Beyond Pairwise:
Higher-Order Interactions in Complex Systems

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Inspiring Awe & Wonder

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I. Introduction

Complex systems are often defined as systems composed of large numbers of individual objects, agents, or parts, that interact in such a way that the global behavior of the collective is difficult to predict or understand from the behavior of the individuals. Such global behavior is often called "emergent." Classic examples include the emergence of cognition from neurons, the emergence of cities from people and their individual choices, or the emergence of life from a soup of chemicals. Some of the deepest, most urgent, and most important questions facing humanity today are about interconnected complex systems: food webs and ecosystems, cities and economies, poverty and systemic racism, diseases and pandemics, sustainability and global warming.

Complex systems are frequently modeled by their collections of pairwise interactions: connections between neurons, exchange of goods and services between individuals, or predator–prey relations between species. Modeling interactions in a pairwise manner frequently allows researchers to apply of the vast, powerful toolbox of linear algebra. As more and more large data sets became available over the last 25 years, this paradigm has been tremendously successful.

But the presence of irreducible higher-order interactions has long been recognized (e.g., Atkin 1972; Alexander 1920; Dür, Vidal and Cirac 2000): those interactions between three or more parties that cannot be explained by any collection of pairwise interactions. Examples include chemical catalysts, interactions between parents and a child, and innovations that use more than two technologies in simultaneous combination. By modeling three-way, four-way, and more general higher-order interactions, not only do our models become more realistic, but they raise questions (and sometimes provide answers!) that are obvious from the higher-order perspective, but can be invisible or obscured by taking only a pairwise perspective.

Applications of higher-order interactions have expanded dramatically in the past 20 years, and especially in the past decade, due to the increase in available data sets, and the concurrent increase in algorithmic methods and computational power. These include understanding drug interactions (Tekin, et al. 2018; Lozano-Huntelman, et al. 2021), individuality (Krakauer, et al. 2020) and collectivity (Daniels, et al. 2016), stability in ecology (Grilli, et al. 2017), contagions (Hébert-Dufresne, Mistry and Althouse 2020; St-Onge, Thibeault, et al. 2021; St-Onge, Iacopini, et al. 2021), distributed computing (Herlihy, Kozlov and Rajsbaum 2014), and neuroscience (Giusti, Ghrist and Bassett 2016; Curto and Itskov 2008; Ellis and Klein 2014), to name just a few.

Our goal in this chapter is decidedly not to survey all the applications and advances in higher-order interactions. Three recent surveys—a "how-to" guide for researchers (Torres, et al. 2020), a survey focusing on higher-order dynamics, especially from the physics viewpoint (Battiston, et al. 2020), and a survey from the mathematical perspective (Bick, et al. 2021)—cite in total more than 1,300 papers. The field is growing so rapidly that surely even these recent surveys together are not exhaustive.

Our goal is rather to give some history, connections, and a bit of a broader perspective, and to

highlight a few recent examples that fit into this story. Although we do spend quite some time discussing hypergraphs and simplicial complexes—two of the most common higher-order generalizations of networks, surveyed in (Bick, et al. 2021; Battiston, et al. 2020; Bick, et al. 2021)—part of our goal is to make clear the connections between myriad different kinds of higher-order interactions, far beyond generalized networks. In addition to higher-order topological generalization of networks, we draw connections between higher-order interactions in information theory, computational complexity, thermodynamics, polynomial equations (algebraic geometry), and dynamics, with a view toward understanding complex systems in general.

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II. Complex Systems

All simple systems are alike in the few possible ways of being simple,
but every complex system is complex in its own way.

(With apologies to Tolstoy)

To put these ideas in the context of complexity and complex systems, in this section we go beyond the common definition of complexity given above. Rather than focusing on a single aspect of complexity—emergence, as above—we support a multifaceted view of complexity.

Before coming to complexity, we focus on simplicity, in some ways its antithesis. There are several different ways in which systems, or we should better say questions about systems, can be simple. For example, they can be sufficiently small that complex behaviors do not appear; linear, and thus easy to analyze in a variety of ways; robust to perturbations, making them easy to analyze in yet other ways; or purely random, so that their statistical properties—the only ones which are well-defined—are easy to predict and understand. This list is not exhaustive, but it covers many of the most well-known ways in which a system can be simple. This is closely related to the idea that there are only a handful of ideas that yield essentially all known efficient algorithms; we will see further relations between complexity and algorithms below.

(S. Ulam famously said that the phrase "the study of non-linear systems" is akin to the phrase "the study of non-elephants". We tend to agree, but still think it is fruitful to say that linear questions are simple, and thus not complex. It then becomes clear the way in which identifying nonlinearity with complexity is at least partially correct, while acknowledging that it is not entirely so. Similarly for the other ways outlined above in which systems can be simple.)

Many attempts at defining complexity have been made in terms of the effects of "intuitive complexity" on our ability to understand, predict, or control certain aspects of a system. In many common situations, understanding precedes prediction, and prediction precedes control, but this

need not always be the case. As a simple example, Ptolemy could accurately predict the motion of the planets long before we had much understanding of why they move the way they do; similarly with quantum mechanics in the early 20th century. As another example, it is quite possible to accurately control a bicycle when riding it, without being able to predict how it would behave in uncontrolled circumstances, and without understanding how it worked!

Understanding, prediction, and control are certainly three important desiderata when it comes to various systems. Often all three are difficult in the case of complex systems. But rather than try to pick a favorite and define complexity in terms of one alone, we simply leave them separate, and view them as three different (if sometimes overlapping) consequences of simplicity or complexity. If one system A is understandable but not predictable, and another system B is predictable but not understandable, we can take these as evidence that both A and B may be complex, but that they are complex in different ways.

Similarly, for complexity more generally: rather than picking one aspect—such as the three commonly used aspects of emergence, nonlinearity, or adaptivity—we recognize that there are many different aspects that can make systems complex in different ways. (This is analogous to the zoo of complexity classes (Complexity Zoo 2002) in computational complexity theory, another facet of the analogy between complex systems and algorithms.) The following is a nonexhaustive list of some of the many ways in which systems can be complex, in no particular order:

- Path-dependence, strong dependence on history, hysteresis, non-Markovianity, memory, feedback
- Hidden variables (difficult or impossible to measure)
- State space of high, unknown, or even infinite dimension (as in the case of phenotypes in biological evolution)
- Sensitivity to initial conditions (sometimes called "chaos")
- Difficulty of prediction or control (for other reasons than listed above)
- Incompressible behavior
- Emergence
- Mix of structure and randomness (the randomness can make the structure hard to see, and the structure can make the randomness hard to predict even in a probabilistic sense)
- Robustness to certain changes in combination with extreme fragility to other changes
- Changes in one part of the system quickly propagate to many other disparate parts in ways that are hard to predict or control
- Downward causation
- Universality (the ability to simulate a large class of other systems)
- Self-organization, "spontaneous order"
- Adaptivity

We emphasize that these are qualitative aspects that different systems may display to differing degrees. There are some relations between some of these, but for the most part they are independent, in that a system may display any subset of these qualities without the others. Many commonly used examples of complex systems display nearly all.

In terms of higher-order interactions, we find such a taxonomy useful, even if (necessarily and always) incomplete. For example, some aspects of complexity can arise simply from having a large number of pairwise interactions. Other aspects can arise from even a small number of higher-order interactions. And still others are most likely when there is a combination of both: a large number of higher-order interactions. Over the past two decades, our ability to handle both large collectives and higher-order interactions—separately and together—has taken off.

Finally, whatever our definition of complexity, we take some care in stating that it is not systems that are complex or simple, but rather the questions we ask of them (Moore and Mertens 2011, p. 16). For example, predicting the total human population to within 0.001% (allowing for an error of around 100,000 people) every month for the next five years is relatively easy and would hardly be considered complex. But predicting almost any indicator of what that human population will do economically to the same accuracy and level of detail, despite being the same underlying system, is both complicated and complex. On this view, when someone (including me!) refers to a system as complex, it can be interpreted to mean that certain standard or frequently asked questions about the system are complex questions.

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III. Why Is Pairwise So Powerful?

Suppose we model a system by a network of pairwise interactions. Each node in the network represents an object or agent in the system, and each connection between two nodes represents some interaction or relationship between the nodes. If we suppose that each node has a quantity of something—dollars, widgets, molecules, energy—then we may consider how those quantities move around on the network. If we suppose, for simplicity, that we have modeled the system so that whenever a widget can move, it does, then the network has the property that if some node has twice as many widgets, then at the next time step twice as many widgets move away from that node. This is the key property that allows for the application of the powerful toolbox of linear algebra.

Linear algebra is essentially the study of functions that are additive, in the sense that if we add two inputs together, the result is simply the sum of their individual outputs: $f(x+y) = f(x) + f(y)$. This additivity property may hold for "mundane" reasons, as when the input is a raw material and the output is a finished product (twice as much material can produce twice as much product), or for deeper reasons, as in the case of the Schrödinger equation: any two solutions to the Schrödinger equation (each corresponding to a possible state of a quantum mechanical system) can be added to get a third such solution, yielding the nonclassical superpositions of quantum mechanics.

Linear algebra provides a toolbox both of conceptual mathematical methods, and of effective computational methods for learning about our world. This toolbox is so successful that it is even able to provide useful insight when applied to linear approximations of nonlinear systems. It remains unclear whether this is a miracle of mathematics, a miracle of the universe, or a case of mathematicians looking for their keys under the lamppost; perhaps a bit of all three.

Why does linear algebra work so well? In our still evolving understanding, there are two main reasons. The first is that linearity enables a lossless, compressed description of a system (usually in the form of a matrix), in a way that the system can be efficiently reasoned about directly from the compressed description.

The second reason is the Fundamental Theorem of Linear Algebra: that several different characterizations of dimension or rank are equivalent. This has recently been called a "miracle" by Landsberg (J. Landsberg 2021, Sec.2; J. M. Landsberg 2021), who emphasized that almost no other measures of rank share this property, and gave a geometric explanation as to why. Interestingly, one of the few other geometric situations that shares some of these properties are curves in two dimensions (but not three or more!), an example of the theme of this chapter.

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IV. Three Is Different: Blessings and Curses

In his famous 1972 essay, "More is Different" (Anderson 1972), Anderson argued that reductionism was independent from the ability to reconstruct descriptions of higher-level systems from lower-level ones (e.g., biology from chemistry). And that the latter reconstruction—usually considered a key aspect of reductionism—is almost never possible. In part, this is because the higher-level system is often determined by symmetry-breaking properties of large collectives, such as an organism made of cells, cells made of molecules, or molecules made of large numbers of atoms (even sugars made of a few tens of atoms). Today, the latter perspective has been taken to extremes, as when Kivelson and Kivelson attempted to define emergent properties in physics (Kivelson and Kivelson 2016) as "qualitative propert[ies] that can only occur in the limit that the number of microscopic constituents tends to infinity."

But Anderson's example of the emergent chirality of sugar molecules, despite none of its 20 atoms being chiral, is quite telling. Indeed, we will see that in many cases, the dividing line of various aspects of complexity is often not between "a few" and "a few million," nor even between "a few" and "a few tens," but is very commonly between 2 and 3.

Each example we cover here highlights different aspects of complexity that can arise in the transition from pairwise interactions to three-way or more. In many cases, one can even argue rigorously that

while four-way or even higher-order interactions are more complex, that no fundamentally new phenomena arise beyond three-way. Also, we will see some of the trade-offs of studying higher-order interactions: they can often make a model more faithful to the real phenomena, but also harder to reason about. Surprisingly, there are nonetheless some cases in which the higher-order phenomena are easier to reason about, because they have certain properties that pairwise phenomena do not.

Dynamics

Consider two stars orbiting in space, influenced only by each other's gravity. What possible trajectories can they take? They can orbit one another elliptically, one can approach the other then fly away in a parabola, or one can approach the other and fly away even faster, in the shape of a hyperbola. The same is true for electrostatic attraction between charged particles. These results have been known for centuries, and can be given as exercises to undergraduate physics students.

Now what happens when we have three particles? In 1767 Euler knew of three periodic trajectories in which all three particles all lie on a line (to see how this is possible, imagine the middle particle fixed and the other two rotating around it). In 1772, Lagrange derived that three particles could orbit a mutual center as the three corners of a rotating equilateral triangle. For a couple centuries, no further periodic trajectories of three equal masses were found (with zero total angular momentum), until Cris Moore found a figure-8 solution numerically in 1993 (C. Moore 1993), formally proved in 2000 (Chenciner and Montgomery 2000). But, much more than a single solution, Moore showed that any possible braiding pattern of three particles was realizable, if one is allowed to choose the strength of the attractive force. So we see our first jump from simplicity at 2 to universality at 3.

Another example also comes from dynamics. Imagine a particle moving around constrained to a flat surface, subject to certain forces, e.g., wind, magnets, electric currents, and so on, so long as the forces are applied consistently, not changing over time. The Poincaré-Bendixson Theorem classifies all the ways such a particle can behave: it can remain fixed forever (at a so-called "fixed point"), it can loop forever (in a so-called "limit cycle"), or it can asymptotically approach a fixed point or limit cycle. This classification theorem precludes exciting phenomena like chaos and strange attractors. But in dimensions 3 and above, these phenomena are quite common (Lorenz 1963).

Why the jump from simplicity in two dimensions to complexity in three? In this case, despite being questions of dynamics, geometry is the key feature. Trajectories through time are one-dimensional curves sitting inside a higher-dimensional space. In two dimensions, a one-dimensional closed curve—corresponding to a limit cycle—divides the space to those points inside the curve and those outside of it (the Jordan Curve Theorem). But in three dimensions or higher, no one-dimensional (smooth) closed curve divides the space in such a way. And indeed, the proof of the Poincaré-Bendixson Theorem relies heavily on the Jordan Curve Theorem. So in this case, we see that the jump in complexity from 2 to 3 is really about the fact that time is one dimensional. And while there are new interesting phenomena that arise in still-higher-dimensional dynamical systems, the jump in complexity from 2 to 3 is certainly the most dramatic.

Topology

Topology is the study of shapes but ignoring distances and lengths, paying attention only to their connectivity properties. On this view, a circle and an ellipse are topologically equivalent (as are two circles of different sizes), but a circle and a line are not. The history of topology touches on many of our other subjects: in some sense it was born combinatorially when Euler introduced networks to study the connectivity properties of the city of Königsberg given by its bridges. Topology's more continuous aspects really arose in Poincaré's work on dynamics, as we got a glimpse of in the previous section. And in topology, there is also a big jump in complexity from two to three dimensions.

In one dimension, the only topological manifolds are circles and lines. In two dimensions, we get the sphere, the surface of a donut, the surface of a two-person inner-tube, and more generally the surface of an n-person inner-tube for any n. These are complete classifications, known for over a century, and easily applied when one encounters a new topological space while studying some phenomenon.

But in dimension three, while there is some sort of classification (Thurston 1982), it is vastly more complicated, was only completed in the last 20 years (Perelman 2002), and is much more complicated to apply. The classification of 3-manifolds involves breaking a 3-manifold up into pieces, each of which falls into one of eight classes (the most well recognized are probably spherical, Euclidean, and hyperbolic).

We may also see evidence of the complexity of classifying 3-manifolds by considering algorithms for identifying whether two manifolds are equivalent. Algorithms for identifying 2-manifolds boil down to linear algebra (again, pairwise interactions), while those for 3-manifolds are both much more complicated and much less efficient (see Kuperberg 2019 for the state of the art, Matveev 2007 for a textbook, and Lackenby 2020 for a survey). It is unknown whether efficient algorithms for identifying 3-manifolds exist, even in theory. For 4-manifolds and higher, it can be proven that there is no algorithm—efficient or not—that will correctly identify any given 4-manifold (Adian 1955; Rabin 1958).

In dimension three, we also see the interesting phenomenon of knots: a mathematical knot is a loop of string that cannot be unknotted without cutting it (see Figure 1). Knot theory has applications across many fields: understanding the knottedness of DNA (Sumners 2011; Flapan 2000), trajectories in three-dimensional dynamics (individual cyclic trajectories can be knotted!) (Birman and Williams 1983), more abstract relations with the foundations of (topological) quantum field theory (Kauffman 1994), and the dynamics of fluids (Kleckner and Irvine 2013) and electromagnetic fields (Kedia, et al. 2013) such as in Earth's outer core and the Sun's plasma.

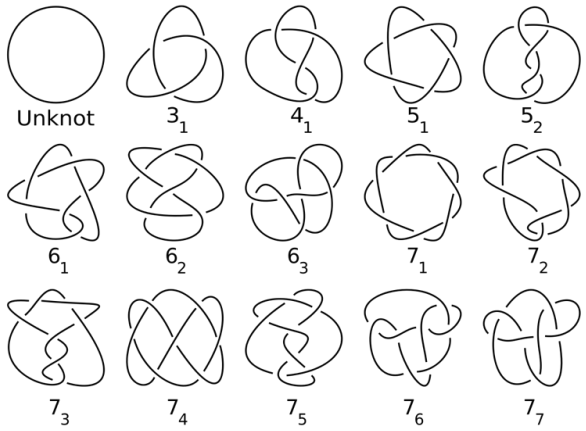

Figure 1 Mathematical knots are closed pieces of string that cannot be unknotted without cutting.

Figure from https://en.wikipedia.org/wiki/File:Knot_table.svg.

As in the case of dynamics, knots cannot exist in two dimensions because of the Jordan Curve Theorem—any closed loop is either just a plain circle, or would have to cross itself, which we don't allow by fiat in our definition of a (mathematical) knot. Loops of string cannot be knotted in four or more dimensions, because there is enough room to pull the knot "away" from itself in the higher dimensions. (And there is indeed a countervailing trend of complexity in topology that there are certain phenomena that become increasingly complex up to three or four dimensions, but thereafter become simpler in even higher dimensions.) But two-dimensional sheets can be knotted in four dimensions, three-dimensional "blobs" can be knotted in five dimensions, and so on.

Knots consisting of more than one piece of string, called "links," can also display higher-order interactions. A classic example is the Borromean rings (see Figure 2), consisting of three pieces of string that together cannot be pulled apart, but once any one of them is removed, it reveals that the other two were not linked together at all. This is an example of a three-way interaction that cannot be explained by any set of pairwise interactions, as here there are no pairwise interactions at all! This example can be generalized to still more pieces of string; such links are called Brunnian links, and were classified in Milnor (1954).

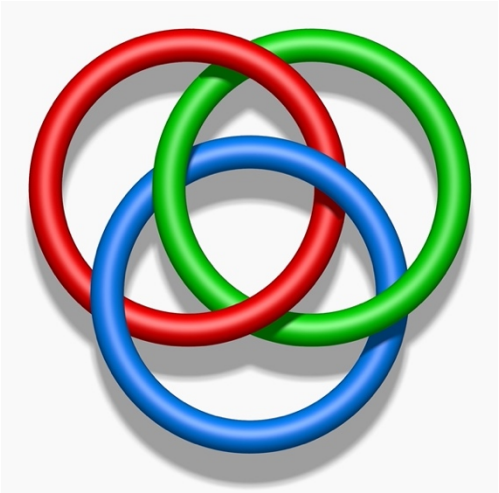

Figure 2 Borromean rings. The three cannot be separated without cutting. But once any one of them is removed, the other two can be pulled apart without any further cutting. This three-way interaction cannot be explained by any set of pairwise interactions. Image from https://commons.wikimedia.org/wiki/File:Borromean_Rings_Illusion.png.

Hypergraphs and Simplicial Complexes

Hypergraphs (a.k.a. hypernetworks) and simplicial complexes are two higher-order analogues of

networks, enabling the combinatorial description and analysis of (certain kinds of) higher-order interactions. As there are several recent surveys on these topics (Torres, et al. 2020; Battiston, et al. 2020; Bick, et al. 2021), we will not belabor the point, but we review them briefly as a starting point and point of comparison.

Just as a graph or network models pairwise interactions, a hypergraph is the least cumbersome model of higher-order interactions. A hypergraph or hypernetwork consists of a set of nodes, and a set of subsets of those nodes, called hyperedges, of arbitrary size. A hyperedge consisting of k nodes represents a k-way interaction between the nodes.

A simplicial complex can be viewed as a particularly topological kind of hypergraph: one in which, if there is a k-way interaction among a set of nodes, then all possible (k-1)-way interactions among that same set of nodes must also occur. Given a hypergraph, one can always build a simplicial complex by adding every subset of every hyperedge as a new hyperedge. A simplicial complex is a hypergraph, but one can also get a "simplified" hypergraph by only retaining those hyperedges that are maximal, in the sense of not being contained in any larger hyperedges. A discussion of the modeling choices involved in deciding to use hypergraphs or simplicial complexes can be found in (Torres, et al. 2020).

The jump from networks to hypernetworks, even those whose hyperedges only consist of three nodes at a time, allows significant modeling flexibility, but often comes at the cost of computational expense. Not only are the corresponding computational problems bigger, but the best-known algorithms are often exponentially worse than the corresponding ones for ordinary networks (Hillar and Lim 2013).

Topographical Data Analysis

The basic idea behind topological data analysis, or more specifically manifold learning, is that data sets that are presented in a very high-dimensional space often occupy only a very low-dimensional subset of that space. On the one hand, the goal is thus to identify low-dimensional structure in seemingly high-dimensional data. On the other hand, "low" rarely means 1 or 2, and the underlying combinatorial objects of manifold learning are the simplicial complexes discussed above. Topological data analysis can thus be viewed as a natural generalization of parts of network theory.

One of the interesting applications of topological data analysis is to data sets with real values, for example, representing the strength of pairwise interactions. To convert such a weighted network into an ordinary network, practitioners will often impose a somewhat arbitrary cutoff value: edges with weights above that value are kept, and those with weights below the value are discarded. Topological data analysis instead asks how the network varies as the cutoff value is varied, thus removing the arbitrary choice, while still learning combinatorial, network-theoretic information from a real-weighted network.

On this view, rather than merely a single network—representing a single pattern of pairwise

connectivities—what one gets is a one-parameter family of networks, one for each possible cutoff value. If we imagine these networks stacked on top of one another, a three-dimensional picture emerges. Each edge in this three-dimensional picture can in fact be viewed as a three-way interaction, between two nodes and one parameter value. A similar viewpoint arises in the use of higher-order interactions in the work of Valverde, et al. (2020) on understanding modularity and nestedness in ecological networks, which we discuss more below.

Coloring Maps and Computational Complexity

Computational complexity is the study of the limitations of efficient algorithms: What algorithmic problems are genuinely hard to solve—in the sense of requiring a certain amount of resources, such as time or computer memory—regardless of choice of software, hardware, or technique?

Interestingly, although computational complexity is formally about computation, it is nearly always the case that the computational complexity of problems lines up with a corresponding intuitive notion of "conceptual complexity." Computational problems that are algorithmically difficult often arise in areas where the mathematical theory is well developed, deep, yet incomplete. When studying a class of systems, we may thus use the computational complexity of associated algorithmic problems as one of many measures of our more general notion of complexity. It is one of the ways in which systems can be complex, that is often correlated with other aspects of complexity.

Within computational complexity, a particular question stands out as one of the deepest across all of computer science and mathematics, namely: Is it the case that any problem that can be solved by a brute-force search, guess-and-check style strategy can also be solved by a much more efficient algorithm (the so-called "P versus NP" problem). Introduced simultaneously on both sides of the Iron Curtain (Cook 1971; Levin 1973), it was soon discovered (R. M. Karp 1972) that many computational problems solvable by brute-force search were equivalent, in the sense that one of them could be solved by a much more efficient strategy only if all of them could. Today such problems are called "NP-complete," and thousands of problems of both practical and theoretical interest fall into this class.

> Terminology: When computer scientists talk about a "problem," they frequently mean a whole family or type of what one might ordinarily call problems. "Sort the list [7,3,1,8,9]" is referred to as a problem *instance*, whereas "sorting lists of integers" is a (computational) *problem*.

For concreteness, here we will focus on just one such representative problem that exhibits a conceptual jump from 2 to 3: properly k-coloring networks. But we emphasize that many of the thousands of NP-complete problems also exhibit a very similar jump from k=2 to k=3, including k-dimensional matching, Boolean k-satisfiability, problems on networks of maximum degree k, and many more.

The problem of properly coloring a network originally arose as the problem of coloring a map. What

is the smallest number of colors needed to color, say, the countries of the world, so that no two adjacent countries receive the same color? To get a network out of this problem, we assign each country a node, and connect two nodes by an edge whenever the corresponding countries share a border (see Figure 3). The kind of map coloring then corresponds to assigning colors to the nodes of this network, so that no two adjacent nodes receive the same color. The problem of k-coloring is this: given a network as input, to decide whether it can be properly colored using at most k colors.

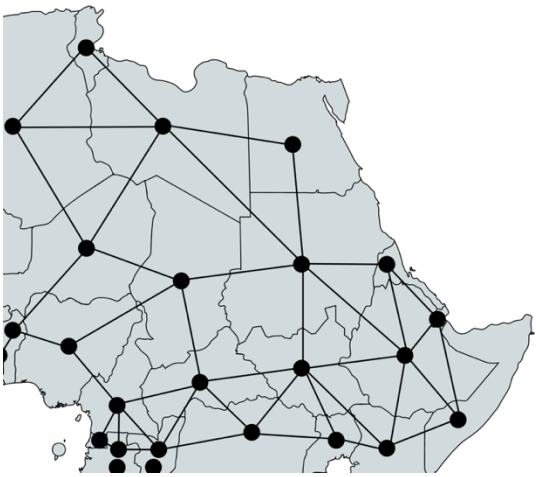

Figure 3 Converting a map to a network for the Coloring Problem.

Two-coloring turns out to be relatively easy: start by assigning one node, arbitrarily, the color red. In any proper two-coloring, there is no choice but for its neighbors to be blue. Their neighbors must be red, and so on. Either this procedure finds a node that we want to color both red and blue—and thus the graph is not two-colorable—or it does not. In the latter case if we imagine all the red nodes on the left side of the page and all the blue nodes on the right, we see that all the edges go between nodes on the left and nodes on the right. Such a graph is called bipartite, which we shall return to later when discussing hypergraphs.

Before proceeding to the case of three-coloring, we pause to observe several ways in which two-coloring turned out to be simple:

1. *Computational simplicity*: It was relatively easy to solve.
2. *Rigid correlations*: The colors of different nodes are linked so rigidly that a single choice completely determined all other choices of colors.
3. *Uniqueness*: If a network is two-colorable, there are only two proper two-colorings, and one can be gotten from the other merely by swapping the colors. So there's essentially at most one way to two-color any network.
4. *Proofs of noncolorability*: There is a simple way to exhibit when a network is not two-colorable, namely, when it contains a cycle of odd length (thus forcing some node to "want" to be both colors). Such an odd-length cycle exists in any non-two-colorable network.

5. *Lack of robustness*: In any two-colorable network, it is possible to add a single edge that makes it not two-colorable: two-color the network, then add an edge between two nodes of the same color.

It turns out that not only is k-coloring NP-complete when k is at least 3, but it will share none of these properties. Three-coloring instead has a whole host of other properties that earn it the moniker "complex."

Now we turn to three-coloring, and we consider each of the above points in turn. Three-coloring is NP-complete (R. M. Karp 1972), which in particular implies that k-coloring for any k is no harder than three-coloring. It also means that there is no algorithm currently known to solve the three-coloring problems on networks of n vertices in less than an amount of time that is exponential in n, nor is any such algorithm expected to exist. In terms of computational complexity, we see a jump from 2 to 3, but not from 3 to 4, nor to any higher number. The jump from 2 to 3 is final.

Next we turn to rigid interactions and information propagation. While it is true that, in some networks, the choice of color of one node fixes the choice of color of a far-away node—propagating information from one part of the network to another—it does so in a way that is much more flexible than in the case of two-coloring. See Figure 4.

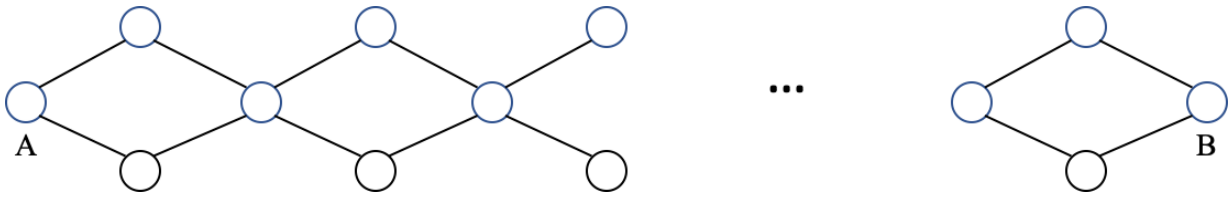

Figure 4 Information propagation in three-coloring. Any proper three-coloring of this network must assign nodes A and B the same color, despite leaving choices of how to color many of the nodes in between.

Figure 4 exhibits just how many different three-colorings a network can have: exponentially many, as a function of the number of nodes! This is in sharp contrast to the effectively unique proper two-coloring.

Figure 4 is also drawn suggestively to highlight an analogy with Watson-Crick-Francis base pairing in DNA. The key is that the crystalline structure provides enough rigidity to encode digital information reliably, but enough flexibility to encode a wide variety of digital information.

As for proving that a network is not three-colorable, there actually is a way! For example, if there are four nodes that are connected to each other by all six possible edges between them, there is no way to properly three-color those four nodes. Such a network is called a four-clique, so the presence of a four-clique is an obstruction that prevents three-coloring in the same way that odd cycles were obstructions preventing two-colorings. However, unlike the case of two-colorings, these are not the only such obstructions. For example, the network in Figure 5 is not three-colorable, despite not

containing any four-cliques.

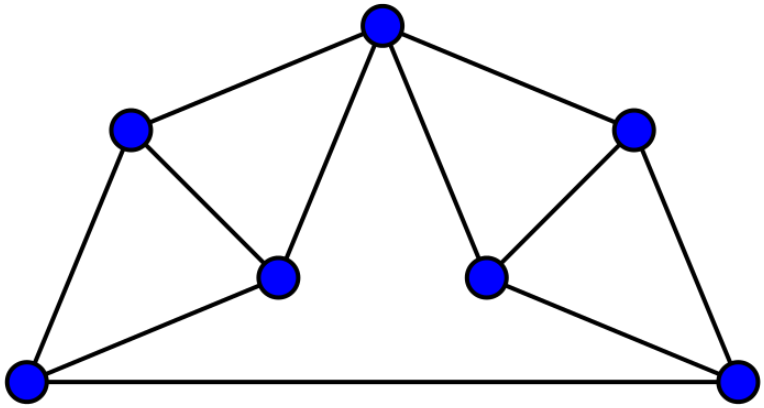

Figure 5 A network that is not three-colorable, despite not containing any four-cliques. This particular network is known as the Moser Spindle. Image by David Eppstein from https://commons.wikimedia.org/wiki/File:Moser_spindle_pseudotriangulation.svg.

However, all hope is not lost. Hajós (1961) showed how to build all obstructions to three-coloring by starting from four-cliques and using certain operations to combine them into larger networks (including the one in Figure 5). He proved that if a network was not three-colorable, it must contain as a subnetwork one of the obstructions gotten by his procedure. However, unlike the case of finding odd-length cycles, in this case finding such an obstruction is itself a hard problem! Pitassi and Urquhart (1995) showed that there are non-three-colorable graphs where the number of steps needed to exhibit an Hajós obstruction was exponential in the number of nodes. So not only are the obstacles to three-coloring infinitely more varied than those for two-coloring, but they are exponentially harder to find!

Finally, we come to the question of robustness. Kun and Reyzin (2014) studied how hard it was to find a proper k-coloring, assuming that the given network was resiliently colorable, in the sense that not only was it k-colorable, but so was any network gotten by adding some number of edges to the original. In particular, for any k at least 3, there exist networks that are k-colorable and such that after adding any k-1 edges they are still k-colorable. (Contrast to the case of two-coloring, where one could always find a single edge to add to make a network not two-colorable.) They also showed that for very resilient networks, coloring actually becomes easy again, but for only mildly resilient networks, coloring remains NP-complete.

Hospitals and Residents and Computational Complexity

The "Hospitals and Residents Problem" is the following computational problem, arising when matching applicants for medical residency to a hospital's resident positions.
Applicants each rank hospitals in their order of preference, hospitals rank residents in their order of preference, and each hospital only has a certain number of positions. The goal is to match residents to positions at hospitals in such a way that no two applicants would both prefer to swap with each

other. The latter property is called "stability." Gale and Shapley (1962) introduced the notion of stable matching and efficient algorithms for it, and were perhaps the first ever to receive the Nobel Prize in Economics for an algorithm. Algorithmic solutions to this problem are still widely used in actual residency matching programs around the world, based on Gale and Shapley's original insights.

However, in real-world matching programs, residents can enter as couples, specifying their joint preferences, e.g., that they would prefer to both be matched to hospitals in the same city. This modified problem, which now includes the three-way interactions of hospital-resident-resident, turns out to be NP-complete (Ronn 1990). The proof of NP-completeness uses instances of the problem in which every resident is part of a couple, which one might reasonably argue is unrealistic. But more recently it was shown that even if the number of couples is small, there is still no efficient algorithm. More precisely, Marx and Schlotter (2011) showed that, under standard assumptions in computational complexity (technically known by the arcane acronym $W[1] \neq FPT$), there is no algorithm whose runtime degrades gracefully as the number of couples grows. Even the presence of a small number of three-way interactions here brings on the spectre of complexity.

Tensors and Multilinear Algebra

Tensors are a generalization of matrices that capture beyond-pairwise interactions (see Kolda and Bader 2009 for a review). Whereas a matrix is a rectangular array of numbers $A1,3$, where i indexes the row and j indexes the column, a 3-tensor is a rectangular box of numbers $T1,3,6$, with three dimensions to it (with a natural generalization to 4- and higher-order tensors). Just as matrices are the basic objects of linear algebra, tensors are the basic objects of multi-linear algebra. Unlike linear algebra, however, most basic questions about tensors are computationally intractable (Hillar and Lim 2013), and even from the abstract mathematical viewpoint are much more difficult to handle. For example, eigenvalues and eigenvectors of tensors are not only much more complicated than in the case of matrices, but their theory is still in active development (Banerjee, Char and Mondal 2017; Xie and Chang 2013; Cartwright and Sturmfels 2013; Cooper and Dutle 2012). This is one example of the relationship we mentioned above: computational complexity going hand in hand with conceptual complexity and deep theory.

One interesting feature of higher-order tensors is that while matrices never have a unique decomposition as a sum of rank-1 matrices, some tensors do have such a uniqueness property. The additional constraints imposed by the higher-order interactions can introduce a sort of rigidity that is simply not possible in the case of the pairwise interactions specified by a matrix. The price paid for this additional rigidity is that computing such a decomposition becomes NP-hard for tensors, whereas for matrices it is computationally easy. But from a conceptual viewpoint, even the existence of a decomposition that is also unique has certain advantages. In particular, if one can find the unique decomposition, the terms in that decomposition should have some meaning, since they depend only on the tensor, and not on an arbitrary choice of how to decompose it.

Polynomial Equations

Polynomials are what we get by starting with variables, and then combining them using the ordinary arithmetic operations of addition, subtraction, and multiplication. They arise in static questions such as measuring areas and volumes, and in dynamical questions such as the rate of change in a population as a function of the populations of its predators and prey.

An equation is of degree 1 if it uses no multiplication of variables, such as $7x + 3y = 1$. Equations of degree 1 have solution sets that look like lines, planes, and hyperplanes (higher-dimensional versions of planes, but still "flat"). These are the so-called linear equations.

An equation is of degree 2 if at most two variables are multiplied together before being added, such as $x9 + 7y - 13y9 = 0$. Solutions to equations of degree 2 can be much more complicated than degree 1. If we allow multiple, simultaneous equations of degree 2, they are in fact universal, in the sense that any system of equations can be mimicked by a system of multiple equations of degree 2. If we call the original system of equations E and the new, degree-2 system of equations F, then solutions to E yield solutions to F and vice versa.

Interestingly, a system of equations of degree 2 can be modeled by a 3-tensor. A single equation of degree 2 can be written as $\sum 1,3\ A1,3x1x3 = 0$; note that it is fully specified by the pairwise interactions in the matrix A. But then when we move to a system of quadratic equations, it becomes $\sum 1,3\ T1,3,6x1x3 = 0$ ($k = 1, \dots, n$) where the third index k denotes which of the equations is being referred to. Thus, we see a jump in universality from 2 to 3.

However, if we stick to single equations (rather than systems of multiple simultaneous equations), we see another jump in complexity from degree 2 to degree 3, but this time in a different way. As before, it's the case that a single degree-2 equation can be expressed by a matrix. The solutions to such equations are generalized ellipses, parabolas, and hyperbolas, a concept known for thousands of years.

In contrast, even for individual degree-3 equations (specified by a 3-tensor), no such classification is known, nor expected to be possible. From the viewpoint of computational complexity, the question of deciding whether two degree 3 equations are equivalent up to a change of basis is at least as hard as the famous Graph Isomorphism problem (Agrawal and Saxena, 2006; Agrawal and Saxena, 2005). Furthermore, it was recently shown to be "universal" in the sense that it is in fact as hard as any tensor equivalence problem, not just for 3-tensors, but for d-tensors for higher d as well (Futorny, Grochow and Sergeichuk 2019; Grochow and Qiao, 2021). Thus we see a different kind of complexity and universality arising in this jump from 2 to 3.

Network Models

When providing null models for some property of a network, a common procedure is to take the network and produce random versions of it that share some of the original properties. Perhaps the

simplest is the so-called configuration model (Newman, 2010), in which one samples from all networks with the same degree distribution (the number of vertices with one neighbor, the number of vertices with two neighbors, and so on) as the original. To produce random samples from the configuration model, a common procedure is edge-swapping (Newman, 2003) (see Figure 6). Edge-swapping is an efficient, mathematically proven process for sampling from the configuration model (see, e.g., Fosdick, et al. 2018 for a review).

Figure 6 Edge-swapping to produce random versions of a network with the same degree distribution

The configuration model asks to preserve the distribution of two-node subgraphs around each node, i.e., edges. What if we want to sample random graphs with the same distribution of three-node subgraphs around each node? In this case, it was found in practice that either the procedure edge swapping combined with a simulated annealing (Grochow, 2006), or swapping multiple edges at once (Tabourier, Roth and Cointet, 2011), could quickly converge to the right counts of three-node subgraphs, though mathematically proving this remains elusive. When we move from three- to four-node subgraphs, it remains an open problem to efficiently sample from the distribution of networks with a given distribution of four-node subgraphs.

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V. Implicit Higher-Order Interactions

There are many mathematical concepts in which higher-order interactions have been considered implicitly, without modeling them explicitly. These include network motifs (Milo, et al. 2002)—small frequently occurring subgraphs—modules, and communities in networks (Newman, 2006; Clauset,Newman and Moore 2004). The advantage of these is that they inherit the ease of working with pairwise interactions, while revealing some of the hidden higher-order structure in a data set. Modeling these concepts explicitly in a higher-order fashion represents an opportunity that might reveal further phenomena and insights.

There are also several dynamical processes on networks that are implicitly higher order, such as majority rule in opinion formation (Poljak and Sura 1983, in which a node takes on the opinion held by a majority of its neighbors. We also speculate that part of the power of agent-based models (see, e.g., Miller and Page 2007; Bonabeau 2002; Arthur 2021)) is that they implicitly define, create, and simulate higher-order interactions, without having to do so explicitly. As with the static

network concepts above, these dynamical processes take advantage of the ease of working with pairwiseinteractions to reveal certain kinds of higher-order structure. We suspect that modeling these higher-order structures explicitly, particularly in the case of agent-based models, could lead to a deeper understanding of their mathematical properties and implications.

Bipartite networks are networks with two types of nodes, such that all the edges connect a node of one type to a node of the other type. Many examples arise from social group interactions, in which individuals are nodes of one type, and groups of people (such as a social group, classrooms, co-authors on a paper) are nodes of the other type. An edge is placed between a person and a group when the person is a member of that group. These are mathematically equivalent to higher-order networks, where each group node corresponds to a single higher-order interaction (hyperedge). However, the viewpoint of "groups as nodes" as opposed to "groups as groups [of nodes]" suggests different methods and different approaches. For example, the linear algebra one gets by considering the pairwise interactions of individual-to-group in a bipartite graph can be very different than the multilinear algebra arising from considering higher-order interactions between multiple individuals in a higher-order network. As with many applications of linear algebra and pairwise interactions, bipartite networks have been incredibly successful modeling tools, but it is natural to wonder how much more is to be discovered by analyzing such systems in their natural, higher-order representations.

Using Higher-Order Interactions to Find Hidden Structure in Pairwise Interactions

Sometimes, even when the data are pairwise, we can use higher-order analyses to reveal "hidden structure" in the data. Given a network G we can define several higher-order networks from it:

- Clique complex or flag complex: include a hyperedge for each set of vertices that form a clique in G; a clique is a subset of vertices between which all possible edges are present. Given a set of points with distances between them, we may define a network by putting edges between two points if they are within distance 1; the clique complex of this network is precisely the Vietoris-Rips complex, one of the starting points for persistent homology and topological data analysis (see above).
- Independence complex: include a hyperedge for each set of vertices that form an independent set in G (a subset of vertices with no edges between them).
- Neighborhood complex: for each vertex v in G, include a hyperedge consisting of all of v's neighbors. The topology of this complex was used to better understand graph colorings and Ising-like models (Lovász 1978).
- Path complex or nerve: include a hyperedge for each set of vertices that form a path in G. (In an undirected network this just reveals the connected components, but in a directed network it can reveal interesting features of the way the strongly connected

components related to one another.) Lambioette et al. (2019) highlight the importance of specifying not just the steps from one state to the next that a system can take, but the higher-order path dependencies. Their suggested method of modeling is to specify a subset of the path complex. This idea was formalized into the notion of "a path complex" (not necessarily coming from a graph) in (Grigor'yan, et al. 2020).

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VI. Explicit Higher-Order Interactions

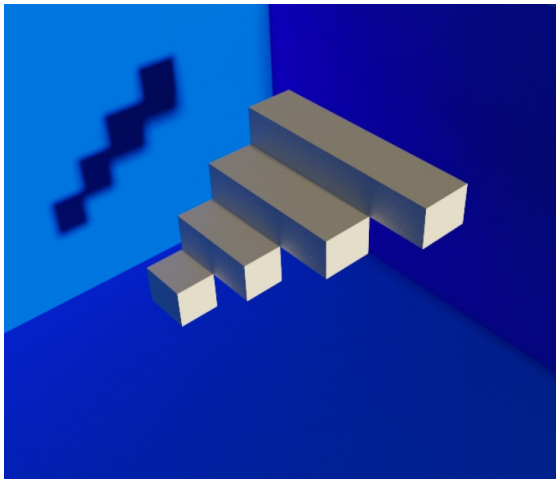
As in the many examples above, we saw that higher-order interactions can be modeled explicitly in a variety of ways. In this final section, we will highlight some recent works using higher-order interactions in the study of complex systems, to understand patterns of interactions in ecology, and to understand how different types of social interactions influence one another.

Vignette 1: Higher-Order Interactions in Ecology

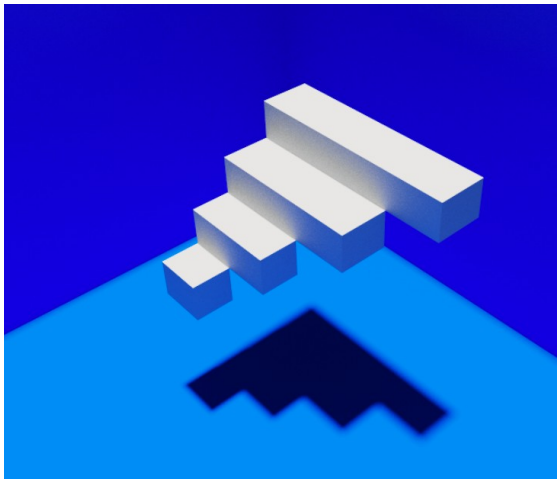
Ecologists frequently use networks to represent interactions between species: nodes represent species (or energy sources or similar), and an edge might represent a predator species that eats a prey species, or a parasite species that parasitizes a host species. To build these data sets, ecologists spend extended periods of time visiting various locations and meticulously recording every species they see, interactions between species, analyzing gut contents of dead animals to see what species they had eaten, and so on.

One of the ongoing mysteries in ecological networks, which a higher-order viewpoint is starting to shed light on, is the seeming dichotomy between nestedness and modularity. We illustrate these concepts by example. A predator–prey network is nested if each species' diet—the set of species it preys upon—is either a subset or a superset of every other species' diet. The caricature here is that of big fish eating littler fish eating still littler fish. On the other hand, a network is modular if it can be broken into groups such that species mostly only interact with other species in their group. These two naturally seem to be at odds with one another.

In a recent paper, (Valverde, et al. 2020) showed how a higher-order viewpoint elucidates the situation. Rather than simple networks, they built a third-order hypernetwork, where some edges represented host species, some pathogens, and others different environments (different locations in which data were collected). A hyperedge was placed between a host, pathogen, and environment if the host and pathogen were seen to interact within (or mediated by) that environment. What one finds in this way is that it is entirely possible for a third-order hypernetwork to display modularity when viewed from the perspective of only two types of nodes, yet nestedness when viewed from the perspective of a different pair of node types (see Figure 7).



Modularity



Nestedness

Figure 7 A pictorial representation of how a third-order hypernetwork can display modularity in one pair of nodes, and nestedness in another pair of nodes. Figure due to Sergi Valverde, Salva Duran-Nebreda, and Blai Videllia; used with permission of S. Valverde.

Vignette 2: Communities in Multilayer Networks Modeled as Third-Order Tensors

A *multilayer network* is a network with multiple kinds of pairwise interactions, each kind corresponding to a layer. These are traditionally modeled either as labels on the edges of a network, as multiple ordinary networks (one for each layer) on the same set of nodes. But one can also model them in a higher-order fashion, as a tripartite hypergraph, where one introduces a new node for each layer, and each hyperedge connects two ordinary nodes together with one layer node. The latter leads naturally to the associated 3-tensor, e.g., De Domenico, et al. (2013).

De Bacco, Power, Larremore, and Moore (2017) took advantage of the tensorial viewpoint on multilayer networks to gain a deeper understanding of the relationships between the layers. In particular, by approximating a low-rank decomposition of the corresponding tensor—something very natural to do for tensors, but somewhat unnatural from the hypergraph viewpoint, and nearly impossible to imagine from the viewpoint of an ordinary bipartite graph—they learned about how the different layers related to one another.

One can ask how independent two layers in a multilayer network are, or more generally how independent various subsets of layers of a multilayer network are. Their framework gives a clean way of answering this question, by saying that one layer gives information about another if adding in that layer results in a lower-rank approximation to the corresponding tensor than one would get by omitting that layer.

When the different layers represent different forms of data collection—as in the social ties in African villages explored in De Bacco, et al. (2017)—understanding these kinds of independence questions can lead to more targeted, less costly data collection. On the other hand, when the different layers represent different genetic loci of the malaria parasite, they found that the layers (genetic loci) were

highly independent of one another, mathematically confirming what malaria geneticists had long suspected, that the parasite takes maximum advantage of mutations at different genetic loci in order to evade immune system defenses. In these two case studies, in which multilayer networks were built from highly different data sources with very different meanings, the higher-order, tensorial viewpoint revealed information not available from the traditional pairwise viewpoint.

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VII. Looking Forward

Despite the rapid increase in the use of higher-order interactions, it still feels very much as though we are just exploring the beginnings of their deeper theory. The examples here highlight the want of a synthesis of different kinds of higher-order interactions, beyond those captured solely by higher-order networks. One can take some inspiration from the history of graph theory and network theory. By the time large network data sets were becoming widely available in the late 1990s and early 2000s, graph theory was already a well-developed, centuries-old subject. However, while the basics of graph theory were crucial in network science, the deeper questions graph theory had explored—for example, about matchings, paths, colorings, embeddings into surfaces, or purely random graphs—were less relevant to network theory than other aspects of graphs such as community structure, generative graph models, network motifs, and global aspects of the degree distribution or path-length distribution (small worlds). So while the two were related, the focus of network theory was quite different. Similarly, the combinatorial theory of hypergraphs is nearly 50 years old, but even from the purely combinatorial viewpoint much remains to be explored (Courtney and Bianconi 2016; Young, et al. 2017; Yen 2021). From the more applied viewpoint, it feels we are just at the beginning of learning what properties of hypergraphs are most relevant for understanding the complex systems arising in the real world, and we hope for many more exciting twists and turns.

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