Emergent Phenomena Practical

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For those who want a worked example of emergent phenomena, we will take as our case study "variations on a theme" – the theme being classic models of collective phenomena, including the Ising model, the XY model, and so forth.

This is not a simple practical; it is open-ended, and you are strongly encouraged to work in groups.

I. GOALS

You will have done well if you can answer the **test your knowledge** questions, understand the mean field solution (Sec. IV) and the **bonus** questions provoke good discussion among your group.

You will have done very well if you can get some code working to examine phase transitions and topological defects in a known system (Ising, XY.)

You will have made a start on a very interesting scientific paper if you have constructed models using internal state structures, and interaction graphs, that reflect a biological, social, or computational system you or your group-mates have familiarity with – particularly if you can explore its defect structures in the event of a phase transition.

II. PREAMBLE

We will define things abstractly in terms of "systems," "components," "interactions," "states," and so forth. However, you may find it helpful to keep a model system in mind – particularly one from your home discipline.

For example, the Ising model has been influential in neuroscience, where the components are neurons, and the states are "on or off." [1] The interactions are effective connections between neurons that tend to correlate the states – neurons switching each other on and off – see, *e.g.*, [2, 3]

Other cases might suggest themselves. In the XY model, for example, states are two-dimensional unit vectors. This might suggest a model where people at different points are moving in different directions, or – just as easily – where an object is held in different fixed orientations at different points.

In a variation you might invent, the vector might be confined to the upper-right quadrant (*i.e.*, all values positive), and have its components sum to unity (as opposed to having the sum of the square normalize to unity.) These states then become like probabilities over two choices, and might be useful when modeling mixed strategies in a game. The interactions could be payoff matrices.

Test your knowledge. Suggest a social or biological system where the internal structure of a component might be a two dimensional vector with unrestricted length.

Consider also the structure of the environment. Physicists like to work in two, three, or four dimensions, in Euclidean, Riemannian, or pseudo-Riemannian space. Biological and social systems might show greater amounts of inhomogeneity (*e.g.*, ecological or national boundaries, where things are odd), their spatial arrangement may be distorted or supplemented by long links, or the system may be not really spatial at all (*e.g.*, they might take place on a clustered, random, facebook or small-world network instead of a lattice.)

Test your knowledge. What network might describe the Ising model at a cocktail party, where guests are perfectly mingling?

Bonus. If you are an evolutionary biologist, what network structures might be more or less amenable to the emergence of cooperation and group selection?

It is suggested you work through the Ising model case first, and then to come back and see how you can adapt more elaborate internal states, network structures and so forth. There is an absolutely enormous amount of literature on these problems, and you should feel free to use the internet to your advantage.

III. GROUND RULES

A. Internal States

Our system is a set of nodes, $\{\sigma_i\}$, i from 1 to N. They have internal structure – in particular, σ_i can take on different values. In the Ising model, σ_i can be either +1 or -1. For historical reasons, this parameter is called **spin**, and sometimes the +1 state is called "spin up", and the -1 state, "spin down."

In the XY model, σ_i is a unit vector (*i.e.*, to be pedantic it might be written $\vec{\sigma}_i$.) The σ_i need not be obviously mathematical structures – *e.g.*, they might be

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drawn from the set {$\texttt{red}, \texttt{black}, \texttt{yellow}$}.

B. Interactions between States

We define an interaction function $H(\{\sigma_i\})$. As you can see, it takes the *entire* system as an input, and gives one output – a number, which I may slip up and call "energy" but which can have many analogies. Systems prefer to be in low-energy states, but the amount of disorder in the system (characterized here by a "temperature") may prevent them from doing so.

The (ferromagnetic) Ising model defines H in the following way:

$$H(\{\sigma_i\}) = -\sum_{i,j} J_{ij}\sigma_i\sigma_j \tag{1}$$

where J_{ij} is a matrix that defines the graph of interactions.

Test your knowledge. In words, what configurations (choices for the values of the nodes) give you lower energy? What give you higher energy?

Test your knowledge. Take N to be three, and have all the nodes connected to each other. Write down the matrix J_{ij}. What is the energy of such a system when σ_1, σ_2 and σ_3 are all $+1$? What about when they are all -1? What is the symmetry of this interaction? How could you alter H to break it?

Bonus. A state space with $+1$ and -1 can at best have an H symmetric on switching sign. Pick a state space that is more interesting than $\{+1, -1\}$. How about one that can have more interesting symmetries? How about a system with n states – now it can be symmetric under the $n!$ permutations?

Bonus. Take n to be three, and write an H that breaks permutation symmetry on {$\texttt{red}, \texttt{black}, \texttt{yellow}$}. Can you find an H that breaks permutation symmetry to a smaller symmetry group – say, to a permutation on only two elements? Can you think of a friend who has this reduced symmetry?

Bonus. Read up on the groups S_n (all permutations on n elements) and A_n (the alternating group on n elements.) Take n to be four, and write an H that breaks S_4 to A_4. What happens if you try to do this in the $n = 3$ case? (S_3 to A_3.)

Bonus. How about a continuous state space, perhaps symmetric under $O(2)$, or $SU(3)$? Develop a model for the condensation of the primordial quark-gluon plasma into atomic nuclei [4].

C. Stationary Distributions

We first consider a stationary, probabilistic distribution over system configurations. In other words, I am going to tell you (how to calculate) the probability of finding the system in a state where the components take some value $\{\sigma_i\}$ (*e.g.*, in the $N = 3$ case above, you will be able to calculate $P(\{+1, +1, -1\})$.)

We will take a one-parameter family of distributions, the Boltzmann distribution, given by

$$P(\{\sigma_i\}) = \frac{\exp\left[-\beta H(\{\sigma_i\})\right]}{Z(\beta)}. \tag{2}$$

where β is the "inverse temperature" (when β is larger, $1/\beta = T$ is smaller, and the system is said to be colder.) $Z(\beta)$ is a constant, just to make sure that P is properly normalized (*i.e.*, so that when you sum over all possible configurations you get 1.) It is called the partition function, and has magical properties – see Fig. 1.

Test your knowledge. Given the $N = 3$ system above, what is $P(\{+1, +1, +1\})$ when β is 1, or 10, or 0.1? How does it compare to $P(\{+1, +1, -1\})$? What does this tell you about the relation between order and (inverse) temperature? You will need to boot up Mathematica, Maple, or some other software to do these computations.

Bonus. Recall the definition of entropy. How does the entropy, S, of the $N = 3$ system change as a function of β? How about the *heat capacity*, defined as $dS/d\beta$? Where is the maximum of the heat capacity? Can you see how to use $Z(\beta)$ to compute quantities like entropy?

Bonus. Read E.T. Jaynes' famous 1957 paper [5] to learn exactly how and why both information theoretic and physical considerations make the form of Eq. 2 is so special.

IV. MEAN-FIELD SOLUTIONS

Eq. 2 is hard to solve in general. Later we will try numerical simulation, but laying bare the qualitative structure of a problem is central to scientific goals of explanation and understanding.

In particular, we will work out an approximate solution to the Ising model, and we will demonstrate the existence of a catastrophic phase transition, where the system properties change dramatically. You can then try your hand at the equivalent approximation for other systems with different structures.

The approximation is called the *mean field solution*. Roughly speaking, it describes the dynamics of the system by considering a single individual, and asking how it interacts with the *average* properties of the system.

Let's start with the Ising model. Consider the contribution to the energy from a single (arbitrarily chosen) spin σ_a,

$$H_a = -\sigma_a \sum_i J_{ia}\sigma_i \tag{3}$$

Test your knowledge. Derive this from Eq. 1, or, conversely, convince yourself that H is $\sum_a H_a$.

The mean field approximation says that we can write

$$H_a = -n_c\sigma_a\bar{\sigma}, \tag{4}$$

FIG. 1. Thanks to the generosity of an anonymous donor, the Institute has its own partition function.

where $\bar{\sigma}$ is the average spin of the system (the "mean field" that the particle sees), and n_c, sometimes called the coordination number, is the number of neighbours of an "average" vertex.

Test your knowledge. What is n_c on a two-dimensional lattice (such as the lines on a Go board, or the street corners in uptown Manhattan.) What is n_c on a fully connected graph? What is n_c on the small world network?

Bonus. What is n_c on a network of particular interest to you?

Following the derivations above, we can now factor the monstrous Eq. 2,

$$P(\{\sigma_i\}) = \frac{\exp(-\beta \sum_a H_a)}{Z(\beta)} = \frac{1}{Z(\beta)} \prod_a \exp(-\beta H_a),$$

where $\prod$, just to remind you, means take the product. Now we can get the probability distribution for a single vertex, since the terms factor. For instance,

$$P(\sigma_a = +1) \propto \exp(\beta n_c \bar{\sigma}),$$

where we only have proportionality, $\propto$, because of the annoying factors of $Z(\beta)$. But we can ask what the average value of σ_a is:

$$\langle \sigma_a \rangle = P(\sigma_a = +1) - P(\sigma_a = -1),$$

and just making sure to normalize the probabilities, we find

$$\begin{aligned}\langle \sigma_a \rangle &= \frac{\exp(\beta n_c \bar{\sigma}) - \exp(-\beta n_c \bar{\sigma})}{\exp(\beta n_c \bar{\sigma}) + \exp(-\beta n_c \bar{\sigma})} \\ &= \tanh(\beta n_c \bar{\sigma})\end{aligned} \tag{5}$$

We now have an expression for the average value of an arbitrary node, $\langle \sigma_a \rangle$, as a function of (1) inverse temperature, β, (2) coordination number n_c, and (3) the average value of all the nodes in the system $\bar{\sigma}$. All that remains is to make things consistent!

In particular, we simply need to find the solutions of

$$\bar{\sigma} = \tanh(\beta n_c \bar{\sigma}), \tag{6}$$

as a function of n_c and β. The simplest way is to plot the left hand and right hand sides on a graph, and vary β to see where things intersect. The case $\bar{\sigma}$ equal to zero will always be a solution, but it may become unstable to small perturbations. In those cases, we have *spontaneously broken symmetry* – H is symmetric under sign flips, but the system finds a new solution which picks a particular sign.

Test your knowledge. Do this for n_c equal to two, three and four. How many solutions are there?

Test your knowledge. In cases where there is more than one solution, which are stable? Hint: displace the "incoming messages" by a small amount, and iterate.

You have now conducted a mean-field analysis of the phase transitions on the Ising model! In particular, the critical temperature, T_c, or $1/\beta_c$, is the point at which the old solution becomes unstable and new solutions, violating some of the symmetries of the interaction, appear.

How well does mean field analysis work? Having done the test your knowledge questions above, you should be familiar with how to go between n_c and lattice dimension. Table I shows the answers.

As you can see, as the dimension (or effective dimension, for a disordered network) goes up, the mean field approximation becomes better and better. When a par-

dimension	T_c (mean field)	T_c (true)	comments
1	2.0	0.0	Ising's dissertation
2	4.0	2.269...	Onsager's "tour de force"
3	6.0	4.510...	by simulation only
4	8.0	6.682...	approximation better...
5	10.0	10.0	mean field works!
$n > 4$	$2n$	$2n$	

TABLE I. Mean field predictions for the critical temperature, compared to true answer. In one and two dimensions, T_c ($= 1/\beta_c$), can be computed analytically – the latter case, however, only by great effort. In three and four dimensions, numerical solutions are necessary (numbers drawn from Ref. [6].) As the dimension of the space gets higher – nodes are connected to more and more other nodes – it is more and more reasonable to neglect fluctuations. Four is the "upper critical dimension" for the Ising model, and for dimensions five and higher, the mean field solution is perfect!

ticle interacts with larger numbers of other particles, it becomes better and better to think of that interaction as an interaction with an "average" member of the system. This is similar to how one reduces the variance on a measurement by averaging together many independent data points.

Conversely, mean field theory fails most drastically when there are few neighbours, and the neighbours themselves are strongly correlated – perhaps because they themselves are connected. Of course, many interesting systems have this property!

Bonus: multistate mean field. Allow σ_i to take on three values, $\{+1, 0, -1\}$. Keep the same interaction structure. What does the mean field solution give? When do unstable solutions appear? Is it easier or harder to get a phase transition? This is related, but not identical, to to the Potts model, introduced in Sec. VI below.

Bonus: XY mean field. Consider the case where σ_i is now a 2D unit vector. Take H to be

$$H(\{\sigma_i\}) = \sum J_{ij}(\sigma_{i,x}\sigma_{j,x} + \sigma_{i,y}\sigma_{j,y}), \tag{7}$$

where $\sigma_{i,x}$ is the x component of the σ_i vector, and so forth. Put differently, the interaction is the dot product between the vectors – you lower your energy by becoming *more* aligned with your neighbours.

Do a mean field analysis of the XY model.

Bonus. Given all of your thoughts on internal state structure (what the σ_i state space is), and the network properties (what the J_{ij} is), do a mean field analysis of your social or biological system.

V. DYNAMICS

Eq. 2 defines the stationary, or equilibrium, distribution of the system. But systems are often out of equilibrium, either because of the initial conditions of the Universe, or because you just dropped it.

We would like to define a (discrete time) dynamics on the system that is *consistent* with the stationary distribution. Another way to say this is "given a configuration A, what is the probability that it will change to configuration A, B, C, D..." at the next step. This is $P(A \to B)$, $P(A \to C)$, and so forth. If you start the system in a state that is rare given the value of β, it will be out of equilibrium, and the dynamics will take some time to drive you to where you are cycling through states in a way consistent with equilibrium. This is called "burn in" – but if you're interested in non-equilibrium phenomena, it's a good thing!

In any case, there will be many possible choices; in order to reach a stationary distribution consistent with Eq. 2, all we (really) need is for the processes to balance

$$\frac{P(A \to B)}{P(B \to A)} = \frac{P(B)}{P(A)}, \tag{8}$$

where $P(A \to B)$ is the probability that, given you are in configuration A, you transition to configuration B.

Only the ratio of switching is fixed. If you are simulating a Boltzmann distribution model for other purposes – for example, if you are doing statistical inference, have a Likelihood function, and are doing what is called Markov-Chain-Monte-Carlo (MCMC) – then you want to pick a dynamics that is super-easy to simulate. Such recipes are common, but may in some cases have unusual properties (*e.g.*, in some cases they may become completely deterministic, transition probability of unity.)

A nice, somewhat "physical," choice, by contrast, is **Glauber dynamics**, which reduces in various continuum and "soft-spin" limits to partial differential equations. It is given by:

$$P(A \to B) = \frac{\exp(-\beta H[B])}{\exp(-\beta H[B]) + \exp(-\beta H[A])}, \tag{9}$$

where $H[A]$ is the energy of configuration A.

Test your knowledge. Show that Eq. 9 is consistent with Eq. 8.

A simple procedure now suggests itself. Start in some configuration, A. Pick a vertex at random. Configuration B is defined to be the same as configuration A, except with that spin flipped. Switch to configuration B with probability given by Eq. 9, otherwise stay in state A. Repeat.

Test your knowledge. For this one spin-flip transition, can you simplify Eq. 9 so that you don't have to compute all of the sums over i and j implicit in $H[A]$ and $H[B]$?

Bonus. Write code to simulate the Ising model in two dimensions. Written well, you should be able to do a 32×32 grid in real time. Roughly, where is the critical point? You can measure this a number of different ways, but plotting average spin as a function of time is one simple way to see if the system is really finding a symmetry-breaking phase. Put in domain wall defects, and show how they evolve.

Bonus – Critical Slowdown. Come up with measures for system timescale. How do these behave near the critical point?

Bonus. Simulate the Ising model on a network close to your heart. How do domain wall defects behave? Where do domain walls, for example, stall out and stop propagating? What network properties are good for dissipating defects?

Bonus. Compare defect dynamics on the 2D model and your network. Given random initial conditions, are your networks more or less susceptible to formation of domain walls?

VI. ADVANCED TOPICS

Defects like domain walls are associated with the breaking of a symmetry. In the case of the Ising model, the energy is symmetric in flipping plus to minus; you investigated other kinds of symmetries in the bonus questions to Sec. III B.

The question of defects in the two-dimensional XY model is somewhat subtle, since there is not actually a true phase transition at any non-zero temperature. However, many online simulations exist to show you how two kinds of vortices arise, and how they compose and dissipate.

A much simpler case to implement and visualize is the Potts model, where you retain the discreteness of the state space, but allow a greater number of states. The n-state Potts model, in particular, can be given two different kinds of interactions. The first just says that states are only lower in energy if they are the same, *i.e.*,

$$H = -\sum J_{ij}\delta_{\sigma_i\sigma_j}, \tag{10}$$

where J_{ij} is the network structure, as before, and $\delta_{\sigma_i\sigma_j}$ is the Kronecker delta, or, more simply "one if $\sigma_i = \sigma_j$, zero otherwise."

The second more tricky one assigns each of the n states an angle between 0 and 2π, equally spaced (*e.g.*, when n is three, σ_i takes on values $\{0, 2\pi/3, 4\pi/3\}$. Then the interaction is given by

$$H = -\sum J_{ij}\cos(\sigma_i - \sigma_j) \tag{11}$$

Test your knowledge. Show how the two-state Potts model can be altered to look exactly like the Ising model. Do they have the same dynamics?

Test your knowledge. What are the symmetries of these two interaction structures? You may wish to consult some of the answers you came up with in the bonus sections of Sec. III B.

Bonus. Simulate the three-state Potts model under the two choices of interaction structure, Eq. 10 and Eq. 11. You will have to generalize the dynamical rules of the previous section only slightly: you might, for example, try a spin *shift* instead of a spin *flip* to get configuration B, or you might just pick a new value of the spin at random. What defects do you see? What dynamical properties do they have?

The classification of defects in symmetry breaking systems proceeds by something called homotopy theory. An informal introduction to these issues can be found in Chapter 9 of Ref. [7].

There are many directions one can go in. If the J_{ij} are taken to be randomly distributed, and possibly negative, one edges closer to spin glass models. These were considered, for many years, the most promising applications of physical reasoning to biological systems, and have become part of the standard lore.

Slightly different dynamics, *e.g.*, the voter model, lead to different defect dynamics – and in some cases, to the disappearance of a phase transition at all.

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[1] This kind of simplification is not for everyone. A friend writes in: "one of my friends from my postdoc days at Rutgers (trained in statistics for his Ph.D.) told me he was at a neuroscience lecture that was being given by a physicist. The lecturer was describing a mathematical object and said 'it can be ON or OFF, so you can think of it as a neuron or as a lightbulb.' A biologist in the audience muttered 'if this can be a neuron or a lightbulb, I'm not interested' and walked out.".

[2] E Schneidman, MJ Berry II, R Segev, and W Bialek, "Weak pairwise correlations imply strongly correlated network states in a neural population," Nature, **440**, 1007 (2006).

[3] William Bialek and Rama Ranganathan, "Rediscovering the power of pairwise interactions," arXiv, **q-bio.QM** (2007), 0712.4397v1.

[4] Just kidding!

[5] E. T Jaynes, "Information theory and statistical mechanics," Phys. Rev., **106**, 620 (1957).

[6] Peter Meyer, "Computational studies of pure and dilute spin models," MPhil Thesis (School of Mathematics and Computing, University of Derby), `http://www.hermetic.ch/compsci/thesis/contents.htm` (2000).

[7] James P. Sethna, "Order parameters, broken symmetry, and topology," in *1991 Lectures in Complex Systems*, Vol. XV, edited by L. Nagel and D. Stein (Santa Fe Institute Studies in the Sciences of Complexity, Proc. Vol. XV, Addison-Wesley, `http://pages.physics.cornell.edu/sethna/StatMech/EntropyOrderParametersComplexity.pdf`, 1992).