

Relating Fisher information to order parameters

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We study phase transitions and relevant order parameters via statistical estimation theory using the Fisher information matrix. The assumptions that we make limit our analysis to order parameters representable as a negative derivative of thermodynamic potential over some thermodynamic variable. Nevertheless, the resulting representation is sufficiently general and explicitly relates elements of the Fisher information matrix to the rate of change in the corresponding order parameters. The obtained relationships allow us to identify, in particular, second-order phase transitions via divergences of individual elements of the Fisher information matrix. A computational study of random Boolean networks supports the derived relationships, illustrating that Fisher information of the magnetization bias (that is, activity level) is peaked in finite-size networks at the critical points, and the maxima increase with the network size. The framework presented here reveals the basic thermodynamic reasons behind similar empirical observations reported previously. The study highlights the generality of Fisher information as a measure that can be applied to a broad range of systems, particularly those where the determination of order parameters is cumbersome.

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I. INTRODUCTION

Critical phenomena and phase transitions have been reported in a very broad range of systems, ranging from physical to biological to computational. Phase transitions have been vigorously studied for many decades, producing fundamental scientific and technological results. Various models have been proposed explaining intricate details of order-disorder transitions under various conditions, universal behavior at critical regimes, dynamics of order parameters, and so on. These models have found applications beyond statistical mechanics, reaching as far as information geometry [1–4] and artificial life [5,6]. The research has produced various metaphors, hypotheses, and theories such as the edge of chaos [6], the enslaving principle in synergetics [7], universality classes of critical exponents [8], self-organized criticality [9], and guided self-organization [10], among many others.

In this paper, we approach the study of phase transitions and relevant order parameters via statistical estimation theory and information theory, aiming to characterize dynamics of order parameters in a fairly general setting. Our tools of choice are Fisher information and the Fisher information matrix, which are well known in statistical estimation theory. We make a few assumptions, most notably we limit our considerations to order parameters representable as a negative derivative of thermodynamic potential over some thermodynamic variable. The resulting representation, however, is general, immediately relating elements of the Fisher information matrix to the rate of change in the corresponding order parameters.

While this paper will turn its attention to information-theoretic concepts, it is beyond our scope to comment here on rich connections between Boltzmann entropy and Shannon entropy. It suffices to point out the seminal works of Jaynes [11,12], who convincingly demonstrated that information theory can be applied to the problem of the justification of

statistical mechanics, producing predictions of equilibrium thermodynamic properties.

It has been suggested in several previous studies [1–4] that the Fisher information matrix provides a Riemannian metric (more precisely, the Fisher-Rao metric) for the manifold of thermodynamic states, and thus can be used as an information-geometric complexity measure for a classification of phase transitions. For instance, it was suggested that the scalar curvature of the thermodynamic metric tensor measures the complexity of the system: the curvature diverges at (and only at) a phase transition point [1]. In this paper, we derive arguably simpler relationships that directly connect first derivatives of order parameter(s) to elements of the Fisher information matrix. This allows us to study second-order phase transitions via divergences of individual (e.g., diagonal) elements of the Fisher information matrix, as exemplified by a computational study of random Boolean networks (RBNs).

We select RBNs as an example because of their generality as discrete dynamical network models with a very large sample space available, making them very suitable for an ensemble study of the required dynamics. In particular, RBNs exhibit a well-known phase transition from ordered to chaotic dynamics, with respect to average connectivity or activity level (magnetization bias). Moreover, Fisher information was recently argued to provide a natural interpretation of the phase diagram in RBNs, where the latter was obtained by maximizing Fisher information of either average connectivity or the activity level [13,14]: i.e., the system dynamics reflected by Fisher information were shown to be most sensitive to control parameters near the critical points. The studies [13,14], however, did not provide underlying reasons for these observations—this paper fills this gap by immediately relating Fisher information (more precisely, elements of the Fisher information matrix) to order parameters. That is, we argue that the maximization of Fisher information reported in [13,14] is a manifestation of the divergences of the corresponding elements of the Fisher information matrix observed in finite-size experimental networks. Specifically, we intend to show

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that such a divergence occurs at a critical point whenever the corresponding order parameter changes continuously, but disappears at the critical point (and its first derivative or the rate of change diverges).

The paper is organized as follows. Section II briefly describes necessary details used in generic models of statistical mechanics, such as the Gibbs ensemble, thermodynamic potential, and derivatives of free entropy. Section III presents the two main components of our analysis: (i) order parameters representable via collective variables and (ii) the Fisher information matrix. Section IV follows with our main observations relating (the rate of change of) order parameters with Fisher information values, exemplified for a simple case of ferromagnetic magnetization. This analysis provides an argument for the divergence of Fisher information values at second-order phase transitions. The divergence of Fisher information is demonstrated in an experimental study of random Boolean networks for different increasing network sizes, presented in Sec. V. This analysis includes a comparison with the rate of change of a well-known order parameter, confirming the analytical relationship reported in Sec. III. Finally, Sec. VI summarizes the findings and suggests several directions for future research.

II. TECHNICAL PRELIMINARIES

A. Gibbs ensemble

Given a physical system in an equilibrium with a large thermal reservoir, models of statistical mechanics typically deal with Gibbs measures of the form

$$p(x|\theta) = \frac{1}{Z(\theta)} e^{-\sum_i \theta^i X_i(x)}, \quad (1)$$

where the configuration variable x varies over the configuration space, $Z(\theta)$ is the partition function, the set $\{\theta^i\}$ includes thermodynamic variables (e.g., inverse temperature, pressure, magnetic field, chemical potential, etc.), and the functions $X_i(x)$ reflect the terms of the system's Hamiltonian and determine the form of action [2]. In other words, the probability $p(x|\theta)$ that the system occupies the microstate x is represented via the time-independent functions $X_i(x)$ of the configuration and time-dependent conjugate variables (forces) θ^i . Generally, one may refer to $X_i(x)$ as collective variables [4]. The configurational probability distribution given by the Gibbs ensemble (1) can be written as

$$p(x|\theta) = \frac{1}{Z(\theta)} e^{-\beta H(x,\theta)}, \quad (2)$$

using the system's Hamiltonian that captures the total energy at x , which is $\beta H(x,\theta) = \sum_i \theta^i X_i(x)$, where $\beta = 1/k_B T$ is the inverse temperature (T) of the environment in natural units and k_B is the Boltzmann constant. This representation (2) makes clear that the partition function “encodes” how the probabilities $p(x,\theta)$ are partitioned among the different microstates x , based on the energies $H(x,\theta)$:

$$Z(\theta) = \sum_x e^{-\beta H(x,\theta)}. \quad (3)$$

For example, a simple model of statistical mechanics may use two thermodynamic variables $(\theta_1, \theta_2) = (\beta, h)$, considering β

as the inverse temperature and h as the external field [1]. This can be exemplified by the Ising spin model with two parameters (β, h) , where h is the magnetic field.

B. Thermodynamic potential

The thermodynamic value of the total energy (i.e., the expected value, or ensemble average for the energy) is defined as the sum of the total microstate energies weighted by their probabilities,

$$U = \sum_x p(x|\theta) H(x,\theta) = \frac{1}{Z(\theta)} \sum_x H(x,\theta) e^{-\beta H(x,\theta)}. \quad (4)$$

Helmholtz free energy is defined as $A = U - TS$, where S is the Boltzmann entropy,

$$S = -k_B \sum_x p(x) \ln p(x), \quad (5)$$

where for clarity we omit parameters θ of the probability functions $p(x)$. This expression is a statistical-mechanics definition of entropy, and it is well known that it is equivalent to the thermodynamic definition (taking Boltzmann's constant k_B into the account).

At this stage, we expand the expression (5) by substituting the probabilities (2) under the logarithm,

$$\begin{aligned} S &= -k_B \sum_x p(x) \ln \left[\frac{1}{Z} e^{-\beta H(x)} \right] \\ &= \beta k_B \sum_x p(x) H(x) + k_B \ln Z. \end{aligned} \quad (6)$$

Then, substituting the definitions of the expected value of the total energy U [given by Eq. (4)] and of S [given by the second line of Eq. (6)] into $A = U - TS$ (and noting $\beta k_B T = 1$) yields the famous expression for Helmholtz free energy:

$$A = -k_B T \ln Z. \quad (7)$$

In thermodynamics, Helmholtz free energy A is a thermodynamic potential which measures the “useful” work obtainable from a closed thermodynamic system at a constant temperature and volume. For our purposes, this concept is important due to its clear relationship with the partition function and the configurational probability distribution, allowing us to treat thermodynamic variables via statistical means.

C. Derivatives of free entropy

Sometimes it is convenient to work with the expression

$$\ln Z = -\beta A = \psi, \quad (8)$$

and the quantity βA may be referred to as the reduced free energy per site (dependent on the context) [1], and ψ is the free entropy (Massieu potential) [4]. In particular, the expression (7) yields

$$\psi = \ln Z = \frac{S}{k_B} - \frac{U}{k_B T} = \frac{S}{k_B} - \sum_x p(x) \sum_i \theta^i X_i(x), \quad (9)$$

where the last step uses the definition of U given by (4) and $H(x,\theta) = \frac{1}{\beta} \sum_i \theta^i X_i(x)$. Following [4], we denote by angled

brackets a weighted average over the appropriate equilibrium ensemble, obtaining

$$\psi = \frac{S}{k_B} - \left\langle \sum_i \theta^i X_i \right\rangle. \quad (10)$$

The first derivatives of the free entropy produce quite revealing expressions for the collective variables:

$$\langle X_i \rangle = -\frac{\partial \psi}{\partial \theta^i}. \quad (11)$$

III. METHODS

A. Order parameters

Basic thermodynamic classification of phase transitions depends on the determination of the “order” of a transition. This typically requires an examination of the thermodynamic potential (e.g., the Helmholtz free energy A) and its derivatives at the transition. If the first derivatives of A are discontinuous at the transition, then the transition is called “first order.” Otherwise, if the first derivatives are continuous but second derivatives are not (and at least one of them is divergent), the transition is a “second-order” transition, identified by a critical point in the phase diagram [15]. A thermodynamic variable distinguishing the phases is called the “order parameter.”

Phase transitions are often related to symmetry breaking. For instance, Jetschke [16] defines a system as undergoing a transition if the symmetry group of its dynamics changes to a less symmetrical one (e.g., a subgroup of the original symmetry group). An example may be given by a ferromagnetic system undergoing a second-order phase transition: (i) in the high-temperature phase, the system has no net magnetization, is “disordered,” and has a complete rotational symmetry (isotropy); (ii) at low temperature, the system becomes “ordered” and the net magnetization defines a preferred direction in space (anisotropy), breaking rotational symmetry. The low-temperature ordered phase is therefore *less* symmetrical and can be fully described by an order parameter—the magnetization vector [8]. It is well known that critical phenomena arise due to a diverging correlation length of the fluctuations of the order parameter [15].

Binder [15] illustrates the concept by considering the thermodynamic potential A , which has the “field” h , i.e., h is one of the thermodynamic variables θ^i . The order parameter ϕ is then given, at constant temperature T , as

$$\phi = -\left(\frac{\partial A}{\partial h} \right)_T. \quad (12)$$

For example, ferromagnetic magnetization $M = -(\frac{\partial A}{\partial h})_T$, given the magnetic field h . The field h is conjugate to the order parameter ϕ as a “natural variable” [15]. Another derivative of A is the entropy $S = -(\frac{\partial A}{\partial T})_h$.

Importantly, in many models there exists a collective variable, the mean value of which is known to be connected with the order parameter [17]. We would like to compare at this stage the representation (12) with (11), where it is easily seen that

$$\phi^i = -\frac{\partial A}{\partial \theta^i} = \frac{1}{\beta} \frac{\partial \psi}{\partial \theta^i} = -k_B T \langle X_i \rangle, \quad (13)$$

for the collective variable X_i connected with the order parameter ϕ^i . That is, if an order parameter ϕ^i is representable as a negative derivative of thermodynamic potential over some thermodynamic variable θ^i , then there exists a collective variable X_i such that Eq. (13) holds.

B. Fisher information

Revisiting the expression (9) for free entropy, we note [4] that its second derivative yields the following expression:

$$-\frac{\partial \langle X_i \rangle}{\partial \theta^j} = \frac{\partial^2 \psi}{\partial \theta^i \partial \theta^j} = g_{ij}, \quad (14)$$

where g_{ij} is the thermodynamic metric tensor. It was pointed out in different studies [1–4] that the thermodynamic metric tensor g_{ij} is identical to the Fisher information matrix,

$$g_{ij}(\theta) = F_{ij}(\theta), \quad (15)$$

where

$$F_{ij}(\theta) = \sum_x p(x) \frac{\partial \ln p(x)}{\partial \theta^i} \frac{\partial \ln p(x)}{\partial \theta^j}. \quad (16)$$

The Fisher information is a measure for the amount of information that an observed random variable provides about an unknown parameter. Fisher information and the Fisher information matrix are well known in statistical estimation theory, and are briefly described in Appendix A.

Appendix B provides additional details needed to establish the equivalence (15). Importantly, as shown in Appendix B, in deriving the equivalence (15) we *do not use* the second form of Fisher information:

$$F_{ij}(\theta) = -\sum_x p(x) \frac{\partial^2 \ln p(x)}{\partial \theta^i \partial \theta^j}, \quad (17)$$

which requires certain regularity conditions to hold [18].

The equivalence (15), together with Eq. (14), leads to the following relationship:

$$-\frac{\partial \langle X_i \rangle}{\partial \theta^j} = F_{ij}(\theta), \quad (18)$$

which will prove to be very useful in relating Fisher information to order parameters in the next section.

IV. PHASE TRANSITIONS AND FISHER INFORMATION

Let us recall that for the collective variable X_i connected with the order parameter ϕ^i , we have the relationship

$$\phi^i = -k_B T \langle X_i \rangle. \quad (19)$$

Taking a derivative over some thermodynamic variable θ^j , assuming conditions for Eq. (13), and using the equivalence (18) produces the representation

$$\frac{\partial \phi^i}{\partial \theta^j} = -k_B T \frac{\partial \langle X_i \rangle}{\partial \theta^j} = k_B T \frac{\partial^2 \psi}{\partial \theta^i \partial \theta^j} = k_B T F_{ij}(\theta). \quad (20)$$

Alternatively, we may use

$$F_{ij}(\theta) = \beta \frac{\partial \phi^i}{\partial \theta^j}. \quad (21)$$

In other words, Fisher information is immediately related to the rate of change in the corresponding order parameter(s), and thus can be used in studying phase transitions—especially the second-order phase transitions where the order parameters change continuously and their derivatives are well defined. For example, one may consider diagonal elements

$$F_{ii}(\theta) = \beta \frac{\partial \phi^i}{\partial \theta^i}. \quad (22)$$

Specifically, during a second-order phase transition, the order parameter changes continuously when an independent variable is varied, disappearing at the critical point, while Fisher information exhibits divergence.

A. An example: Ferromagnetic magnetization

Let us consider a simple example of ferromagnetic magnetization. It is well known that during a second-order phase transition, the order parameter (magnetization M) changes continuously when an independent variable T is varied, and disappears at the critical point T_c according to $M = \phi \propto (1 - T/T_c)^b$, where b is the well-known critical exponent. The derivative of the order parameter over the variable h (i.e., $i = 1$) is equal to the negative second derivative of the thermodynamic potential,

$$k_B T F_{11}(h) = \left(\frac{\partial \phi}{\partial h} \right)_T = - \left(\frac{\partial^2 A}{\partial h^2} \right)_T, \quad (23)$$

and hence, for the case of ferromagnetic magnetization $M = -(\frac{\partial A}{\partial h})_T$, can be thought of as the susceptibility [15]

$$\chi_T = - \left(\frac{\partial^2 A}{\partial h^2} \right)_T \propto (1 - T/T_c)^{-\gamma}, \quad (24)$$

where γ is another well-known critical exponent. The susceptibility has a power law singularity diverging at the critical point T_c ,

$$k_B T F_{11}(h) = \chi_T \propto (1 - T/T_c)^{-\gamma}. \quad (25)$$

Noting that another derivative of A is the entropy $S = -(\frac{\partial A}{\partial T})_h$, we point out that entropy plays a somewhat dual role to the order parameter:

$$k_B T F_{22}(T) = \left(\frac{\partial S}{\partial T} \right)_h = - \left(\frac{\partial^2 A}{\partial T^2} \right)_h. \quad (26)$$

Expressing the specific heat C_h as

$$C_h = -T \left(\frac{\partial^2 A}{\partial T^2} \right)_h \propto (1 - T/T_c)^{-\alpha} \quad (27)$$

yields

$$k_B T^2 F_{22}(T) = C_h \propto (1 - T/T_c)^{-\alpha}. \quad (28)$$

This shows the divergence of the diagonal elements of the Fisher information matrix at the critical point in this example.

B. A more general case

The general relationship (derived in Appendix B)

$$F_{ij}(\theta) = \langle [X_i(x) - \langle X_i \rangle][X_j(x) - \langle X_j \rangle] \rangle \quad (29)$$

gives the covariance matrix between the collective variables X_i and X_j . Thus, the Fisher information F_{ij} can be seen to measure “the size of fluctuations about equilibrium” of the collective variables, X_i and X_j [19].

Using this general expression, one may consider a generic case of a d -dimensional Ising-type magnetic model with a probability density expressible in the form of Eq. (1) [2]. For this model, Brody and Rivier [2] have shown that the critical behavior of thermodynamic quantities can be analyzed in terms of the reduced temperature, $t = T/T_c - 1$, via scaling:

$$\begin{aligned} & \langle [X_1(x) - \langle X_1 \rangle]^n [X_2(x) - \langle X_2 \rangle]^m \rangle \\ & \sim \int d^d r (t^{1-\alpha})^n (t^b)^m \Lambda(r t^\nu), \end{aligned} \quad (30)$$

where α , b , and ν are critical exponents, Λ is some scaling function, r is the d -dimensional vector labeling the lattice sites, and $n + m$ is an even integer. Combining this formula with the expression (29) results in

$$F_{ij}(\theta) \sim |t|^{n(1-\alpha)+mb-d\nu}, \quad (31)$$

where $n = 2$ and $m = 0$ if $i = j = 1$; $n = 0$ and $m = 2$ if $i = j = 2$; and $n = m = 1$ if $i \neq j$. Assuming hyperscaling relations $d\nu = 2 - \alpha$ and $\gamma = d\nu - 2b$ that explicitly use the number of space dimensions d , one may obtain the general expression [2]

$$F_{ij}(\theta) \sim \begin{pmatrix} |t|^{-\alpha} & |t|^{b-1} \\ |t|^{b-1} & |t|^{-\gamma} \end{pmatrix}. \quad (32)$$

One may demonstrate divergence of certain elements of the Fisher information matrix at the critical point (where $T \rightarrow T_c$ and $t \rightarrow 0$) for specific cases of d and the corresponding values of critical exponents (e.g., for the three-dimensional Ising model, all matrix elements diverge).

C. Divergence of Fisher information at phase transitions

Thus, the simple relationship (20) not only establishes a clear connection between thermodynamic order parameters and the Fisher information matrix, but supports the argument that phase transitions can be systematically studied in information-theoretic terms. *In particular, rather than trying to determine an order parameter, one could compute appropriate Fisher information values.* The location of second-order phase transitions can be identified where the Fisher information values diverge. In finite-size computational studies, the divergence can be approximated by maximization of Fisher information [13,14]. Not only does this avoid the issue of identifying order parameters, but it also provides a natural interpretation of localizing the critical point where the observed variable is most sensitive to the control parameter(s) and/or thermodynamic variable(s) (an interpretation applicable in both infinite and finite systems). For first-order phase transitions, the Fisher information terms cannot be defined where the first derivative(s) of A are discontinuous, also indicating a possible transition.

As mentioned in Sec. I, several previous studies [1–4] reported that the Fisher information matrix provides a Riemannian metric (more precisely, the Fisher-Rao metric) for the manifold of thermodynamic states. In particular,

Janke *et al.* [1] noted that the Fisher information matrix can lead to an information-geometric complexity measure for a classification of phase transitions. For instance, it was suggested that the scalar curvature \mathfrak{R} of the thermodynamic metric tensor $g_{ij}(\theta) = F_{ij}(\theta)$ measures the complexity of the system. Specifically, a flat metric implies that the system is not interacting, while, conversely, the curvature diverges at (and only at) a phase transition point for physical ranges of the parameter values [1]. However, we believe that even the individual relationships like (21) can be useful in studying phase transitions. This will be exemplified in the next section.

V. RANDOM BOOLEAN NETWORKS

In this section, we revisit our earlier numerical study [13,14] of Fisher information through a second-order phase transition in random Boolean networks (RBNs), interpreting the results there in light of the above discussion on the fundamental link between Fisher information and such phase transitions.

A. Background

Random Boolean networks are a class of generic, discrete, dynamical network models. They were proposed as models of gene regulatory networks by Kauffman [5]. See also Gershenson [20] for another thorough introduction to RBNs.

An RBN consists of N nodes in a directed *network* structure. The network topology (i.e., the adjacency matrix) is determined at *random*, subject to whether the in-degree for each node is constant or stochastically determined given an average in-degree \bar{K} (giving a Poissonian distribution).

Each node in the network has a *Boolean* state value, which is updated in discrete time. For each node, the new state value is a deterministic Boolean function of the current state values of the nodes from which it has incoming links (i.e., its neighbors). When the network is initialized with a given topology, this Boolean update function is decided at *random* for each node, subject to a probability r of producing “1” outputs. Note that r is symmetric around 0.5: r close to 1 or 0 gives low activity and close to 0.5 gives high activity. In pure RBNs, the nodes here are heterogeneous agents: there is no spatial pattern to the network structure (indeed there is no inherent concept of locality), nor do the nodes have the same update functions. In classical RBNs (CRBNs), the nodes all update their states synchronously [21].

Interestingly, the variable r is sometimes called the magnetization bias. For example, Aldana *et al.* [22] note that the word magnetization comes from the possibility of identifying each element with an atomic spin (a very small magnet), and the analogy has been used in the seminal works of Derrida *et al.* [23,24].

RBNs are known to exhibit three distinct regimes of dynamics, depending on their parameters: ordered, chaotic, and critical. At relatively low connectivity (i.e., low degree K) or activity (i.e., r close to 0 or 1), the network is in an ordered phase, characterized by high stability of states to perturbations and strong convergence of similar macro states in state space. Alternatively, at relatively high connectivity and activity, the network is in a chaotic phase, characterized by low stability of states to perturbations and divergence of similar macro

states. In the critical regime (the *edge of chaos* [6]), there is percolation in nodes remaining static or updating their values, and uncertainty in the convergence or divergence of similar macro states.

The first description of a phase transition in RBNs in terms of an order parameter (in the thermodynamic limit as the network size $N \rightarrow \infty$) was provided by Derrida and Pomeau [25]. There are a number of ways to study the critical regime, and it has been shown that there is a second-order phase transition both with respect to activity r and average connectivity \bar{K} . For example, Luque *et al.* [26] contrasted different order parameters: (i) the normalized Hamming distance obtained by means of Derrida’s annealed approximation [25], (ii) Flyvbjerg order parameter defined via the asymptotic stable core [27], and some others, with (iii) the percent of 1’s in the Jacobian matrix that represents the Boolean derivative of the system, and observed that all these parameters undergo a continuous change in the vicinity of critical activity r .

Similarly, it can be shown that there is a second-order phase transition near critical average connectivity \bar{K} . For example, there is a continuous phase transition in terms of the frozen component, defined as the fraction of nodes that do not change their state along an attractor, as shown by Rohlf and Bornholdt [28].

To quantify the phase transitions in the r - \bar{K} phase space, we shall use the well-known state-based measure of sensitivity to initial conditions, or damage spreading—that is, the normalized Hamming distance.

Following Gershenson [29], we take a random initial state A of the network, invert the value of a single node to produce state B , then run both A and B for many time steps (enough to reach an attractor is most appropriate). We then use the normalized Hamming distance,

$$D(A, B) = \frac{1}{N} \sum_{i=1}^N |a_i - b_i|, \quad (33)$$

between A and B at their initial and final states to obtain a convergence or divergence parameter δ ,

$$\delta = D(A, B)_{t \rightarrow \infty} - D(A, B)_{t=0}. \quad (34)$$

[Note that $D(A, B)_{t=0} = 1/N$. Finding $\delta < 0$ implies the convergence of similar initial states, while $\delta > 0$ implies their divergence. In infinitely sized networks, for fixed r , the critical value of \bar{K} between the ordered and chaotic phases is [25]

$$K_c = \frac{1}{2r(1-r)}. \quad (35)$$

B. Experimental results

We aim to study Fisher information $F(r)$ in RBNs as a function of the magnetization bias, i.e., the probability r of each node producing an output of “1”. This would identify the peaks of $F(r)$ (for a given \bar{K}) with the critical point on the r - \bar{K} plane. Tracing these critical points allows us to build a phase diagram, contrasting it with such a diagram obtained by using a traditional approach, e.g., using Eq. (35). However, finite network size N is known to have an effect on the locations

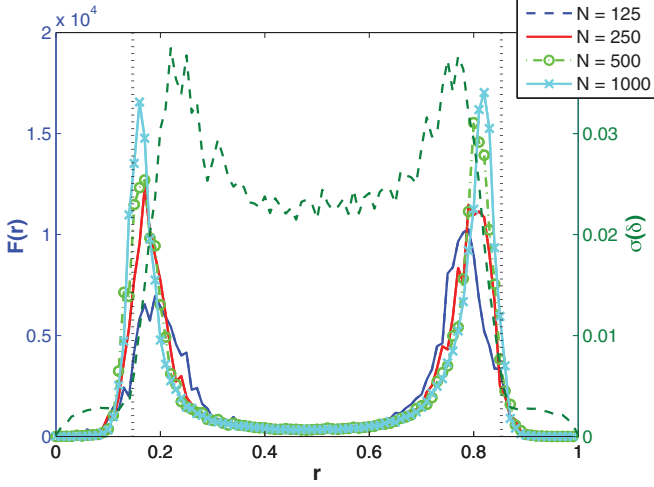


FIG. 1. (Color) Standard deviation σ_δ vs the bias of the network r , network size $N = 250$ (dashed line). Average Fisher information $F(r)$ vs the bias of the network r for different network sizes. Theoretical critical points are indicated by vertical dotted lines. Average connectivity $\bar{K} = 4.0$.

of the ordered and chaotic phases (moving the critical regime to more active r and higher K), and so theoretical values inferred by (35) for infinitely sized networks are not directly comparable to maxima of $F(r)$ in our finite-sized networks. As described in [14], maximal values of the standard deviation σ_δ of δ are more appropriate as a guide to the relative regions of dynamics in finite- N networks. We select σ_δ then as our baseline measure for finite- N networks, noting that it also serves as a proxy to the rate of change in the order parameter. Further details of computational experiments are described in Appendix C.

Figure 1 contrasts the Fisher information $F(r)$ with our baseline measure for studying the phase transition σ_δ . The dashed curve shows the standard deviation σ_δ as it changes over r , with $\bar{K} = 4.0$. We can see that there are two separate peaks in this curve, representing the edge of chaos for this finite-sized RBN. This is expected, since the probability distribution function is symmetrical about $r = 0.5$, when there is no bias between choosing 0 and 1. These two peaks occur at $r = 0.22$ and 0.77 , which as expected are “inside” the theoretical edge of chaos of an infinite-sized RBN at $r = 0.147$ and 0.853 yielded by Eq. (35) (shown as vertical dotted lines).

Figure 1 also shows Fisher information $F(r)$ for four different network sizes: $N = 125, 250, 500$, and 1000 , with $\bar{K} = 4.0$. $F(r)$ has two peaks almost mirrored about $r = 0.5$ for all the network sizes. These peaks are close to those of the baseline measure σ_δ for finite-sized networks, locating the phase transition between the chaotic phase and the ordered phase for the RBNs. The values of $F(r)$ for r that are away from the phase transition are at least one order of magnitude smaller than the peaks. Importantly, as the network size grows, the peaks of Fisher information approach theoretical critical points (for $N = 1000$, this occurs at $r = 0.16$ and 0.82). In addition, the peaks become sharper at the edge of chaos, as expected [30,31]. The peaks in Fisher information are close to those of the baseline measure σ_δ for finite-sized networks, though since our arguments in Sec. IV directly tie

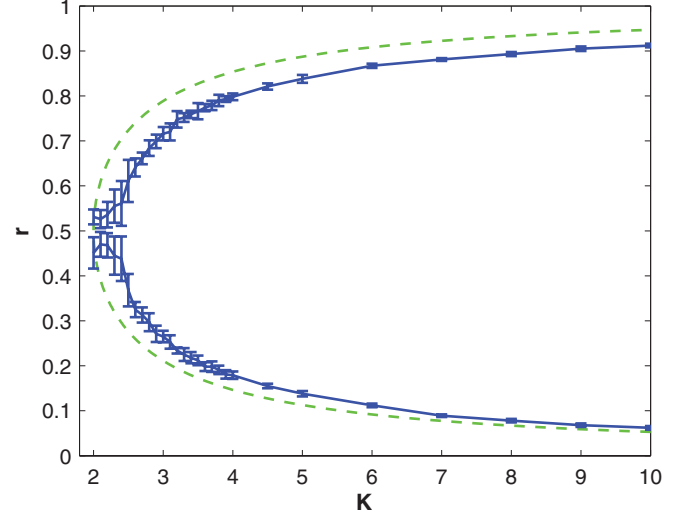


FIG. 2. (Color) Phase diagram tracing the maximum Fisher information $F(r)$, with respect to r , as a function of \bar{K} . The error bars on the curve show the standard deviation of r . The dashed line is the theoretical curve for critical K_c vs r .

the maximization of Fisher information to the location of the phase transition (while σ_δ is only a proxy to the rate of change in the order parameter), we suggest that the maximization of the Fisher information is a more appropriate measure to locate the critical points.

The peaks of Fisher information can be represented on the r - \bar{K} plane (see Appendix C for the details). The dashed curve in Fig. 2 shows the theoretical critical regime (edge of chaos) of the RBNs, generated using Eq. (35). It is evident that the phase diagram obtained by maximizing Fisher information generally follows the same shape, but is bounded by the theoretical curve as expected for finite-size RBNs (for finite-size networks, the critical point is known to shift toward the chaotic region—this is elaborated in Appendix C).

These experiments verify the general representation (20)–(22) introduced in this study, and confirm our conjecture that Fisher information may be used instead of the rate of change in the order parameter when one needs to determine the critical point(s). In particular, as argued in Sec. IV C, while the Fisher information diverges at a second-order phase transition, for finite-sized systems (where second derivatives of A only approximate divergence) the corresponding location of the critical point can be identified by maximization of the Fisher information instead. While being more computationally intensive in the case of RBNs, we have argued that maximization of the Fisher information is a more appropriate locator of the critical point than the baseline measure for finite-sized networks σ_δ . Importantly, it can also be applied to systems where the precise nature of the order parameter is unclear.

VI. CONCLUSION AND DISCUSSION

In this paper, we approached the study of phase transitions and order parameters via Fisher information. First of all, we pointed out that if an order parameter ϕ^i is representable as a negative derivative of thermodynamic potential over some thermodynamic variable θ^i , then there exists a collective

variable X_i such that Eq. (13) holds. We then examined the known relationship between the Fisher information and the derivatives of (the expectation value of) these collective variables X_i in (15) and therefore the second derivative of the free entropy, demonstrating that the relationship holds even without the regularity conditions for the second form of the Fisher information. This led to a set of general representations (20)–(22) immediately relating Fisher information to the rate of change in the corresponding order parameter(s). That is, thermodynamic variables were related to statistical estimation theory and information theory in a fairly general setting.

These relationships can be used in practical studies of phase transitions, especially the second-order phase transitions where the order parameters change continuously and their derivatives are well defined. Specifically, during a second-order phase transition, the order parameter changes continuously when an independent variable is varied, disappearing at the critical point, while Fisher information exhibits divergence. While several information-geometric studies [1–4] have recently pointed out that the Fisher information matrix provides a Riemannian metric for the manifold of thermodynamic states, and thus can be used as a complexity measure for a classification of phase transitions, our contribution is in explicitly relating Fisher information to the rate of change in the corresponding order parameter(s).

As pointed out by Crooks, Fisher information may provide a more general and fundamental definition of a metric than the thermodynamic definition, “just as the statistical definition of entropy is widely considered more general and fundamental than the original thermodynamic definition:” in particular, the characterization via the Fisher information matrix naturally extends to the situation where the system is not in thermal equilibrium [4]. In addition, Fisher information provides a natural interpretation of critical points applicable in both infinite and finite-size systems. That is, critical points are localized where the observed variable is most sensitive to the control parameter and/or thermodynamic variable, diverging in infinite systems and maximized in finite-size systems (where it is often easier to detect the corresponding maxima of Fisher information than the fluctuations of the order parameter).

The reported relationships were illustrated in random Boolean networks—a well-known class of generic, discrete, dynamical network models that exhibit three distinct regimes of dynamics (ordered, chaotic, and critical), depending on their parameters, such as average connectivity \bar{K} and magnetization bias r . We used a well-accepted baseline measure of phase transitions in RBNs: the sensitivity to initial conditions, or damage spreading (i.e., the normalized Hamming distance) δ . This is a proxy to an order parameter, and the standard deviation σ_δ of δ served as a proxy to the rate of change in the order parameter.

Following earlier studies [13,14], we observed that Fisher information about the magnetization bias r has maxima at the critical (r, K) points (in finite-size systems), and these maxima increase with the network size. This is because $F(r)$ measures (locally) the amount of information that RBN dynamics carry about the parameter r , and these dynamics are most sensitive to the parameter near the critical point. These observations experimentally demonstrated that Fisher information can be used to information-theoretically locate the critical points

in RBN dynamics. Moreover, the results presented here reveal the basic thermodynamic reasons behind the empirical observations reported in [13,14], which related the square of the first derivative of Shannon information to Fisher information without uncovering an underlying representation like (26). In addition, Fisher information should be able to locate the critical points in the dynamics of Boolean networks with heterogeneous topologies also, e.g., with scale-free [32] or small-world topologies [33], though this remains to be verified in future work.

In examining *average* computational properties as a function of system (e.g., network) parameters, we emphasize that there is in general a very large range of system realizations and consequently of behaviors possible for each parameter set. The local information dynamics of computation will provide much more detailed insights *for a given network* (as for Cellular Automata in [34–38]) than the averages over configurational elements (e.g., nodes, networks, and network sets discussed here). That being said, these averages can provide important insights into the computational properties as a function of system parameters, only if we remember that the average results are akin to likelihoods rather than certainties, albeit likelihoods that are much stronger in the limit of infinite system size. In parallel, tracing *local* profiles of Fisher information within a system (e.g., highlighting different levels of Fisher information for individual nodes of an RBN) may provide, in the future, another tool for studies of critical phenomena.

In summary, we suggest that in many studies the critical point(s) of second-order phase transitions can be determined by divergence of the Fisher information (or its maximization in finite-sized systems), instead of tracing the rate of change in the order parameter. While computation of Fisher information may often be more intensive, it is more appropriate and much more naturally interpretable than other measures that are only proxies to the order parameter (e.g., σ_δ for RBNs). Crucially, Fisher information is a generic measure that requires only appropriately defined probability measures and therefore can be applied to a broad range of systems, particularly those where the precise nature of the order parameter is unclear or its computation is cumbersome.

APPENDIX A: FISHER INFORMATION

Fisher information [39] is a measure of the amount of information that an observable random variable \mathcal{X} has about an unknown parameter θ , upon which the likelihood function of θ depends. Let $p(x|\theta)$ be the likelihood function of θ given the observations x . Then, Fisher information can be written as

$$\begin{aligned} F(\theta) &= E \left\{ \left[\frac{\partial}{\partial \theta} \ln p(x|\theta) \right]^2 \middle| \theta \right\} \\ &= \int_x \left\{ \frac{\partial \ln[p(x|\theta)]}{\partial \theta} \right\}^2 p(x|\theta) dx, \end{aligned} \quad (\text{A1})$$

where $E\{\dots|\theta\}$ denotes the conditional expectation over values for $x \in \mathcal{X}$ with respect to the probability function $p(x|\theta)$, given θ . Thus, Fisher information is not a function of a particular observation, since the random variable \mathcal{X} has been averaged out.

Fisher information can be represented as

$$F(\theta) = -E \left[\frac{\partial^2}{\partial \theta^2} \ln p(x|\theta) \middle| \theta \right] \\ = - \int_x \left\{ \frac{\partial^2 \ln[p(x|\theta)]}{\partial \theta^2} \right\} p(x|\theta) dx, \quad (\text{A2})$$

if $\ln[p(x|\theta)]$ is twice differentiable with respect to θ and some other regularity conditions hold [18].

The discrete form of Fisher information is

$$F(\theta) = \sum_x p_x \left[\frac{\Delta \ln(p_x)}{\Delta \theta} \right]^2, \quad (\text{A3})$$

where $\Delta \ln(p_x) = \ln(p'_x) - \ln(p_x)$ and $p_x = p(x|\theta)$, $p'_x = p(x|\theta + \Delta\theta)$. In this case, $p(x)$ is a discrete probability distribution function, such that $x \in \{x_1, \dots, x_D\}$, where D is the number of states for the variable \mathcal{X} .

Similarly, the $n \times n$ Fisher information matrix is defined for several parameters, $\theta = [\theta_1, \theta_2, \dots, \theta_n]^T$, as follows:

$$F_{ij}(\theta) = E \left\{ \left[\frac{\partial}{\partial \theta_i} \ln p(x|\theta) \right] \left[\frac{\partial}{\partial \theta_j} \ln p(x|\theta) \right] \middle| \theta \right\}. \quad (\text{A4})$$

Again, under some regularity conditions,

$$F_{ij}(\theta) = -E \left[\frac{\partial^2}{\partial \theta_i \partial \theta_j} \ln p(x|\theta) \middle| \theta \right]. \quad (\text{A5})$$

APPENDIX B: EQUIVALENCE OF FISHER INFORMATION AND SECOND DERIVATIVE OF FREE ENTROPY

Here, we will explicitly demonstrate the equivalence $g_{ij}(\theta) = F_{ij}(\theta)$ from (15). First, following [4,19], we show that the Fisher information takes the form of a covariance expression. Starting from

$$F_{ij}(\theta) = \sum_x p(x) \frac{\partial \ln p(x)}{\partial \theta^i} \frac{\partial \ln p(x)}{\partial \theta^j}, \quad (\text{B1})$$

we have, by definition of the configurational probability distribution (1),

$$\ln p(x) = - \sum_i \theta^i X_i(x) - \psi, \quad (\text{B2})$$

$$\frac{\partial \ln p(x)}{\partial \theta^i} = -X_i(x) - \frac{\partial \psi}{\partial \theta^i} = -[X_i(x) - \langle X_i \rangle], \quad (\text{B3})$$

where the last step uses the first derivatives of ψ (11). Substituting the second line of (B3) into (B1) gives

$$F_{ij}(\theta) = \sum_x p(x) [X_i(x) - \langle X_i \rangle] [X_j(x) - \langle X_j \rangle] \\ = \langle [X_i(x) - \langle X_i \rangle] [X_j(x) - \langle X_j \rangle] \rangle. \quad (\text{B4})$$

The resulting expression gives the covariance matrix between the X_i and X_j . Though they are related, we must carefully note that these X_i and X_j are different variables than those directly considered by the Fisher information (which studies the information contained in the observations x about the thermodynamic variables θ).

Turning our attention to the second line of (B3) once more, and using $\frac{\partial p(x)}{\partial \theta^j} = p(x) \frac{\partial \ln p(x)}{\partial \theta^j}$, we obtain a useful expression [40] for any j :

$$\frac{\partial p(x)}{\partial \theta^j} = p(x) [\langle X_j \rangle - X_j(x)]. \quad (\text{B5})$$

Second, we demonstrate that $g_{ij}(\theta)$ also takes the covariance form of (B4) (which is stated but not proven in [4]). We have

$$g_{ij}(\theta) = \frac{\partial^2 \psi}{\partial \theta^i \partial \theta^j} = - \frac{\partial \langle X_i \rangle}{\partial \theta^j} = - \sum_x \frac{\partial [p(x) X_i(x)]}{\partial \theta^j} \\ = - \sum_x p(x) [\langle X_j \rangle - X_j(x)] X_i(x), \quad (\text{B6})$$

where the last step uses $\frac{\partial X_i}{\partial \theta^j} = 0$ and the expression (B5).

Now, by definition of $\langle X_j \rangle$,

$$\sum_x p(x) [X_j(x) - \langle X_j \rangle] \langle X_i \rangle \\ = \langle X_i \rangle \sum_x p(x) [X_j(x) - \langle X_j \rangle] = 0, \quad (\text{B7})$$

and hence we can include an $\langle X_i \rangle$ term in (B6) [i.e., effectively adding (B7) to the right-hand side of (B6)] to construct the *symmetric* covariance expression

$$g_{ij}(\theta) = \frac{\partial^2 \psi}{\partial \theta^i \partial \theta^j} \\ = \sum_x p(x) [X_i(x) - \langle X_i \rangle] [X_j(x) - \langle X_j \rangle] = F_{ij}(\theta), \quad (\text{B8})$$

where the last step uses the first line of expression (B4). This proves the required equivalence (15), as well as (18).

This demonstration of the equivalence (15) is an important one because *we have not used* the second form of the Fisher information from (A2), which requires certain regularity conditions to hold [18].

The equivalences can be demonstrated using this second form (and therefore assuming regularity conditions as done, for example, in [1,2]), and indeed this is a faster demonstration. The second form of the Fisher information for the discrete case is given by

$$F_{ij}(\theta) = - \sum_x p(x) \frac{\partial^2 \ln p(x)}{\partial \theta^i \partial \theta^j}. \quad (\text{B9})$$

We use now the first line of equation (B3), taking the partial derivative of the first line of (B3) with respect to the thermodynamic variable θ^j , and obtaining the second derivative of $\ln p(x)$,

$$\frac{\partial^2 \ln p(x)}{\partial \theta^i \partial \theta^j} = \frac{\partial [-X_i(x) - \frac{\partial \psi}{\partial \theta^i}]}{\partial \theta^j} = - \frac{\partial^2 \psi}{\partial \theta^i \partial \theta^j}. \quad (\text{B10})$$

The right-hand side does not depend on x , and so averaging over $p(x)$ yields

$$F_{ij}(\theta) = - \sum_x p(x) \frac{\partial^2 \ln p(x)}{\partial \theta^i \partial \theta^j} = \frac{\partial^2 \psi}{\partial \theta^i \partial \theta^j}, \quad (\text{B11})$$

establishing the equivalence (15).

APPENDIX C: EXPERIMENTAL DETAILS OF RBN EXPERIMENTS

We model the RBNs using enhancements to Gershenson's RBNLAB software [41]. For each simulation from an initial randomized state of an RBN, we ignore a short initial transient of 30 steps, then observe another 400 time steps (similar to the approach in [42]). The experiments are repeated 10 times with 250 different networks.

We calculate $p(x^k|r)$ of each node k in a given RBN over multiple runs with different initial conditions of a specific RBN. Due to computational constraints, we calculate the average Fisher information of the individual nodes,

$$F(r)_{\text{RBN}} \triangleq \langle F^k(r) \rangle, \quad (\text{C1})$$

where $F^k(r)$ is the Fisher information of the k th node of the RBN computed according to (A3). This is repeated then for multiple networks with the same r (and the same

\bar{K}), producing the average Fisher information for the value r , $F(r) = \langle F(r)_{\text{RBN}} \rangle$. Each $F(r)$ is an average of Fisher information $F(r)_{\text{RBN}}$ over 250 networks and 10 runs [14].

The phase diagram is obtained by plotting r_{max} (i.e., the value of r attaining the maximum Fisher information) for different \bar{K} . Formally, r_{max} for every \bar{K} is set to locations of the global maxima of $F(r)$ in two regions: $0 \leq r \leq 0.5$ and $0.5 \leq r \leq 1$. For example, r_{max} correspond to the peaks shown in Fig. 1.

The finite-size nature of the simulated networks is the reason why the loci of the divergent maxima of Fisher information do not meet as $K \rightarrow 2$ (Fig. 2). For $r = 0.5$, the phase transition with respect to K shifts toward the chaotic regime at around $K \approx 2.5$ in these finite-size RBNs, rather than the theoretical $K = 2.0$. Our experimental curve should converge or diverge at around $K \approx 2.5$. The fact that it does not converge is an artifact of our explicit search for two maximum values of $F(r)$ for $0 \leq r \leq 0.5$ and $0.5 \leq r \leq 1$.

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