produced, the more energy they will cost, even if the register into which each copy is written was blank.

For processes that must occur in a finite time, a more natural (and useful) measure is the power efficiency, which is given by the *Gouy-Stodola theorem* [16]:

$$\frac{dW_{\text{rev}}}{dt} - \frac{dW_{\text{use}}}{dt} = T \frac{dS}{dt} \quad (2)$$

where T is the temperature of the environment into which the entropy S is released. The Gouy-Stodola efficiency is maximized when the rate of entropy production per unit of power supplied to the system is minimized [16].

We seek expressions for expected (mean-field) values for an otherwise unknown RBN drawn at random from some ensemble defined by some macroscopic parameters, such as the bias, p . We therefore have only partial information about this RBN. Since BNs evolve in a discrete time steps, we use a finite-difference version of this equation. and a mean-field approximation to the discrete dynamics to calculate the *expected entropy production rate*. As this method finds an average value per node, we will write the mean k instead of k_i for the in-degree of a typical node i . This approach should also allow discussion of the expected power requirements of the RBN under different initial conditions.

Reversible simulation of an irreversible TM incurs overheads in either time, space, or both [17, 18]. Since we must supply power to the BN for each time step [12], any increase in the time taken will cost us, so we focus on time-parsimonious simulations. A large space overhead [18] raises the problem of where that information can be stored. If there is insufficient memory, then some bits will need to be erased [10]. Even so, additional memory can only delay the inevitable, after which the rate of copying information cannot exceed the erasure rate; writing a bit of information requires somewhere to write it. For each directed edge leaving a node, a copy is made of that node's bit onto that edge; thus for a node with out-degree m , and since $m = k$, k edges must be prepared locally. We also assume that every node has at least one incoming edge, without loss of generality.

In 2004, Shmulevich and Kauffman [19] defined a new measure of the average dynamical properties of BNs that they called the *sensitivity*, s of the Boolean function f_i , which is the number of inputs to f_i for which flipping that input bit alone changes the value of f_i . Such input bits are said to be *relevant* to that node. The more sensitive a BN is, the better it remembers perturbations; thus the rate it erases the information that distinguishes one computational path from another is low.

Shmulevich and Kauffman showed [19] that for a Boolean function of bias p , the probability that an input edge is relevant to any given node (its "activity") is $\alpha = 2p(1-p)$. Whether or not an input bit is locally erased at a particular node depends on its *relevance* to that node. This will typically depend on the values of other input edges. However, the irrelevant bits may not have been erased from the network *as a whole*. If an edge is *irrelevant*, the local copy on that edge is lost, since it is not recoverable by any procedure that is independent of the state of the larger RBN, if at all. If all edge-copies of a bit are irrelevant under at least one set of values of the other edges (it need not be the same set) then that bit is irreversibly erased [10].

A lower bound for the expected entropy production rate per node: To make an BN as efficient as possible, we must minimize the number of irreversible erasures at each step, or equivalently, the number of copies used by each

node per step. We use Landauer's principle and the non-zero energy cost of copying a bit at a finite speed [12] to find a lower bound for the entropy production rates for RBNs. Writing Eq. (2) in finite difference form gives

$$\frac{\Delta W_{\text{in}}}{\Delta t} = \frac{T\Delta S}{\Delta t} + \frac{\Delta W_{\text{use}}}{\Delta t} \quad (3)$$

where $T\Delta S$ is the dissipated energy lost due to Landauer's principle and ΔW_{use} is the free energy available per step to drive the computation forward. We divide (3) by the finite difference ratio $\Delta W_{\text{rev}}/\Delta t$ to obtain the corresponding power efficiency measure:

$$E_P := \frac{\Delta W_{\text{use}}}{\Delta W_{\text{rev}}} = \frac{\Delta W_{\text{rev}} - T\Delta S}{\Delta W_{\text{rev}}} = 1 - \frac{T\Delta S}{\Delta W_{\text{rev}}}. \quad (4)$$

Let A_{in} be the expected number of edges that need to be prepared for each node for each time-step. Let A_{out} be the expected number of bits of information erased per node per time step as a result of the computation. Then \mathcal{D} , the *specific dissipation rate per node* is

$$\mathcal{D} := |(A_{\text{in}} - A_{\text{out}})/A_{\text{in}}|, \quad (5)$$

which will give us $E_P = 1 - \mathcal{D}T$. (The modulus function is needed because for some ranges of the parameters there is a net loss of information at the node, whereas for others, the network is sending bit-copies into the node's equivalent finite TM that are not erased at this time-step since they are relevant to the function at that node.)

Shmulevich and Kauffman also demonstrated [19] that the sensitivity can be defined for every BN. They calculated this value to be $s = k\alpha$ and show that when $s = 1$, the RBN is critical. We use this to show that the dissipated power \mathcal{D} is minimized for critical networks, and thus E_P is maximized accordingly. Since the expected activity of each edge is α we see that on average every node will have at least $k(1-\alpha)+1 = k-s+1$ copies which must be deleted in the process of computing the Boolean function for the associated node, since they are inactive at that node. (The additional +1 is from the deletion of the output bit from the previous time-step.) Since these input bits are irrelevant, their information content cannot be retrieved from the output of that node. Since $A_{\text{in}} = k$, this allows us to write down an expression for the expected rate of information loss per node:

$$A_{\text{out}} = k(1-\alpha) + 1 = k - k\alpha + 1 = 1 + k - s. \quad (6)$$

Using Eq. (6), it is possible to approximate the erasure rate \mathcal{D} for a BN given any two of p , s , or k .

$$\mathcal{D} = |(k - (1 + k(1 - \alpha)))/k| = |\alpha(s - 1)/s|, \quad (7)$$

where $k = s/\alpha$. Thus when $s = 1$ (i.e. $k = \alpha^{-1}$) we have $\mathcal{D} = 0$ at the critical line. Since \mathcal{D} is the average erasure rate per node, the power efficiency E_P is maximized at the dynamical critical line for RBNs. As long as every node has at least one incoming edge, the minimum lower bound for $\mathcal{D} = 0$ occurs at critical values of k .

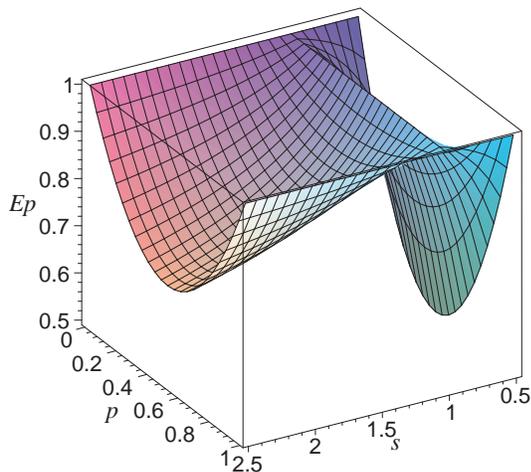


FIG. 1: Power efficiency E_P at $T = 1$, as a function of s and p , showing maximized power efficiency in a ridge at criticality; E_P is maximized at the critical line of Derrida and Pomeau [22]. As $p \rightarrow 0$ or 1 the input bits at each node have a lower Shannon entropy, so less information is lost if the output bit is subsequently erased. Thus $E_P \rightarrow 1$ when $p \rightarrow 0$ or 1 .

A “maximum power principle” and other questions: Suppose we have an expression for the power available to drive the RBN, $\Delta W_{\text{in}}/\Delta t$. A reversible TM computing at a rate r consumes energy $k_B T \ln r$ per time step. The form of the rate function r will depend on the implementation of the RBN. Thus we have an expression for the maximum possible “metabolic rate” per node for the RBN with bias p ,

$$r = S(p)e^{-\mathcal{D}}e^{P_{\text{in}}\Delta t/k_B T}. \quad (8)$$

The RBNs most closely approaching these upper bounds are dynamically critical; this suggests the existence of a “maximum power principle” [20, 21] for RBNs. Figure 1 shows how E_P varies with s and p when k is fixed; similar behavior occurs for other distributions of k .

It should be noted that the distinction between the copy-cost and the available energy cost may not be sharp in some implementations. In the molecular computer mentioned above, the driving power is supplied via the chemical potential terms in the Gibbs free energy. Maintaining the reactants in such non-equilibrium concentrations requires the larger system to do work.

Conclusion We have shown that critical RBNs maximize power efficiency; critical RBNs also maximize pairwise mutual information [23]. We conjecture a direct causal link between these three phenomena. Moreover Odum has proposed a maximum power principle for ecosystems [20] and Ulanowicz has argued that mature ecosystems maximize their mutual information content [24]. Furthermore, cells may be critical [3] and the rate of accumulation of biomass in an ecosystem may also be

maximized at criticality [25, 26]. In more detailed and realistic models that include more modes of energy expenditure, our lower bound should increase. Future work will look for direct relationships between criticality, mutual information and power efficiency in causal networks.

This work was supported by iCORE, NSERC and the University of Calgary. The authors would also thank Mircea Andrecut, Ilya Shmulevich and Matti Nykter for some stimulating discussions.

* Electronic address: hcartere@qis.ucalgary.ca

† Electronic address: kjrose@gmail.com

- [1] S. Kauffman, *J. theor. Biol.* **22:3**, 437 (1969).
- [2] S. Kauffman, *The Origins of Order: Self-Organization and Selection in Evolution* (Oxford University Press, New York, 1993), ISBN: 0195079515.
- [3] M. Nykter, N. D. Price, M. Aldana, S. A. Ramsey, S. A. Kauffman, L. E. Hood, O. Yli-Harja, and I. Shmulevich, *Proc. Natl. Acad. Sci. USA* **105**, 1897 (2008).
- [4] E. Smith, *Chemical Carnot cycles, Landauer’s principle, and the thermodynamics of natural selection* (2006), Working Paper, Santa Fe Institute.
- [5] L. Onsager, *Phys. Rev.* **37**, 405 (1931).
- [6] L. Onsager, *Phys. Rev.* **38**, 2265 (1931).
- [7] R. Landauer, *IBM J. Res. Develop.* **5**, 183 (1961).
- [8] Y. Lecerf, *Comptes Rendus* **257**, 2597 (1963).
- [9] C. H. Bennett, *Int. J. Theoret. Phys.* **21**, 905 (1982).
- [10] M. Li and P. Vitányi, *Proc. Roy. Soc. Lond. A* **452**, 769 (1996), arXiv:quant-ph/9703022.
- [11] W. H. Zurek, *Nature* **341**, 119 (1989).
- [12] R. P. Feynman, *Feynman Lectures on Computation* (Addison-Wesley, 1996), edited by A.J.G. Hey and R.W. Allen, ISBN: 0-14-028451-6, sections 5.1-5.3.
- [13] C. E. Shannon, *Bell Sys. Tech. J.* **27**, 379 (1948).
- [14] C. H. Bennett, *IBM J. Res. Develop.* **17**, 525 (1973).
- [15] C. H. Bennett, *IBM J. Res. Develop.* **32:1**, 16 (1988).
- [16] A. Bejan, *J. Appl. Phys.* **79**, 1191 (1996).
- [17] C. H. Bennett, *SIAM J. Comput.* **18**, 766 (1989).
- [18] H. Buhrman, J. Tromp, and P. Vitányi, *J. Phys. A: Math. Gen.* **34**, 6821 (2001), arXiv:quant-ph/0101133.
- [19] I. Shmulevich and S. A. Kauffman, *Phys. Rev. Lett.* **93**, 048701 (2004).
- [20] H. T. Odum, *Maximum Power: The Ideas and Applications of H.T. Odum*, Chapter 28: Self-organization and maximum empower (University Press of Colorado, 1995), edited by Charles A.S. Hall, ISBN: 0870813625.
- [21] A. J. Lotka, *Proc. Natl. Acad. Sci. USA* **8**, 147 (1922).
- [22] B. Derrida and Y. Pomeau, *Europhys. Lett.* **1**, 45 (1986).
- [23] A. S. Ribeiro, S. A. Kauffman, J. Lloyd-Price, B. Samuelsson, and J. E. Socolar, *Phys. Rev. E* **77**, 011901 (2008), arXiv:0707.3642.
- [24] R. E. Ulanowicz, *Proc. Natl. Acad. Sci. USA* **80**, 305 (1987).
- [25] H. V. Westerhoff, K. J. Hellingwerf, and K. V. Dam, *Proc. Natl. Acad. Sci. USA* **80**, 305 (1983).
- [26] S. E. Jørgensen, *J. theor. Biol.* **175**, 13 (1995).