A graph-theoretic approach to understanding emergent behavior in physical systems

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Abstract

The exact dynamics of emergence remains one of the most prominent outstanding questions for the field of complexity science. I first discuss various perspectives on emergence, then offer a perspective on understanding emergence in a graph-theoretic representation. To test this, I analyze the dynamics of all possible spatial state spaces near the critical temperature in a 2-D Ising model. The size of different state spaces constrains a system's ability to explore various states within a finite time frame. In addition, the distribution of topological "determinism" for these state spaces remains constant for any particular temperature. At the critical temperature, this distribution is nearly linear, which is distinct from other temperatures. This approach may provide a path forward in building a mathematical framework that captures the dynamics of emergent phenomena. This is key to understanding emergence in biological systems, which are layered with various state spaces and observational perspectives.

What are the exact mechanisms of emergent phenomena and how can we predict when they will happen in a system? For the field of complex systems, this remains one of the most prominent outstanding questions. Emergence is at the heart of the evolution of species, resurgence of pandemics, the development of human technologies, and our impact on climate change, just to name a few.

The exact definition of emergence differs in a variety of ways from one field to another, but most rely on describing a single system in terms of microstates (a smaller, fine-grained description) and macrostates (where emergent behavior occurs on a larger scale). Deutsch (2013) define emergence as "certain sets of collective phenomena can be explained in terms of emergent laws relating them only to each other, without reference to the underlying particles and laws." Bedau (1997) distinguishes emergence as weak and strong forms. Weak emergence can be found in a macrostate that can be derived from internal dynamics and known external conditions only via simulation. By contrast, strong emergence cannot be predicted using this same information.

What defines a microstate or a macrostate (or any other state space) depends on what aspects of a system an observer is able to enumerate (Longo and Montévil (2013)). Any system can be described in multiple state spaces, depending on the observer and what sorts of variables an observer can access. Transitions between states are determined by the rules of the dynamics in that system. If states are nodes and transitions between them are directed edges, the connectivity of a state space is determined by the dynamical rules that evolve a system over time (Adams et al. (2017)). Depending on these rules and the choice in state space, it may be possible to move from one state to any other state.

To be able to make reliable predictions about emergent phenomenon such as biological evolution, we would need to better understand the relationship between randomness, determinism, and our choice of description (our chosen state space) in a system that employs randomness (at least on a microstate level). This paper tests some of these ideas in a small computational experiment of a 2-dimensional Ising model. The 2-D Ising model is one of the best-known examples of a phase transition that emerges as a result of pseudo-random transitions between microstates at a particular temperature.

Materials & Methods

As an exploratory first step, only the results of a 3x3 classic 2-D Ising model are shown. In this model, each cell can be a 1 or a -1. At each time step, each cell can "flip" depending on the configuration of its neighbors and external factors such as temperature and a magnetic field[1]. For this experiment, the magnetic field remained constant and varying the temperature confirmed the model behaved as expected, with a phase transition occurring at the expected critical temperature ($T = 2.27$). Monte Carlo simulations of this Ising model ran for 1000 time steps at several temperatures between the values of 0 and 5. The model was simulated 100 different times for each temperature to get a statistical average of results.

All possible spatial state spaces were considered for this analysis. Since a 3x3 Ising model has 9 cells, there are 512 possible state spaces. The topology of each state space was discovered by representing the states as nodes and directed edges as transitions between the states. Each state within a

[1]See Onsager (1944) for more details

state space is a particular configuration of 1's and -1's. For any state space, there are A^N possible states, where A is the number of possible spins and N is the size (number of cells) of the state space.

In a state space that is completely deterministic, the transitions between different states are not probabilistic. The "amount of determinism" (here, called the **deterministic fraction**) in a state space topology can be estimated by counting the fraction of nodes with more than one out-degree to the total number of nodes (states) in the state space:

$$\text{deterministic fraction} = \frac{\text{\# nodes with out degree} > 1}{\text{\# nodes}} \quad (1)$$

A state space topology that is completely random will have all nodes with an out-degree higher than 1. In contrast, a completely deterministic topology will only have nodes with an out-degree of 1 (or 0 if it an absorbing state). Since each state space topology is inferred from the state trajectory within that state space, it is possible to count the number of times an existing directed out-edge "switches" directions and points to a different node than it did previously. Since all edges are directed in these graphs (not counting multi-edges in the same direction and self-loops), it is possible to track how many edges switch direction in a single step of the Ising model simulation. The number of "edge switche" in a single step is called the number of **determinism bit flips**.

Results & Discussion

From Figure 1, the average number of out-edge switches (pointing to one state node in one time step to a second state node in a future time step) does *not* scale linearly with respect to the size of the state space. State spaces that are 5 or 6 cells large switch their outgoing edges much more often than any of the other state space sizes, including the largest state space (9x9) of the model.

In biology, systems that operate in relatively larger state spaces may not have sufficient time to explore all possible states and evolve regardless of the fraction of states left unexplored. These results are reminiscent of nested state spaces in biological systems. Smaller state spaces have the potential to explore all possible states and their transitions more thoroughly than larger ones. This relationship between state space size and the finite time to explore possible states could be a driving factor in the evolution of open-ended systems, particularly in irreversible "ratcheting mechanisms". As new state spaces are discovered and employed by evolutionary mechanisms, the size of the state space seems to have a relationship with the amount of "determinism" within that state space.

But regardless of the state space size, the distribution of the deterministic fraction over all state space topologies in Figure 2 remains almost exactly the same over multiple simulations. The distribution only changes as a function of temperature, with lower temperatures resulting in more deterministic topologies. This distribution is nearly linear around the critical temperature and curved at higher and lower temperatures, suggesting the phase transition can be understood in terms of the structure of all possible state space topologies. Together, these results suggest a similar analysis can be done for other systems capable of phase transitions. This approach may provide a path forward in building a mathematical framework that captures the dynamics of emergent phenomena.

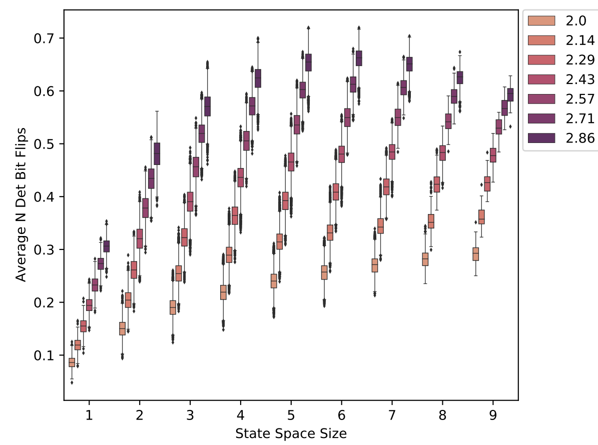

Figure 1: Average number of determinism bit flips at various temperatures over all possible state spaces. Results are grouped according to the size of the state space.

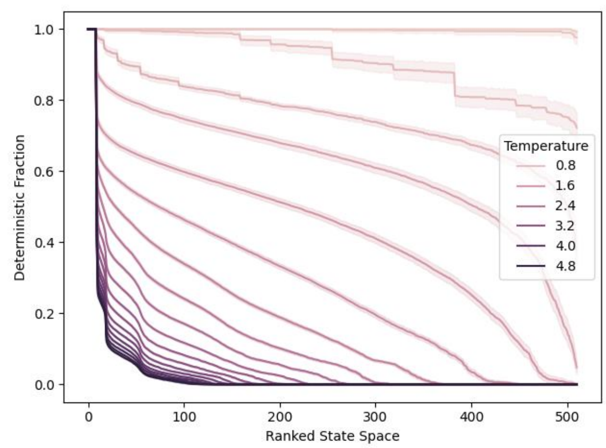

Figure 2: Rank-order distribution of the deterministic fraction of all state spaces for various temperatures. The size of the individual state spaces is not denoted and the ordering of state spaces is not preserved across the 100 simulations. Error bars showing a 95% confidence interval are shaded. The critical temperature for this Ising model is 2.27.

References

Adams, A. M., Berner, A., Davies, P. C. W., and Walker, S. I. (2017). Physical universality, state-dependent dynamical laws and open-ended novelty. *Entropy*, 19(9).

Bedau, M. A. (1997). Weak emergence. *Noûs*, 31(s11):375–399.

Deutsch, D. (2013). Constructor theory. *Synthese*, 190(18):4331–4359.

Longo, G. and Montévil, M. (2013). Extended criticality, phase spaces and enablement in biology. *Chaos, Solitons & Fractals*, 55:64–79. Emergent Critical Brain Dynamics.

Onsager, L. (1944). Crystal statistics. i. a two-dimensional model with an order-disorder transition. *Phys. Rev.*, 65:117–149.