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Hypergraphs and Simplicial Complexes in Focus: A Roadmap for Future Research in Higher-Order Interactions

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Abstract. Higher-order interactions are increasingly being recognised as fundamental to our understanding of complex systems, networks, and the development of the next generation of AI algorithms. However, modelling higher-order interactions requires us to go beyond graphs and networks, which can only encode pairwise interactions, and so demands a new theory. Hypergraphs and simplicial complexes (also called higher-order networks), which arise as natural mathematical representations of higher-order complex systems, are therefore attracting increasing attention. The mathematics of higher-order networks is already providing important insights, yet many fundamental mathematical questions remain unsolved; for instance, in spectral graph theory, discrete topology, and higher-order network dynamics. This roadmap summarizes the scientific discussions that took place on these topics between pure mathematicians, theoretical physicists, computer and network scientists at the Newton Institute Satellite meeting on 'Hypergraphs: Theory and Applications'. We survey the current state-of-the-art in higher-order network research, and propose some trajectories for future research, including in areas such as extremal and spectral hypergraph theory, discrete topology, higher-order dynamics, higher-order machine learning, and applications in the brain and social sciences.

1. Introduction

Networks are graphs that represent complex interacting systems formed by vertices representing system components and edges representing pairwise interactions between them [1, 2]. The underlying structure of these networks encode the information content present in the web of interactions and provides new fundamental insight on the rich interplay between network structure and function of real-world complex systems [1,3]. In the last two decades, it has been shown that networks provide an abstract mathematical representation of numerous complex systems which has proven to be fundamental in several domains – including technological systems such as power networks and the internet; biological systems such as complex food webs and intracellular molecular regulatory networks; and online social networks.

However, such approaches only consider system components and their pairwise interactions. In many important cases, so-called higher-order interactions [4–7] are also important and can play a significant role in characterizing system topology [8] and function [9–11]. There is growing interest in modeling these higher-order structures in representations of complex systems: for instance by encoding them as simplicial complexes that can be analysed using methods from topology or, more generally, as hypergraphs. Both of these approaches are successful and active areas of research [7, 12–15].

Because higher-order networks account for many-body interactions, they can be used to represent communities of elements of any size. If, for instance, we want to model an epidemic, we can model individuals as vertices in a graph or hypergraph, and connect individuals (in pairs or in communities) if they come into contact with each other. Importantly, because they only capture binary relationships, graph-based representations may fail to effectively capture important information such as social events that involve numerous people. As another example, proteins typically perform their functions in cells by physically interacting to form chemical complexes. Although protein-protein interaction networks enumerate possible pairwise interactions, they are not able to unambiguously capture the formation of higher-order complexes involving three or more proteins. In both these cases higher-order interactions – relating to spreading events or protein complexes, respectively – carry important information that is missed in graph representations. Other important applications include among other microbial communities [16], and brain functions [17]. Higher-order networks include hypergraphs that provide the most general combinatorial framework to encode interactions between two or more nodes, simplicial complexes that fully account for the higher-order topology of data, and networks with triadic interactions which encode regulatory interactions between nodes and edges (see Figure 1). Simplicial complexes [7, 15, 18] provide a way of representing higher-order interactions that allow powerful tools from algebraic topology to be applied to data analysis, typically by representing interactions, or similarities, between data points as a simplicial complex. Accordingly, simplicial complexes have a prominent part in topological data analysis [8]. Despite

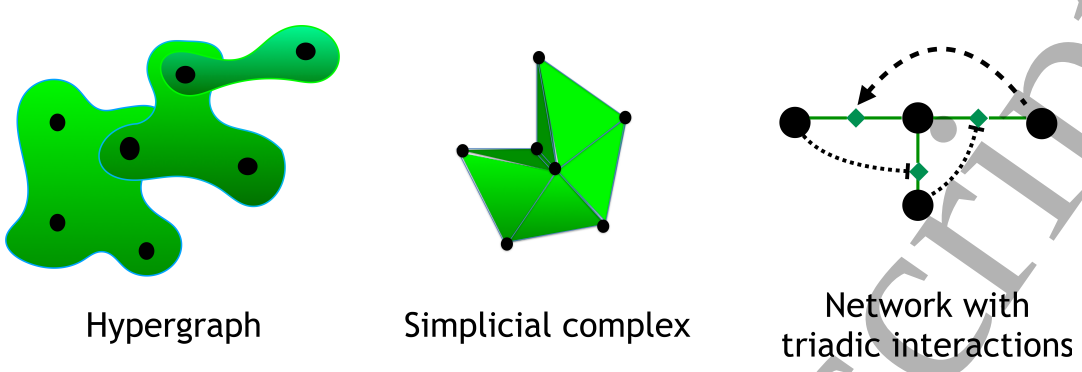

Figure 1. Hypergraphs are formed by nodes connected by hyperedges representing the interactions between two or more nodes. Simplicial complexes can be seen as a type of hypergraph that allow algebraic topology approaches to uncover the topology and the geometry of higher-order networks and the dynamics of topological signals. Networks with triadic interactions occur when one or more nodes can regulate the interactions between other two nodes.

clear conceptual similarities, hypergraph theory and topological data analysis have historically been (practically speaking) largely separated from one another – some notable connections notwithstanding [19].

However, simplicial complexes can be seen as a type of hypergraph formed by simplices representing all-to-all interactions among constituent vertices that are closed under the inclusion of their faces (subsets of vertices) – a constraint that is not present in the definition of a hypergraph. This is easily be understood from a topological/geometrical point of view: for example, we cannot have a triangle (a 3-way interaction between three vertices) with a missing edge. Despite this restriction, however it was recently shown [20] that if one considers weighted simplicial complexes it is actually possible to encode any hypergraph data without loss of information. The benefit of using simplicial complexes to represent higher-order interactions is that this is the ideal framework for encoding the topology and geometry of higher-order interactions. Thanks to powerful tools provided by algebraic topology, in particular Topological Data Analysis (TDA) and Topological Deep Learning, simplicial complexes can be used to characterize the topological structure of data and of the higher-order dynamical processes unfolding on them.

Recently, networks with triadic interactions have begun to attract significant interest [10, 21]. Triadic interactions occur when one or more nodes regulate the interaction between other two nodes. This occurs for instance in ecosystems when one species regulates the interaction between two other species, or in neuronal systems when one glial cell modulates the synaptic signal between other two neurons. Triadic interactions can also occur in chemical reaction hypergraphs, for instance when one node, such as an enzyme, affects the rate of chemical reactions between substrates. Abstracting from these examples, triadic interactions cannot be recast into hyperedges between the nodes, and a formal mapping between network with triadic interactions and a hypegraphs can only be performed by extending the notion of hypegraphs to

factor graphs (see for details Ref. [22, 23]). Therefore in this case, the attribution of different functional roles to the triadic regulatory interactions can significantly enrich the dynamics that arise from these types of higher-order networks.

Currently, there is increasing interest in using hypergraphs and higher-order networks to analyze the structure and function of real-world complex systems [6, 9, 10, 24–27]. However, despite this interest, the potential of hypergraphs and higher-order networks has not yet been properly realized because the theory needed to address the pressing theoretical questions is not yet fully developed. Indeed, the interdisciplinary interest in a subject that involves mathematicians, theoretical physicists, computer scientists and network scientists generates a fertile ground for the formulation of new theoretical challenges and the development of new frameworks to extract relevant information from networks with higher-order interactions.

At the Newton Institute Satellite Programme 'Hypergraphs: Theory and Applications', held in summer 2024 at the Alan Turing Institute, London, we discussed the recent progress and open perspectives of the field of higher-order networks. Arising from those discussions, we have identified core mathematical topics in pure and applied mathematics/theoretical physics that we believe are essential for the development of network science and machine learning tools in the context of higher-order interactions, with wide applications in the study of real-world complex systems – from brain research and drug discovery, to social networks, epidemic spreading and game theory (see Figure 2). In the following, we will present an overview of the general themes discussed during the Programme, which range from pure mathematical questions to increasingly more applied topics. These topics are: spectral hypergraph theory (Sec.2), discrete topology (Sec.3), higher-order network dynamics (Sec. 4) higher-order Machine Learning (Sec.5) and higher-order Network Science (Sec. 6).

This Roadmap is intended to guide a wide range of scientific readers in this very active interdisciplinary field transcending discipline boundaries. We have adopted a widely accessible style which will provide a comprehensive reference for the researchers that are either already working on higher-order networks or that desire to approach this field. At the same time different sections address topics and discuss results from different perspectives. Sec. 2, and Sec.3 present a discussion of recent progress in modern pure mathematics while Secs. 4, 5 and 6 provide an ample overview of this very active research field focusing mostly on the applied mathematics/theoretical physics, computer and network science perspective respectively.

2. Extremal and Spectral Hypergraph Theory

Raffaella Mulas, *Aida Abiad, Ágnes Backhausz, József Balogh, Krystal Guo, Jürgen Jost*

When considering the foundational theories of hypergraphs and their roles in modeling higher-order interactions, it is important to examine two key areas — extremal

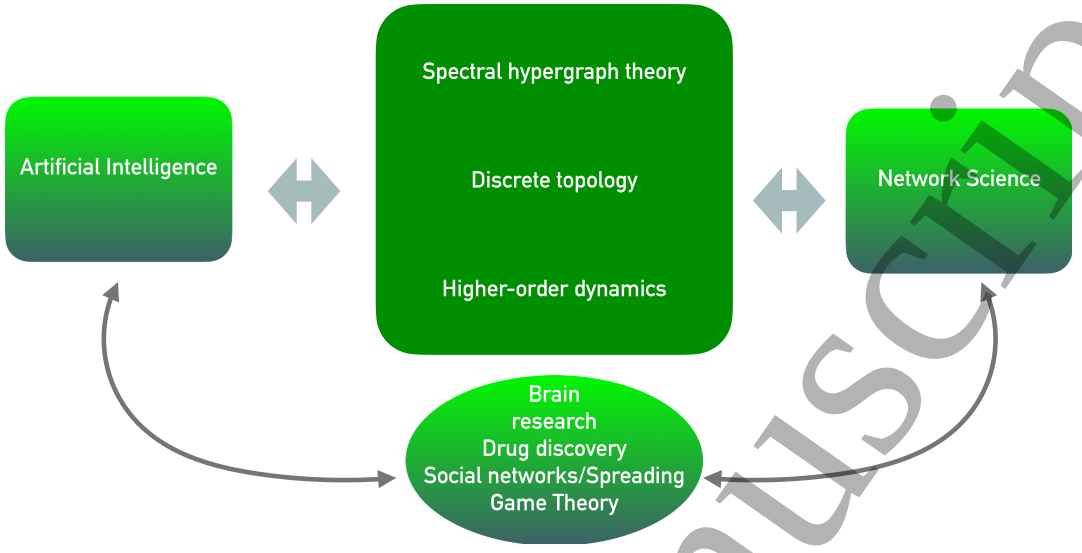

Figure 2. Hypergraph and higher-order network challenges discussed during the Newton Institute Satellite: 'Hypergraphs: theory and applications'. Advances in spectral hypergraph theory (pure mathematics), discrete topology and geometry (pure mathematics) and dynamics of higher-order networks (applied mathematics/theoretical physics). Such advances can inform and provide solid mathematical grounds for Network Science and Artificial Intelligence with the potential to significantly improve our understanding of, and ability to predict, the behaviour of complex interacting systems such as brain dynamics, social systems and epidemic spreading, with important applications, for instance in drug discovery and game theory.

hypergraph theory and spectral hypergraph theory — which, while abstract, have significant c onnections t o r eal-world a pplications. F or i nstance, c hemical s pace, that is, the system of all chemical substances and reactions ever reported in the literature, forms a gigantic hypergraph, with the substances being the vertices and the reactions the hyperedges connecting the input and output sets [28]. The Laplace operator introduced in [13] captures that structure, and its spectral properties will yield deeper insight into the structure of chemical space, for instance by identifying particular motives like closed systems of reactions. Likewise, coauthorship networks are naturally modelled as hypergraphs, see e.g. [29], and again, hypergraph spectral theory should be able to provide structural insight similar to what it can do for ordinary networks, see [30, 31]. These fields thus have not only advanced the mathematical understanding of hypergraphs but are also crucial for addressing problems in network science and dynamical systems.

Extremal hypergraph theory focuses on identifying structural boundaries, such as the maximum or minimum number of vertices or hyperedges given certain constraints. Meanwhile, spectral hypergraph theory extends well-established results from spectral graph theory to hypergraphs, making it an essential tool for analyzing the dynamics of systems with higher-order interactions and for interpreting complex network data. The interplay between extremal and spectral methods presents a promising direction

for future research and opens up new possibilities for both theoretical advancements and practical applications.

A schematic overview of the topics covered in this section is given in Figure 3.

2.1. Extremal hypergraph theory

While hypergraphs have grown into a broad and international area of study, their origins and early development are deeply rooted in the Hungarian extremal combinatorics. In [32], Paul Erdős wrote:

> *As far as I know, the subject of hypergraphs was first mentioned by T. Gallai in a conversation with me in 1931. He remarked that hypergraphs should be studied as a generalization of graphs. The subject really came to life only with the work of Berge.*

The work of Claude Berge that Erdős referred to are the two books [33, 34] that laid the foundation for the study of hypergraphs. Some classical (and partially, still open) problems on extremal hypergraph theory include, for example, the *Turán Tetrahedra Problem* that was introduced in 1941 by Pál Turán [35]. Another well-known problem is the 50 year old *Erdős Matching Conjecture:* What is the maximum size of a family of k-element subsets of an n-element set if it has no $s+1$ pairwise disjoint sets?

Moreover, in recent years, a major contribution in extremal hypergraph theory was made by József Balogh, Robert Morris, and Wojciech Samotij, and independently by David Saxton and Andrew Thomason, who developed the *hypergraph container method* as a new tool for bounding the number of finite objects with forbidden substructures [36–38]. This approach not only advances our understanding of extremal problems but also opens new directions for exploring hypergraphs.

2.2. Spectral hypergraph theory

Recent years have seen increasing interest in applying hypergraph tools to real-world data analysis. However, while network science tools are now very well-established, based on rigorous notions from underpinning graph theory, the theoretical tools and techniques needed to make the most of the potential of hypergraphs have not yet been fully realized. Besides active research activity on statistical models of hypergraphs and simplicial complexes, great attention has been recently addressed in spectral hypergraph theory where we expect that new progress will bring a fundamental change of paradigm with respect to the simple graph setting.

In the graph context, spectral theory refers to the study of the eigenvalues and eigenvectors of a given graph operator, such as the adjacency matrix, the Kirchhoff Laplacian and the normalized Laplacian matrix associated with a graph [39–42]. While two graphs cannot always be distinguished by their spectra, the spectra reveal some important graph properties – such as their bipartiteness, completeness, and connectivity. This has implications for various applications, including clustering,

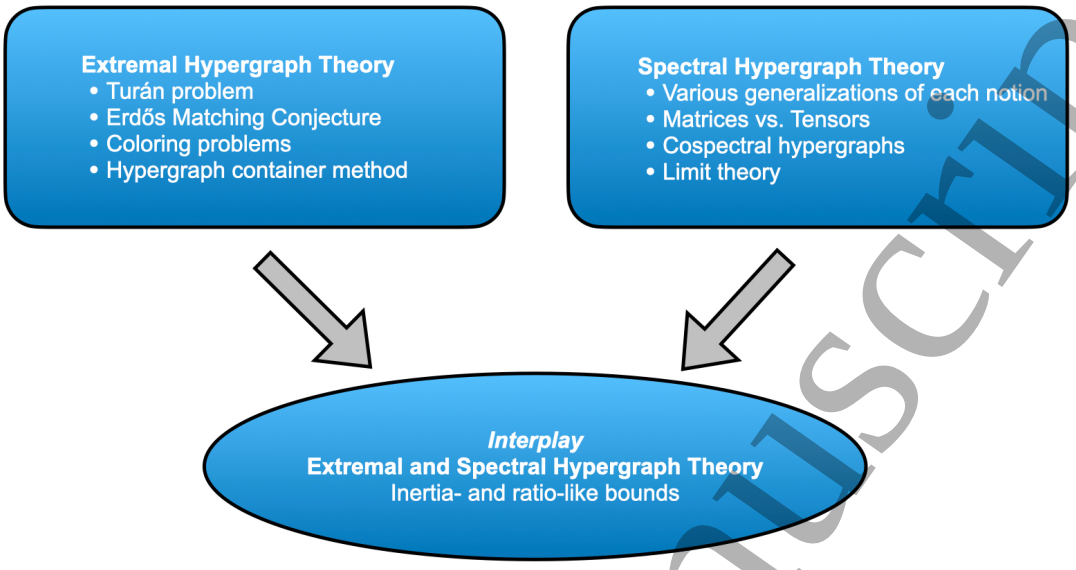

Figure 3. A schematic overview of Section 2 covering extremal graph theory, spectral graph theory and their interplay.

community detection, graph partitioning, and diffusion processes on networks [42–44]. Additionally, key problems in spectral graph theory include eigenvalue bounds, spectral clustering, and spectral characterizations, among others, forming the basis of many modern applied techniques in data analysis and network science [45, 46].

In recent years, various generalisations of spectral graph theory to hypergraphs and their analysis have been proposed [47–55] and some have applied to network science and dynamical systems [56, 57], but many important questions remain open. For instance, is any particular generalisation better suited for the analysis of real-world data, or for the study of higher-order dynamics?

A key challenge in extending spectral graph theory to hypergraphs is that there are multiple ways to generalize graph operators. For example, while for graphs the degree of a node is uniquely defined, for hypergraphs, the notion of degree can vary depending on whether one considers the number of hyperedges a node belongs to or the size of those hyperedges. Moreover, the definition of adjacency for vertices can vary in the case of hypergraphs. This flexibility leads to different ways of constructing hypergraph analogs of classical graph matrices, such as the adjacency matrix or the Laplacians.

In addition to these choices, there is a fundamental distinction between representing hypergraphs using matrices versus tensors. While tensors offer a complete representation of the hyperedges, they also introduce significant computational complexity. On the other hand, matrix-based representations—by flattening or projecting hypergraph structures—allow for the application of more established matrix-based techniques (see [58, 59] for example), but at the cost of losing some structural information inherent to hypergraphs. Thus, one important question is whether matrix-based methods, with their computational simplicity, can capture enough of the hypergraph structure to provide meaningful insights, or whether tensor-based approaches, despite their complexity, are

necessary to fully explore higher-order relationships and dynamics.

These choices—between different degree and adjacency notions, and between matrices and tensors—pose important questions for future research.

Another interesting direction to pursue is the study of cospectral hypergraphs, which is important since it reveals which hypergraph properties cannot be deduced from their spectra. Several papers proposed methods to obtain cospectral uniform hypergraphs based on well-known hypergraph representations [50, 60, 61]: adjacency tensors and adjacency matrices. Extensions of the known constructions of cospectral uniform hypergraphs to non-uniform hypergraphs and to other hypergraph generalizations, such as oriented hypergraphs, are interesting open problems

Going further in the direction of spectral hypergraph theory, we can also think about connections with graph limits and their extensions to hypergraphs. Graph limit theory has been successfully used to analyze the behavior of random d-regular graphs [62]; a generalization of the limit notion and the methods to tensors might lead to new results in the hypergraph case as well.

2.3. Merging extremal and spectral frameworks

Interestingly, there are deep connections between spectral properties and extremal combinatorics in graphs. For example, the *inertia bound*, due to Cvetković [63], and the *ratio bound*, developed by Hoffman, establish relations between the independence number of a graph and its eigenvalues. Both bounds can be used to prove an important result in extremal combinatorics (EKR theorem).

Hypergraph methods have also been used in the field of combinatorial designs, where they provided powerful tools for tackling longstanding existence problems. A *combinatorial design* is a system of finite sets meeting specific criteria. Hypergraph methods made an appearance in the field in 1985, in [64] where Rödl found an approximate design with the probabilistic method. In a recent breakthrough, Keevash [65] resolved a long-standing existence conjecture for combinatorial designs, a problem originating in the 19th century, by proving the existence of Steiner systems for nearly all admissible parameters using Randomized Algebraic Constructions. Recent advances by Glock, Kühn, Lo, and Osthus [66] extend Keevash's work by solving the existence problem for F-designs for arbitrary r-uniform hypergraphs F, using probabilistic and combinatorial methods.

While some of these results have already been extended to hypergraphs (see e.g. the several extensions of the ratio bound for hypergraphs [67, 68]), many potential generalizations and their applications remain open. The complexity of hypergraph structures—where multiple definitions of adjacency, degree, and eigenvalues exist—presents new challenges for extending these classical spectral bounds to the hypergraph setting. Addressing these challenges promises to advance both spectral hypergraph theory and extremal combinatorics.

Several directions appear particularly promising. On the extremal side, long-

standing problems such as the Erdős Matching Conjecture and Turán questions for hypergraphs remain major open challenges. On the spectral side, the ongoing development the mathematical theory of hypergraph matrices and tensors opens the understanding their roles in applications. The known cospectral constructions are limited to uniform hypergraphs and the extension of these to non-uniform and oriented settings would be an interesting future direction of research. Finally, the interplay between extremal and spectral approaches is only beginning to be understood: for instance, extending classical eigenvalue bounds relating invariants such as independence or coloring numbers to eigenvalues in the hypergraph setting (and for different types of hypergraph operators) could lead to powerful new methods. Together, these examples illustrate the rich landscape of open problems at the interface of extremal and spectral hypergraph theory.

In Subsection 3.2, we will also explain how insights into (hyper)graph spectra can augment the topological approach (which only needs the eigenvalue 0) to obtain a richer picture of local and global properties of networks and to understand the properties of coupled dynamics on networks.

3. Discrete Topology

Jürgen Jost, *Ginestra Bianconi, Magnus Botnan, Heather Harrington, Cerene Rathilal, Ruben Sanchez-Garcia, Martina Scolamiero, Francesco Vaccarino, Kelin Xia*

The interplay between discrete topology and geometry offers insights into complex systems, providing a structured way to understand connectivity and shape of data. We highlight the importance of concepts from algebraic topology and discrete geometry in tackling problems in both pure and applied mathematics. We introduce concepts and the evolving role of discrete structures in modern mathematics, discussing recent advances and open perspectives in homology and cohomology of simplicial complex and hypergraphs and important recent progress on the characterization of the spectral properties Laplacians and generalized algebraic topology operators. While in this section the emphasis is more on the pure mathematics aspects of this field, we frame our discussion highlighting key illustrative applications. The wider spectrum of applications of these two topics will be discussed in the following sections. In particular, cohomology and the spectral properties of algebraic topology operators are key to define topological dynamics on higher-order networks and topological signal processing that will be treated in Secs. 4 and 5 respectively, while homology is pivotal for the formulation of persistent homology algorithms to uncover the shape of data of fundamental importance for topological machine learning (see Sec. 5), as well as for brain research and network neuroscience (see Sec. 6).

3.1. Homology and cohomology of simplicial complexes and generalizations

Mathematically, homology theory works by constructing a boundary operator ∂ whose square is 0, and from which the homology groups of the object in question, here a simplicial complex, are constructed. The dimensions of these groups, the Betti numbers, provide the number of higher-dimensional holes, yielding basic topological invariants. In cohomology theory, one can additionally use scalar products to construct adjoints of the dual δ of ∂, and from these one then obtains Dirac [5] and Laplace operators [69]. These can be used to define more refined invariants. In particular, the spectra of the Laplace operator provide important geometric invariants — see, for instance, the textbook [70].

Homology theory is applied in Topological Data Analysis (TDA) to families of simplicial complexes depending on a parameter r. As an example, Vietoris-Rips simplicial complexes are constructed from metric data sets, with points forming a simplex at scale r if their mutual distances are at most r, resulting in an increasing family of simplicial complexes $X_r \subseteq X_{r'}$ whenever $r \leq r'$ (a *filtration*). We can keep track of the homology as the scale parameter r varies, and in particular of those generators of the homology groups that persist for a wide range of r — this is the basis of *persistent homology* in Topological Data Analysis [8, 71, 72] which will be discussed further in the Higher-order Machine Learning section (see 5.2). The resulting persistence diagrams uniquely describe the persistent homology of the underlying dataset and can be shown to be stable to data noise: small changes in the dataset result in small changes on the persistence diagram. At the same time, improved computational techniques, including on scalability and efficiency, allow the calculation of persistent homology for large datasets [73]).

Another active area of research is multiparameter persistence [74], where data and simplicial complexes are filtered along two or more parameters. This approach is particularly useful for analyzing data with meaningful structures across multiple scales and densities, as well as functional and time-varying data. For a recent overview of the field and its applications, see [75]. This approach can be extended to hazy metrics and fuzzy simplicial sets, that is, where distances are only statistical [76, 77], linking it with state-of-the-art schemes for data analysis like Isomap or UMAP and providing an improved version (IsUMap [78]).

For hypergraphs, only a partial theory is possible in principle because a hypergraph need not contain the faces of a hyperedge; see [70]. Another generalization is the path homology of digraphs (directed graphs) [79], which can also be used for hypergraphs; see [80].

3.2. Laplacians and their spectral properties

The Laplace operators for simplicial complexes were introduced in [69], for a Hodge type cohomology theory on simplicial complexes. But the Laplacians can tell us more than purely topological invariants and, indeed, their spectra encode basic geometric invariants. In graph theory, this has been systematically exploited; see for instance

[39, 42, 53]. In fact, not only individual eigenvalues, like the smallest non-vanishing or the largest one, encode important information, but also the distribution of all eigenvalues can reveal qualitative properties of networks, e.g. [30, 31, 81]. For higher order simplicial complexes, the Laplacian framework was developed in [82]. This can be further generalized: if we consider vector spaces of functions on the k-simplices and transition operators between them satisfying suitable properties so that they square to 0 as the (co)boundary operators in (co)homology, this leads to the notion of *sheaf Laplacian*; see [83] for applications to persistent (co)homology.

A natural question is whether this can also be turned into a useful tool for hypergraphs. Different Laplace operators have been proposed; for a comparison see for instance [84]. For the most general theory, we need an additional structure on the hypergraph. Namely, we assume that each hyperedge h consists of two (not necessarily distinct) sets $V_0(e), V_1(e)$ of vertices, like the educts (input) and products (output) in a chemical reaction. Such hypergraphs, in [13], are called *chemical hypergraphs*. One can then construct a Laplace operator that evaluates differences between inputs and outputs and quantifies flows through the hypergraph and develop a spectral theory in full analogy to the above, and the eigenvalues encode crucial structural properties of the underlying hypergraph [13, 53].

In particular, the eigenvalues control the collective behavior of diffusively coupled chaotic dynamics in networks. Kaneko [85] discovered the surprising phenomenon of synchronization of chaotic dynamics on diffusively coupled networks, and in [86], stability conditions were derived. The stability depends on the cohesion of the network, and the latter is controlled by the smallest positive eigenvalue of the coupling Laplacian, while the largest eigenvalue controls oscillations of period 2, as shown in [87]. Synchronization is of course interesting and useful in many applications, but in many systems, there exist collective dynamics of a richer nature. It was observed in [57, 88, 89] that such dynamics can result from the diffusive coupling of chaotic dynamics on hypergraphs. Here, the hypergraph Laplacian of [13] is used to lump together the activities on the inputs as well as those on the outputs of a chemical hypergraph. It remains to explore the potential for global pattern formation from such diffusive coupling of chaotic dynamics further. What can be generated in such a way beyond the rich patterns already observed in [88]? The general principle behind all these phenomena is that local, strongly nonlinear, chaotic dynamics at individual components are diffusively coupled via a linear operator, a Laplacian, on a network. The eigenvalues of that Laplacian encode geometric properties of the network, and these then are crucial for understanding the emergence of collective phenomena that cannot be predicted from the individual dynamics themselves. In this context, we can also look at the pattern generation potential of the Dirac operator that links the dynamics in simplicial complexes in different dimensions; see for instance [5, 90]. The role of these algebraic topology operators in shaping the higher-order dynamics of simplicial complexes will be extensively discussed in Sec. 4.

The topological and spectral theory of simplicial complexes and hypergraphs

currently constitutes a very active research field, where both deep mathematical structures and novel applications in machine learning emerge. For instance, we can ask for the persistence of spectral properties in filtered simplicial complexes and what they tell us about the underlying data set. The resulting persistent eigenvalues recover the barcode from persistent homology while also providing additional geometric information [91–93]. This approach to studying filtered complexes has shown to outperform persistent homology on image data, though efficient computation remains a challenge [94].

We expect that in the next few years, this extensive research activity will contribute to a comprehensive theory of spectral properties of hypergraphs and higher-order networks. Many problems for this new field remain open. For example, is any particular operator (not limited to those sketched above) better suited for the analysis of real-world data, or for the study of higher-order dynamics? In the absence of a clear answer to this question, can we provide guidelines for indicating under which hypothesis we should adopt a given spectral operator? Are the different definitions of spectral operators for hypergraphs and simplicial complexes orthogonal or complementary?

4. Higher-order dynamics

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Higher-order networks provide a framework to unveil the basic mathematical mechanisms driving higher-order dynamics, [9–11,95] of wide relevance for a large variety of complex systems ranging from the brain to the climate. Here we discuss the recent progress in the field [9–11, 95] by distinguishing among higher-order node dynamics, and higher-order topological dynamics [10]. This latter approach combines algebraic topology with the theory of non-linear dynamics and requires a more radical change of perspective with respect to the traditional node-centered description of the dynamical state of the network. In particular, in higher-order topological dynamics, dynamical variables, also called topological signals (see Figure 4), are not only associated with nodes but also with edges, and with higher-dimensional simplices of simplicial complexes. Thus while in the node-centered approach the dynamics can be associated with hypergraphs as well as to simplicial complexes, for higher-order topological dynamics, simplicial complexes provide a powerful framework to uncover how topology shapes dynamics and how dynamics learns the topology. After discussing the important process in both node-centered higher-order dynamics and higher-order topological dynamics, we conclude this Perspective by highlighting the role of triadic interactions in determining new dynamical states of higher-order networks that cannot be accounted for by considering standard higher-order interactions such as hyperedges or simplices.

Due to space constraints we will not be able to overview here the large literature on classical and quantum spin models that includes the p-spin, combinatorial optimization problems such as K-sat, and the Sachdev-Ye-Kitaev model. For the interested reader

who wants to be introduced to these subjects we suggests Refs. [96–98].

4.1. Higher-order dynamics at the node level

In the traditional field of network dynamics, the dynamical state of the network is fully captured by the dynamics associated to the nodes of the network and evolves thanks to the pairwise interactions existing between them. This framework leads to many fundamental results in network theory, highlighting not only the interplay between network structure and dynamics [99,100] but also the rich variety of dynamical behaviours that emerge by considering different coupling functions between the nodes [101]. Indeed, if one considers the same dynamics on different network structures one can observe paradigmatic shifts in the phase diagram of critical phenomena, such as the vanishing of the epidemic threshold in scale-free networks [99,100]. On the other side, by keeping the underlying network structure fixed, and by changing the coupling functions between the nodes it is possible to formulate models that generalize classical models such as the famous Kuramoto model [102] and models of nonlinear oscillators [103] which display a large variety of surprising dynamical phenomena [104, 105].

Embracing the framework of higher-order networks [4, 7, 9, 15] by continuing to assume that the relevant dynamics is only encoded on the nodes, entails considering the effect of many-body higher-order network interactions between more than two nodes. In this context, higher-order dynamics gives rise to surprising effects such as discontinuous "explosive" phase-transitions in both synchronization [7, 9, 106–108] and contagion processes [109–111] while the corresponding pairwise models only display continuous second order transitions.

Leaving the discussion of contagion models to Section 6, let us discuss here the proposed higher-order synchronization models for node signals. These models include generalization of the Kuramoto model taking into account higher-order couplings associated with higher-order interactions leading to a wealth of dynamical phenomena, including abrupt synchronization transitions [106,107], heteroclinic dynamics [112,113], and chaos [114]. Alternative approaches [57,115] to higher-order synchronization defined on generic hypegraphs, assume that the oscillators associated with the nodes of the higher-order networks are identical and thus generalize the classical pairwise approach of coupled identical oscillators [86]. Interestingly, an important open research question is the identification of the dynamical properties associated to the different representations for higher-order networks. This includes hypergraphs versus simplicial complexes [116] but also aspects like directionality of higher-order interactions [117, 118], that may be needed for cluster synchronization or more complicated dynamics to arise [119].

All these approaches assume that the higher-order interactions are given and propose mechanisms [9] for higher-order dynamics at the node level. This research direction has raised large attention also because predicting the dynamics of the nodes present in real networks, such as brain networks, is a significant scientific challenge. Here, we mention two of the main research questions that have been raised in this

context. The first one is whether it is possible to disentangle the role of higher-order interactions from the role of the choice of the coupling functions. As the choice of the coupling function might already provide an explanation of the exotic dynamical states observed, such as the discontinuous transitions [108], answering this question might involve considerations on the nature of the physical system under study. The second observation is that in absence of the actual knowledge of the structure of the higher-order interactions and the coupling function, the observation of the dynamical state of a real complex system might lead to effective higher-order behaviours [11] emerging from pairwise interactions. Indeed one finds that upon linearization some of the considered higher-order interactions [106, 107] are indistinguishable from pairwise interactions, while phase reductions of pairwise interactions can lead to effective higher-order models [89, 120]. The quest for a comprehensive theoretical framework that can address these two important aspects of this theory is likely going to be a central theme of this vibrant research topic.

Another fundamental class of dynamical processes taking place at the node level are random walks. Extensions of random walks on regular [121] or generic hypergraphs [122] have been recently proposed; transition probability among nodes can depend on the hyperedges size, determining thus a different behaviour with respect to a random walker moving on the (weighted) clique projected network. This observation determines two relevant consequences. First, when using random walks to rank nodes, it can happen that node relevance is not the same if considering a hypergraph structure or a network one [122], for instance, the h-factor of authors of scientific papers can depend on the number of co-authors. Second, random walks can be used to detect communities by using Markov Stability [123, 124], in this case the bias introduced by the hyperedges size on the transition probability can determine different community structures.

4.2. Percolation on simplicial complexes and on hypergraphs

Percolation a fundamental critical phenomenon defined on networks, typically investigated in order to probe and assess the robustness of complex systems ranging from biological networks to complex infrastructures [100, 125, 126]. Percolation monitors the fraction of nodes in the giant component of a network as a function of the probability that nodes or edges are deactivated or removed from a network. Since the giant component of the network ensures the required connectivity to allow communication among different nodes of the network or to sustain diffusion processes from one node to other distant nodes of the network, observing a percolating cluster can be considered the minimal prerequisite for studying relevant collective phenomena on a network. Moreover the nature itself of the percolation process is suitable to investigate the impact of different types of failures coming from different stochastic processes or dismantling network strategies.

Given the great relevance of percolation for simple networks, an important research question is to what extent the higher-order network representation of complex systems changes the nature of the percolation transitions and the conclusions on the underlying

complex system robustness. This is a very active area of research with multiple applications: on one side, percolation processes are strongly connected to processes of contagion and epidemic spreading that will be discussed in Sec. 6 on the other side percolation properties reflect the robustness of the network under study to random failures of either nodes, edges (hyperegdes) or higher-order simplices.

Since, already in pairwise networks, percolation can result from damage of nodes or damage of edges, we discuss this process separately from the previous section in which we considered exclusively the dynamics of the nodes. As we will see, this research field will provide also an important introduction to higher-order topological dynamics that we will discuss next.

We distinguish three major types of percolation dynamics on higher-order networks. Percolation on hypergraphs where we could damage either nodes or hyperedges, and if a node is damaged its incident hyperedges in the original hypergraph reduce their number of nodes by one. This is also called *factor graph percolation*. This percolation like dynamics reflects a common situation encountered, for instance, in social media, where a social group, upon the deactivation of one node, is not dismantled, but it is just redefined as the group with one less member (the deactivated member). This percolation problem can be enriched by further combinatorial dynamics if one considers a representation of a hypergraph as a multiplex network [21, 110] in which each layer comprises exclusively hyperedges of a given cardinality. Indeed the correlations encoded in the resulting multiplex hypergraphs can be exploited to define cooperative hypergraph percolation phenomena displaying tricritical points and discontinuous transitions [21], demonstrating how the robustness of hypergraphs can be affected by the combinatorial rules defining the interdependencies in the multiplex hypergraph structure. This type of percolation like dynamic is also fundamental to define (k, q)-core percolation problems [127] with important implications in social dynamics [128].

In marked contrast with the above definition of hypergraph percolation there is a definition of the model in which hyperedges become immediately deactivated if one of their nodes becomes inactive. This is the situation occurring for instance in chemical reaction networks, where the absence of a reactant impedes a reaction from happening, or in supply networks in which the absence of a supply will impede the production of a commodity. This second definition of the hypergraph percolation leads to a significant decrease of the robustness of hypergraphs, i.e., a larger percolation threshold, with effects particularly severe for hypergraphs with hyperedges of large cardinality and whose effect is strong not only for percolation but also for the corresponding (k, q)-core percolation problems [129,130]. Interestingly, factor-graph percolation and hypergraph percolation can be combined in a recently proposed approach for hypergraph percolation in the presence of anchor nodes [131]. In this setup, anchor nodes are essential for defining the activity of a hyperedges, while the damage of non-anchor nodes only reduces the cardinality of the hyperedge. This leads to interesting critical phenomena both on single and on multiplex hypergraphs.

Finally, it is also possible to define Topological Percolation, which characterizes

different types of percolation problems, defining the connectedness of the simplicial complex under topological damage [132]. By topological damage, it is indicated that the damage not only addressed to nodes and edges but also addressed to higher-dimensional simplices such as triangles or tetrahedra of a simplicial complex. The topological percolation transitions indicates when the k-connected giant component disappear as a function of an increased fraction of simplices affected by topological damage. In Ref. [132] it has been shown that the same simplicial complex can display multiple topological percolation transitions, having different percolation thresholds depending on the dimension of the simplices under consideration. For instance triangle percolation can have a different threshold than edge percolation on the same simplicial complex. Moreover, and even more surprisingly, also the nature of the transition can also depend on the dimension of the simplices under consideration. In particular, in Ref. [132] an example of simplicial complex is provided where triangle percolation is in the Berezinskii–Kosterlitz–Thouless universality class while edge percolation displays an exponential critical behavior.

4.3. Synchronization and diffusion of topological signals

Embracing a higher-order approach to network dynamics entails associating a dynamical variable, also called topological signals, not only to the nodes but also to the edges and to higher-order simplices of simplicial complexes (see Figure 4). The emergent field of higher-order topological dynamics [10] combines algebraic topology to non-linear dynamics and reveals new dynamical states for topological signals. The field has wide applications in complex systems and opens new perspectives in the study of the brain, the climate and lead to dynamical processes underpinning of a new generation of AI algorithms.

Although traditionally the characterization of the network dynamics has been dominated by the node-centered point of view, topological signals [133] are ubiquitous and include molecular transportation fluxes in cells, synaptic signals in the brain and edge signals among brain regions [134]. Interestingly, also vector fields such as the one representing currents in ocean [135] or velocity of wind at a given altitude can be projected into the edges of a tesselation of the Earth and can be treated as topological signals, i.e., cochains.

Higher-order topological dynamics includes important collective phenomena such as Topological Synchronization captured by the Topological Higher-order Kuramoto model [25, 136], Global Topological Synchronization [90, 137] and topological diffusion and random walks [135, 138]. Such collective phenomena occur when topological signals defined on different simplices (for instance, edges) are locally coupled via shared nodes and/or higher-order structures (such as shared triangles). In higher-order topological diffusion the steady state is static, while in the higher-order Topological Synchronization one observes a collective phenomenon where the resulting dynamics are localized on the holes of the simplicial complex. In both cases, topology and higher-order dynamics are

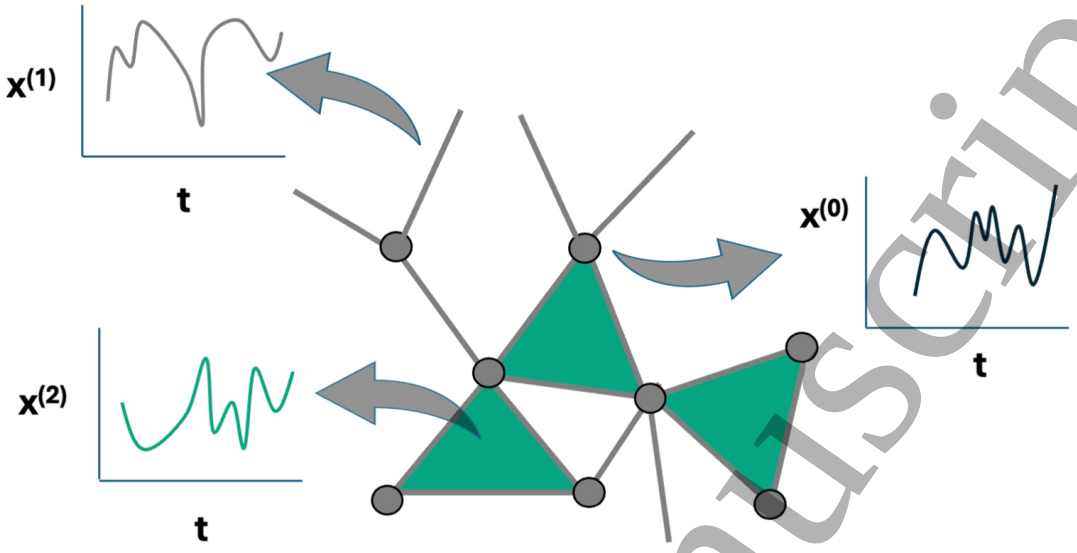

Figure 4. Schematic representation of the topological dynamics of a simplicial complex captured by topological signals, i.e., dynamical variables associated to nodes, edges, triangles and higher-order simplices of a simplicial complex. Topological signals undergo collective phenomena revealing on one side how topology shapes dynamics and on the other side how dynamics learns topology [10].

intimately connected.

Topological Synchronization leads to a completely new interpretation of the synchronized state on higher-order networks which demonstrates the strong interplay between topology and dynamics. In particular, higher-order topological synchronization learns the topology by establishing a spatial pattern of the synchronized dynamics that is not delocalized over all the simplices of the simplicial complex but localized on the n-dimensional holes of these structures. Results have been generalized in different directions, for instance, considering directed, weighted simplicial complexes [139]. These novel results connecting the synchronized state of higher-order networks are among the most promising theoretical frameworks to understand the interplay between topology and dynamics in the brain and open new perspectives for research. In particular a central question is whether the localization of the synchronized dynamics over one hole or the other, can carry information and be associated with attractors that store memory. A related question is whether it is possible to formulate the approach to control and modulate, on which of the possible degenerate states the topological synchronization will occur.

While the synchronized state of the Topological Higher-order Kuramoto is localized on the holes, one important question is whether Global Topological synchronization can ever be observed [90]. In this respect, it has been shown that Global Topological Synchronization, i.e., the state in which the topological signals on each n-dimensional simplex (edges, triangles, etc.) display the same behavior, can only occur for some specific and very regular topologies. Indeed, Global Topological Synchronization will be localized on the n-dimensional holes of the simplicial complex, similarly to what happens

for the Topological Kuramoto model. However, to require a globally synchronized state, we need to consider topologies in which the n-dimensional hole is "spanning the entire structure" and is not localized into a few simplices. A major example of topology in which we can observe Topological Global synchronization is square lattice tessellations of high-dimensional tori, where we can observe Global Topological Synchronization of topological signals of every dimension. Note, however, that in general the Topological Global Synchronized state is very rare, and that if the simplicial complexes are not weighted [137], they might also impede synchronization of odd dimensional topological signals.

4.4. Dynamics of coupled topological signals driven by the Topological Dirac operator

Until now, we have exclusively discussed the dynamics of topological signals of a given dimension, edge signals, triangle signals, and so on, taken in isolation. However, the dynamics of a simplicial and cell complex comprises the evolution of the topological signals of every dimension, which can be coupled to each other in a non-trivial way. The Topological Dirac operator [5] is the key operator that allows for cross-talk of topological signals of different dimension co-existing on the same simplicial or cell complex. The Topological Dirac operator can be interpreted as the "square-root" of the Laplacian and it acts effectively as a topological version of a derivative: on a network it performs the gradient of the node signal and attributes that to the edges, while it performs the divergence of the edge signal and attributes it to the nodes of the network. The Topological Dirac operator has its roots in the Kogut-Susskind [140] staggered fermions defined in lattice gauge theory, but only recently it has been proposed [5] to be a key operator to study topological dynamics on higher-order networks. The Topological Dirac operator can indeed by used to define the Topological Dirac equation of higher-order networks [5] that is pivotal to define the mass of simple and higher-order networks [141]. Moreover the Topological Dirac operator is fundamental to study Topological Synchronization of coupled topological signals both in the framework of Topological Kuramoto-like models [142,143] and in the framework of Topological Global Synchronized models [144]. As the dynamics of higher-order networks is encoded on all the topological signals defined on these structures, the Topological Dirac operator can shed new lights into Topological Turing and Dirac-like patterns, which include both static [145] and dynamical pattern formation [146]. In this context one observes interesting new phenomena. For instance, in this context one can have Turing patterns for interacting node and link signals where both are inhibitors, a combination that can never give rise to patterns in the case of species reacting and diffusing on nodes of a network. Finally, as we will see in the Machine Learning section, the Topological Dirac operator is raising increasing attention as a fundamental algebraic topology operator for Topological Machine Learning.

4.5. Dynamics driven by triadic interactions

Triadic interactions are higher-order interactions that cannot be accounted by simplices or hyperedges between the nodes of a higher-order network. Triadic interactions occur when the interaction between two or more nodes is regulated or modulated by other nodes of the network significantly affecting the dynamics of the higher-order network. Evidence for triadic interactions in natural systems are multiple: in neuronal networks the synaptic activities between neurons are modulated positively or negatively by glia [147]; in ecological networks the competition between two species can be affected by the presence of a third species [148]. Although triadic interactions are widely accepted in neuroscience and ecology, only recently triadic interactions are attracting the interest of mathematicians and theoretical physicists for investigating higher-order network dynamics at the fundamental level.

It has been shown recently [22, 149] that triadic interactions can lead to triadic percolation and account for situations in which the giant component of a network or of an hypergraph is time-varying as it happens in brain or climate networks. The proposed triadic percolation model assumes that the regulatory interactions can be signed, and shows that in this scenario percolation becomes a fully-fledged dynamical process, with the size of the giant component displaying a period doubling and a route to chaos. The result sheds light on real systems in which the functional connectivity of the network is strongly dependent on time such as brain networks. Interestingly, triadic percolation on spatial networks [150] can account also for changes in the topology of the giant component.

Triadic interactions are becoming increasingly studied to investigate the properties of neuronal networks, and work in these directions include neural network models such as the Hopfield model and general models of associative memory [151, 152] in the presence of triadic interactions and models of neural mediums [150], providing insights into the spatiotemporal dynamic properties of brain networks.

Besides models that capture the dynamics in the presence of triadic interactions, recently, a new information theory approach to infer triadic interactions implemented by the TRIM algorithm has been proposed [153]. This algorithm has been applied to the inference of triadic interactions in gene regulatory networks, but the methodology can be also applied to generic network data such as climate data.

While hypergraphs, simplicial complexes, and networks with triadic interactions are often the combinatorial structure of choice to capture higher-order interactions, the question arises whether other combinatorial structures are relevant for network dynamical systems. Examples of these possible extensions include the coupled cell network formalism for higher-order network dynamics [118], directed hypergraphs [117, 154]), that may be needed for cluster synchronization or more complicated dynamics to arise [119], and further multisets generalization of higher-order interactions [155]. Elucidating the combinatorial properties of such new combinatorial structures provides an exciting opportunity; see also Section 2.

5. Higher-order Machine Learning

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Higher-order networks are at the forefront of research in machine learning and AI. The interest and relevance of this field is fueled by two important considerations. First, there is a recognition of the relevance of going beyond the pairwise description of the interactions existing in real complex systems. Secondly, there is the realization that topological signals are ubiquitous and that, in many contexts, it is important to go beyond the node-based description of higher-order network dynamics.

At the structural level, AI algorithms might adopt either a hypergraph representation or a simplicial complex representation of the higher-order networks. One central question in higher-order machine learning is to determine how information can be extracted from data associated with elements of a topological space. On one side, this is achieved by Topological Data Analysis (TDA), whose main idea is to capture the information encoded in higher-order network structure by associating nested topological spaces to the observed data and extracting information from their properties. On the other side, this is achieved by Topological Signal Processing (TSP), where the focus is on extracting information from signals defined over the elements of a topological space. Broadly speaking, a signal is a map from the elements of the space, be they points, edges, polygons, etc., onto the real domain. Examples of signals can be potential values defined over points in space and time, flow data defined over the edges of a graph, colors of the faces of a simplcial complex associated to the triangular mesh used to represent the surface geometry of a 3D object. The distinguishing feature of TSP is that the operators used to extract information from the signals are tailored to the domain where the signals are defined. In particular, TSP tools can be used to develop learning algorithms that are rooted on topological descriptors, leading to Topological Deep Learning (TDL). In TDL, learning includes both learning from data defined over a topological space as well as learning the structure of the space to be associated with the observed data.

5.1. Hypergraph representation learning

Higher-order interactions reveal structural patterns that cannot be always reduced to pairwise relations, but can be formally represented using hypergraphs [156]. Because of their pervasive presence in so many applications, there is an increasing interest in exploiting hypergraphs to extract meaningful information from their structure or from data that can be associated with the elements of a hypergraph. Merging hypergraph-based representation and machine learning is becoming an intense area of research because of its immense potential. Hypergraph representation learning (or hypergraph embedding) aims to embed the hypergraph into a low-dimensional space such that structural information is preserved, facilitating subsequent tasks such as

node clustering. A seminal work on machine learning using hypergraphs, including clustering, classification, and embedding, was proposed in [157]. For a comprehensive review of hypergraph learning, see [158, 159]. More recently, extending the potential of graph neural networks (GNNs), hypergraph neural networks (HNNs) have been proposed [160], showing significant results in a variety of applications, including missing metabolic reaction prediction [161], functional brain network classification [162], traffic flow forecasting [163] and computer vision [164]. A recent survey on HNNs is given in [165]. Growing attention is also addressed to formulate efficient hypergraph solvers for classical optimization problems such as coloring [166], matching [167,168] as well as for hypergraph partitioning [169] (we point the reader to Ref. [170] for a recent survey on the topic).

Hypergraph-based learning can occur in different ways, depending on whether the hypergraph structure is a priori known or has to be inferred from data. Furthermore, when the hypergraph is given, we might have labels (features) associated with its nodes and hyperedges. In this case, we refer to the hypergraph as the *domain* and to the space of features living on the hypergraph as the *co-domain*. The co-domain is typically a multi-dimensional vector space, but not necessarily, because the features can also be categorical. When the data are numerical, a hypergraph signal is defined as the mapping from the domain to its co-domain. The interesting aspect of this framework is that the identification of the domain allows the derivation of tools for analyzing signals defined over the domain using tools tailored to the domain and able to capture properties of the domain itself. A paramount example is Graph Signal Processing (GSP), where the Graph Fourier Transform has been defined as the projection of the signals defined over the nodes of the graph onto the space spanned by the eigenvectors of the graph Laplacian [171]. However, a graph is just a very simple case of a hypergraph, able to encode only pairwise relations. In recent years, several contributions have generalized this approach to develop processing tools suitable for topological spaces capturing higher-order relations, such as simplicial or cell complexes [133, 172–175].

5.2. Topological Data Analysis (TDA)

Topological Data Analysis (TDA) is a framework that utilizes concepts from algebraic topology to study the shape and structure of data [8]. One of the key tools in TDA is persistent homology, which provides a multiscale representation of data by tracking the birth and death of topological features such as connected components, loops, and voids across different scales [71]. TDA is particularly useful for analyzing high-dimensional, noisy, and complex datasets where traditional statistical or machine learning methods may struggle to capture underlying geometric structures.

A fundamental concept in TDA is the notion of a *filtration*, which is a sequence of nested topological spaces that describes the evolution of structures as a function of a scale parameter. Given a point cloud dataset, a filtration is constructed by progressively connecting points based on their pairwise distances, typically using a Vietoris–Rips

or Čech complex [72]. As the scale parameter increases, topological features such as connected components, loops, and voids appear and disappear, and their persistence across multiple scales is recorded in the form of *persistence diagrams* or *barcodes*.

TDA is widely applied in various domains, including biology (e.g., protein structure analysis), neuroscience (e.g., brain connectivity), and machine learning (e.g., feature extraction for classification) [72]. The core idea behind TDA is to build a topological space from data points using simplicial complexes and then extract meaningful topological invariants. These invariants provide insights into the data's shape and connectivity. A key strength of TDA is its ability to generalize across different data types and its robustness to noise. Unlike graph-based models, which primarily capture pairwise relationships, TDA considers higher-order structures, making it a powerful tool for uncovering complex interactions within datasets. Advances in TDA have inspired new approaches in topological machine learning, where persistent diagrams and topological features are integrated with neural network architectures for tasks like classification, clustering, and generative modeling [176].

Recent advancements in TDA have extended its application to data defined over hypergraphs. Hypergraphs, which generalize graphs by allowing edges (hyperedges) to connect multiple nodes, naturally encode higher-order interactions present in complex datasets [177]. Standard graph-based TDA techniques often fail to capture these rich relationships, necessitating new frameworks for topological analysis on hypergraphs.

Persistent homology is naturally defined on simplicial complex representation of data. However, persistent homology can be adapted to hypergraphs by constructing simplicial complexes from hypergraph structures, such as the clique expansion or other higher-order representations [178]. By analyzing the resulting persistence diagrams, researchers can extract meaningful insights into the higher-order topology of the data, allowing for improved clustering, anomaly detection, and feature extraction [179]. Further, based on infimum chain complexes and supremum chain complexes derived from hypergraphs, persistent embedded (co-)homology has been developed to characterize the intrinsic hypergraph topology, instead of its associated simplicial complex [80, 180].

Applications of hypergraph-based TDA include material science [181–183], where higher-order interactions encompass a wide range of couplings that extend beyond simple two-body forces, biological networks [184] including gene interaction studies, and molecular interactions such as protein-ligand interactions [180], and higher-dimensional embeddings in machine learning [185]. The integration of TDA with hypergraph representations provides a promising avenue for understanding complex datasets beyond traditional graph structures.

Persistent homology is computationally demanding, and typically restricted in practice to homological classes of low order. If this is an over-simplification, typically one selects a subset of essential simplices of higher order. To face this challenge, significant attention is devoted to the study of quantum algorithms based on the use of the Topological Dirac Operator [186–189] which aim to overcome the computational limitations of classical persistent homology algorithms. Note, however, that the

quantum speed up of these algorithms is achieved only once the full information on the higher-order interactions (simplices, cliques) is known [190]. To face this challenge, recently [191] a universal programmable photonic quantum processor has been physically implemented. This processor can identify weighted k-cliques and estimate Betti numbers by leveraging the Gaussian boson sampling algorithm's ability to preferentially select high-weight, dense subgraphs of a weighted network. Therefore this photonic quantum computing approach opens new perspectives for quantum-enhanced TDA.

5.3. Topological Signal Processing (TSP)

Recently algebraic topology has been combined with machine learning to reconstruct topological signals opening a entire new perspective in signal processing, leading to the emergent field of *Topological Signal Processing* (TSP) [133, 172, 192] and the further development of *Topological Deep Learning* (TDP) that we will discuss in the next paragraph. This field is attracting increasing attention because topological signals have a broad relevance in numerous applications, including, most relevantly, brain research [134].

The distinctive feature of Topological Signal Processing (TSP) is that it is able to derive operators that capture the intrinsic properties of the space where the signals are defined. Historically speaking, the first important framework where this idea was thoroughly investigated is Graph Signal Processing (GSP), where the data are associated with the vertices of a graph and where relations between pairs of signals are encoded by the presence of an edge between the corresponding vertices [193]. In GSP, a key operator is the Graph Fourier Transform (GFT), defined as the projection of the vector associated with the whole set of (scalar) parameters living over all the vertices, onto the space spanned by the eigenvectors of the graph Laplacian. The underlying idea is that if the signal is smooth on the graph – i.e., if it is slowly varying within each cluster, although it may vary arbitrarily across different clusters – then the GFT of the signal is approximately sparse. Recovering a sparse representation of the signal is a key property that enables sampling and recovery of the overall signal from the observation of a subset of values [194]. The existence of a GFT is also fundamental to study the properties of filters operating over graphs [193]. Typically, a filter is defined as a localized operator that aggregates data associated with neighboring vertices and is used to reduce the effect of noise or to emphasize certain parts of the spectrum with respect to others [195].

In GSP, the signals are typically only associated with the vertices of a graph (i.e., singleton sets). However, there are many applications where the data are associated with sets of higher cardinality, for example: flow data, associated with pairs of nodes; or the number of co-authored papers, where each number is associated with the set of all the co-authors. In general, we may then talk about Topological Signal Processing (TSP), i.e, methods for processing signals defined over topological spaces. In these cases, higher order relations between the data can be encoded using simplicial complexes. Restricting the attention to more structured domains, such as a simplicial complex, makes it possible

to derive, in a principled way, a well-defined spectral representation, with consequent sampling theory and spectral filter design [133,172,196]. The extension to cell complexes has also been provided [173–175].

One of the main aspects of the topological approach to signal processing is represented by the Hodge decomposition, which provides a principled way to process signals with operators that can discriminate different components in a way that reflects some fundamental properties of the space where the signals are defined. An interesting application of these methodologies is the processing of a vector field defined over a set of points (i.e., a point cloud). Through proper triangulation, it is possible to build a mesh representation of the point cloud. A vector field – that is, a set of vectors defined over the vertices of a graph – can then be transformed into a set of scalar values defined over the edges of a simplicial complex [133]. These (flow) signals can then be filtered, exploiting Hodge decomposition to highlight, for example, rotational or divergence components, and the result can be mapped back onto a (filtered) vector field, as suggested in [133].

As mentioned before, using simplicial or cell complexes, reveals a number of properties that can be efficiently exploited, but lacks the full generality of hypergraph formulations. Recent work has introduced a tensor-based representation to deal with the more general case of signals defined over a hypergraph [197]. Extracting information and learning from hypergraph data enriched with topological signals has huge potential to advance our understanding of complex system dynamics [19]. Interestingly, however, the authors of [20] showed that signals defined over a hypergraph can be translated into signals defined over a *weighted simplicial complex*. This approach makes possible to circumvent the limitations of unweighted simplicial complexes to represent higher-order interactions.

An interesting application of TSP and Hodge decomposition is the analysis of brain networks. The study in [198] applies Hodge decomposition to brain network analysis by decomposing connectivity patterns into gradient, curl, and harmonic flow components, effectively capturing complex topological features. Leveraging a Wasserstein distance-based topological inference framework, the method identifies statistically significant differences in the topological organization of male and female brain networks using resting-state fMRI data. Further advancements in [199, 200] introduce a persistent homology-based approach that employs the Hodge Laplacian to detect and analyze cyclic structures (topological cycles) in brain networks. These methods are validated through both simulations and resting-state fMRI experiments. In a related direction, [201] presents a noise-resilient EEG analysis technique that integrates persistent homology with a Bayesian framework, enabling robust classification of EEG signals that are typically noisy, nonlinear, and nonstationary.

5.4. Topological Deep Learning (TDL)

Advances in TDA have inspired new approaches in topological machine learning, in which persistent diagrams and topological features are integrated with neural network

architectures for tasks like classification, clustering, and generative modeling [176]. Neural networks (NNs) can be extremely effective when the architecture of the network is designed to incorporate geometric key properties of the domain in which the signal is defined. This is the case for convolutional neural networks (CNNs), which exploit the translation equivariance of convolution operator when applied to data defined on a regular grid, such as sounds or images. The resulting architecture significantly reduces the number of parameters that need to be trained and makes the learning process much more robust [202]. This idea has been generalized to applications where the data are defined on a graph or a manifold [203], [204]. More recently, deep neural networks have been generalized to data living over higher order structures such as simplicial complexes, giving rise to various forms of simplicial neural networks [205–207] – see also [208] for a review. Simplicial neural networks and Hodge representation of networks have been applied, for instance, in power outage detection [209] and in false data injection attacks in smart grids [210].

An interesting field of application is biological data modeling. In this field, a central challenge in graph-based learning is the classification of molecules—or even the generation of novel ones—using only a limited training dataset [211, 212]. Many advancements in message-passing neural networks (MPNNs) have been specifically developed to address the limited expressivity of Graph Neural Networks (GNNs) under the Weisfeiler-Lehman (WL) framework for graph classification tasks [192], [213]. Molecules, in particular, can be naturally modeled as structurally complex graphs that encode both explicit features and implicit topological information [214]. By introducing higher-order structures, such as simplicial complexes or cellular complexes, into molecular graphs through a process known as lifting [215], topological neural networks (TNNs) can capture and exploit these topological dependencies to learn more expressive representations. Hodge theory has also been used in [216] to analyze biomolecular structures. In this context, biomolecules are modeled as simplicial complexes with defined edge flows, where the spectrum of the associated Hodge Laplacian encodes structural properties and provides insight into molecular folding and compactness.

An interesting challenge that arises when dealing with data defined on subsets (chains) of different order – such as vertices, edges, and polygons – is whether these features should be handled in parallel and how. A principled way to address this question is to use the (discrete) Dirac operator [5]. In [217], this idea was used to derive filters as polynomial functions of the Dirac operator, giving rise to the so called simplicial attention neural network architecture, which also includes an attention mechanism operating over signals (co-chains) of different order.

A further mathematical framework that could have a significant impact on topological learning is sheaf theory [218]. The application of sheaf theoretic principles to signal processing was analyzed in [219]. A structure that may be particularly relevant for signal processing and learning is a *cellular sheaf*. If applied to data defined over a graph, a cellular sheaf consists of vector spaces associated with each vertex and to linear maps,

called *restriction maps*, associated with each edge in the graph [220]. This definition can be extended to higher order structures such as simplicial complexes, including linear maps from edges to triangles, and so on. Within such a model, a fundamental operator is the *sheaf Laplacian operator*, which generalizes the classical Hodge Laplacian operator, incorporating the restriction maps.

A fundamental step in applying sheaf theory to machine learning is the inference of the sheaf Laplacian from data; a possible solution to this problem was suggested in [221]. More recent work has extended this work to infer the structure of the restriction map as well as the graph topology from data [222]. Sheaf-based models have also been used in conjunction with deep neural networks, as a generalization of graph neural networks (GNNs) – for example, in [223], where sheaf diffusion models are shown to possess many desirable properties that address the limitations of classical graph diffusion equations (and corresponding GNN models) and obtain competitive results, especially in heterophilic settings.

6. Higher-Order Network Science: from Theory to Applications

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Higher-order interactions represent the next natural step in the mathematical analysis of dynamical processes on network topologies in practical settings [4]. Embracing higher-order structures, such as hypergraphs, simplicial, and more general cell complexes, allows parsimonious yet expressive representations of group-mediated mechanisms across domains. Incorporating higher-order dynamics (Sec. 4) sharpens our understanding of emergent phenomena and reveals behaviors absent in pairwise models: higher-order interactions can reshape thresholds, stability, and response, with documented consequences for synchronization [106], contagion [109], and percolation [132], among others. Beyond node states, topological signals supported on edges and higher-dimensional simplices encode fluxes in complex systems, such as ocean currents or dynamic connectivity in brain networks. The study of collective dynamics (Sec. 4.3)—including abrupt or multistable synchronization—can be intrinsically different from node-based counterparts [25].

In what follows, we organize the discussion around four application fronts where higher-order modeling is already altering the agenda. In epidemic spreading, group exposure and nonlinear transmission rules modify effective transmissibility and phase structure, with implications for inference and control. In game theory, multiplayer interactions embedded in higher-order structures reveal cooperation patterns and transitions unattainable on dyads alone. In social network analysis, higher-order representations align naturally with affiliation and group data, enabling centrality, mesoscale, and motif analyses consistent with multilevel structure. In brain research, directed higher-order motifs, edge/face-level signals, and topological descriptors connect

micro- to mesoscale organization with functional dynamics.

Network science ultimately relies on empirical data, and the next step is to co-design experiments where higher-order interactions and their associated dynamics can be observed, measured, and integrated into models [224]. This perspective ensures that higher-order network science remains tightly coupled to data, enabling robust theory–experiment feedback loops across disciplines.

6.1. Epidemic spreading

Epidemic spreading is a pivotal dynamical process on networks, where the topology of the underlying contact network plays a crucial role in shaping the characteristics of epidemic. Traditional models often represent contacts as pairwise interactions between individuals, neglecting the fact that real-world social and biological systems frequently involve higher-order interactions, such as group meetings, shared environments, or concurrent transmissions in small groups [4]. These higher-order structures can fundamentally alter epidemic dynamics by modifying the effective transmissibility [109, 225–228], introducing non-linear effects, and influencing outbreak thresholds. However it is worth noticing that heterogeneous group weights can induce an apparent superlinear signature even for simple contagion, complicating mechanism inference [229]. Incorporating higher-order interactions into epidemic models through frameworks such as simplicial complexes and hypergraphs offers a more realistic representation of contagion processes [6, 230, 231].

The simple contagion framework is widely used in epidemic modeling. It assumes infection can occur between an infected and a susceptible individual after a single exposure. However, real-world epidemic dynamics often involve complex contagion, where exposure to multiple infected individuals is necessary for transmission [232]. Higher-order networks provide an ideal framework for capturing complex contagion in epidemics.

From the theoretical perspective, higher-order interactions can lead to non-linear relationship between the exposure to infected contacts and the risk of infection, which can induce novel critical phenomena [233] such as discontinuous hybrid phase transition, super-exponential spread and hysteresis [111], which are partially supported by empirical studies [234, 235]. Control-oriented analyses further show bistability and parameter domains in multi-group simplicial SIS [236]. In addition, the structure of the underlying higher-order network strongly affects the critical properties, such as hyperdegree correlation [21, 237], and hyperedge overlap [228, 238–241].

From an empirical perspective, [242] provided experimental evidence that behaviors often spread as 'complex contagions', requiring multiple sources of reinforcement, a hallmark of higher-order interactions. The authors demonstrated that centrality measures and seeding strategies based on the classical definition of path length frequently fail to identify the network features most effective for spreading complex contagions.

Beyond memoryless single-pathogen settings, non-Markovian higher-order conta-

gion and competing pathogens on simplicial complexes introduce additional bifurcations and regimes [243, 244]. Despite the rich phenomenology induced by higher-order interactions and the rich insights gained from analytical and numerical studies, applying higher-order network models to real-world epidemics remains challenging. A major challenge in applying higher-order network models to real-world epidemics is the limited availability of higher-order contact network data. Distinguishing between simple and complex contagion from empirical data remains an open problem, crucial for selecting the most suitable epidemic modeling framework [245, 246].

6.2. Game theory

Since its inception, game theory has provided a framework for n-body strategic interactions [247, 248]. When applied to structured populations, mainly in evolutionary game theory, the emphasis has historically been on pairwise games on networks, which have been extensively used to study social dilemmas such as the Prisoner's Dilemma, Stag Hunt, and Snowdrift [249–251]. These models emphasised the role of network reciprocity in sustaining cooperation [252]. Building on this foundation, group games on pairwise networks, notably the Public Goods Game (PGG), extended the analysis to collective interactions [253–255].

In parallel, game-theory-focused studies explored equilibria in general multiplayer settings but often neglected the role of structured populations [256–258]. More recently, strategic interactions have been modelled beyond pairwise dynamics using higher-order structures such as simplicial complexes and hypergraphs [259–263]. In these settings, payoffs are generated at the group level, so the size and composition of each hyperedge directly modulate marginal returns, thresholds, and the balance between synergy and discounting. Overlapping group membership couples multiple games that a single player participates in, which creates cross-group feedback and can shift both equilibrium selection and basin size. These mechanisms yield phenomena that are absent or rare in dyadic models, including bistability and discontinuous transitions to cooperation, now observed in higher-order social dilemmas [264]. Higher-order frameworks also allow different strategic scenarios to coexist within the same population, for example by assigning distinct payoffs or rules to different hyperedge types, which provides a versatile setting for comparing public goods, coordination, and anti-coordination within a single model [264–266]. Adaptive higher-order games further reveal stability properties under the coevolution of topology and strategy [267], and higher-order settings reshape interactions beyond classical dilemmas, including signalling games [268].

Despite this progress, a unified framework that combines the flexibility of higher-order networks with the generality of multiplayer games remains an open goal. Such a framework would enable systematic exploration of strategic interactions across social, biological, and economic systems, clarifying how group structure, overlap, and composition shape strategic behaviour and collective outcomes.

6.3. Social network analysis and social contagion

Traditional pairwise representations often underfit the mechanisms that drive social systems, where interactions are generated by groups, multiway affiliations, or temporally ordered pathways. Higher-order models capture these features along two complementary axes. First, group-based representations (hypergraphs, simplicial complexes) encode interactions among sets of actors, enabling direct analysis of mesoscopic structures such as overlapping groups, higher-order motifs, and their role in diffusion and coordination [261, 263, 269]. Second, path-based higher-order (memory) models capture non-Markovian dependencies in sequences of social interactions, which strongly affect diffusion speed, reachability, and controllability [224, 270, 271].

A core task is to infer higher-order structure from data. Beyond projecting groups to pairwise links, recent work exploits time-stamped simplices to track how open triplets or k-tuples close into higher-order interactions, and uses this to formulate higher-order link prediction benchmarks ("simplicial closure") and learning tasks [272]. This program has produced practical predictors that favor local higher-order features over long-range information and has been extended to feature-aware settings, e.g., higher-order homophily that conditions which groups form [273,274]. In parallel, centrality and mesoscale structure have been generalized to the higher-order setting: tensor/nonlinear eigenvector centralities quantify node and hyperedge importance [275, 276], while community detection in hypergraphs now enjoys consistency and recovery guarantees under planted models, including sparse regimes [277–279]. These tools allow analysts to reason about influence, mixing, and roles at the group level rather than only on dyads.

Social contagion provides a particularly clear arena where higher-order modeling changes conclusions. Empirically, many behaviors require multi-source reinforcement (complex contagion), which privileges clustered or overlapping group structure [280,281], see Fig.5.

Higher-order contagion models on simplicial complexes and hypergraphs formalize these mechanisms and reveal qualitative shifts relative to pairwise diffusion, including discontinuous transitions, hysteresis, and topological prerequisites for global cascades [109, 111, 228, 230, 231]. Methodologically, distinguishing simple from complex contagion from a single cascade is feasible by exploiting order-of-infection patterns and local topology, providing a bridge from data to mechanism [245]. Together, these results suggest that seeding, targeting, and evaluation strategies should be designed in the higher-order space (hyperedges, motifs, pathways) rather than solely with node-level centralities or shortest-path metrics.

Finally, because network science relies on data, progress will hinge on co-designed experiments and platforms that record group interactions [282] and temporal pathways at sufficient resolution. This includes instrumentation of online communities and field studies to capture explicit group events, annotated higher-order ties, and time-resolved participation, enabling direct estimation of higher-order exposure, reinforcement, and their causal impact on adoption.

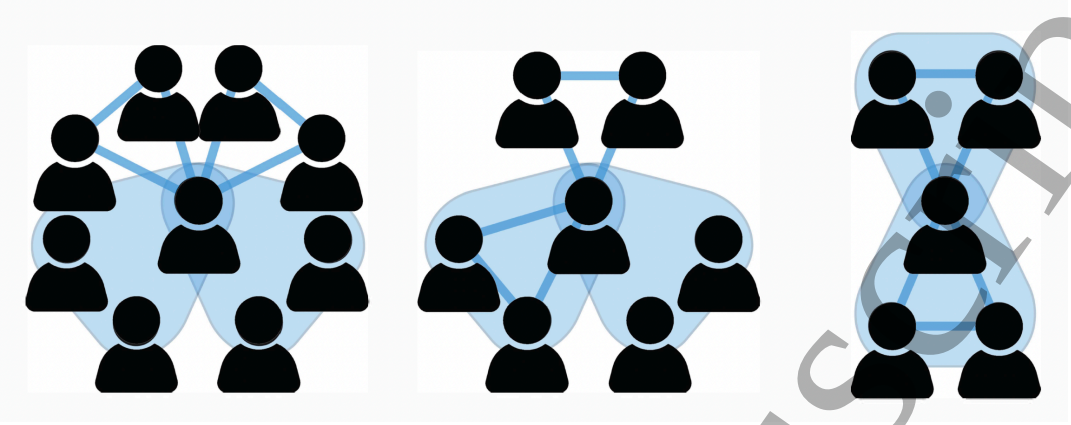

Figure 5. Representative patterns of overlapping group structure underlying multi-source contagions. From left to right the panels illustrate scenarios in which pairwise and higher-order interactions do not have any overlap (left), do partially overlap (middle) or do completely overlap (right). Only structural configurations are shown (no dynamics); such overlap can condition the resulting contagion behaviour.

6.4. Brain networks

Understanding brain function requires capturing interactions that extend beyond pairs of elements. Cognitive and behavioral dynamics often emerge from collective activity among groups of neurons or regions, and both experimental and theoretical work has shown that pairwise descriptions are insufficient. For instance, analyses of rat somatosensory cortex recordings demonstrated that synchronous population discharges can only be explained by including third- or fourth-order interactions, not by pairwise statistics alone [283]. This result stands in contrast to the seminal findings of Schneidman and colleagues [284], who showed that maximum entropy models constrained only by pairwise correlations could already capture much of the collective activity of retinal populations, suggesting that strong collective states may arise from weak pairwise interactions alone. Together, these studies highlight an ongoing debate at the neuronal level: whether higher-order models are genuinely required, or whether low-order interactions suffice once considered at the right scale. This tension motivates current efforts to determine when higher-order dependencies are irreducible, and frames the importance of investigating both microcircuit activity and mesoscale organization.

Two complementary scales are particularly relevant. At the *cellular and microcircuit level*, directed connectivity is essential: synapses transmit signals from presynaptic to postsynaptic neurons, and generalizations such as directed simplicial complexes allow one to model cliques of neurons with unique sources and sinks. Directed cliques have been identified in neocortical models, where they shape stimulus–response patterns [285], and in striatal circuits, where disease-linked degeneration alters motif distributions [286] and functional connectivity [287] with implications for Parkinson's disease. Another microscopic example comes from *triadic interactions*, which capture modulatory influences such as axo-axonal synapses or astrocytic regulation at the

tripartite synapse. Modeling schemes based on triadic percolation [150, 288] show how such regulations can dynamically rewire neuronal connectivity and generate complex spatiotemporal patterns of activity.

At the *mesoscale of brain regions*, functional connectomes are often represented as weighted graphs, but edge-centric and higher-order representations provide richer views. Edge time-series and edge functional connectivity reveal overlapping mesoscale organization and moment-to-moment cofluctuations [289, 290]. Higher-order connectomics and multivariate higher-order time-series methods extract genuine interactions among triples or larger sets of regions, improving task decoding, subject identification, and brain–behavior associations compared to pairwise baselines [291]. Recent work further demonstrates how *homological* structure and higher-order models capture subject identity and functional organization beyond and better than pairwise descriptors, as well as systematically compare HOI metrics across tasks and states [292, 293]. Perturbational studies indicate that neuromodulation can reshape redundancy–synergy balances and higher-order network plasticity [294].

Inferring genuine higher-order dependencies from data remains a methodological frontier. While topological approaches typically assume interactions are given, information theory provides tools for discovery. Partial entropy decomposition and related frameworks extend mutual information to decompose interactions into redundant, unique, and synergistic components [295]. Applications to fMRI, EEG, and MEG have revealed robust signatures of synergy—information present only in the joint activity of multiple regions—that correlate with cognitive functions and decline with aging, shifting toward redundancy [296, 297]. Such measures show promise as biomarkers, complementing structural and functional connectivity.

Topological Data Analysis (TDA) offers complementary approaches to detect and summarize higher-order organization. Clique topology and cavity structure have been reported in human connectomes [298], supporting the view that computation leverages densely connected assemblies and loop-like pathways. Persistent homology pipelines have been applied to brain networks across conditions, from schizophrenia to pharmacological modulation, while homological scaffolds extract cycle representatives that differentiate between clinical and control cohorts [299–301]. Emerging clinical applications highlight potential for surgical planning and outcome prediction, as in epilepsy surgery where resected tissue exhibits distinctive topological signatures [302].

Finally, methodological advances that bridge higher-order dynamics and brain data—such as edge/face signals, Dirac and simplicial synchronization, and higher-order inference—suggest a path toward integrative models linking micro- and mesoscale organization to functional dynamics [10, 25, 142, 143]. These efforts underline how structural, dynamical, topological, and informational perspectives can be woven into unified models of brain function. Future progress will hinge on engineered measurement programs—combining dense neurophysiology, multimodal imaging, and large-scale cohorts—with methodological advances in higher-order inference and topological signal processing. By bridging these layers, higher-order frameworks may yield not only

more faithful descriptions of brain organization but also actionable insights for clinical translation.

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