1 The Relevance of Higher-Order Networks in Network Science

1.1 Simplicial Complexes as Generalized Network Structures

Network science [1–4] is rooted on the idea that the complexity of interacting systems can be captured by the network of interactions between their constituents. This very powerful framework has enabled the scientific community to make unprecedented progress in the understanding of complex systems ranging from the brain to society. In the last 20 years, network theory has revealed the rich interplay between the network topology and dynamics [3, 5]. It has been shown that universal statistical properties of complex networks, such as the scale-free degree distribution and the small-world nature of complex networks, are responsible for the surprising dynamical properties that processes such as percolation, epidemic spreading, Ising model and synchronization display in these networks.

Recently, mounting evidence reveals that to make the next big leap forward in understanding and predicting the behavior of complex networks it is important to abandon the framework of a simple network formed exclusively by pairwise interactions and use generalized network structures that can better capture the richness of real data. Multilayer networks [6] are well-studied generalized networks that are able to treat datasets in which interactions have different nature and connotation displaying a rich interplay between structure and dynamics. More recently the research attention has been focusing on higher-order networks [7–11] that allow capture of the many-body interactions of complex systems going beyond the pairwise interaction framework.

Consider for example three regions of the brain. These three regions can be correlated with each other pairwise via three two-body interactions or might be related by a higher-order (three-body) interaction, revealed by the fact that these three regions of the brain are typically activated at the same time. These two scenarios correspond to very different dynamics that can be distinguished only by considering higher-order networks. Indeed in the first case the higher-order network between the three regions of the brain will include just three links, while in the second case the three brain regions would form a three-body interaction indicated by a filled triangle (also called a two-dimensional simplex). In social networks a notable example of a higher-order network is constituted by the set of face-to-face interactions at a party or during a coffee break at a conference. In this context the people will form conversation groups, often involving more than two individuals, in which ideas are shared and elaborated in a way that is not reducible to a set of pairwise conversations.
Likewise in protein interaction networks proteins bind to each other forming protein complexes typically including more than two different proteins. Only when the protein complex is fully assembled is the protein complex able to perform its biological task. This indicates that the biological function of the protein complex is the result of many-body interactions between its constituent proteins and cannot be reduced to a set of pairwise interactions.

Higher-order networks fully capture the interactions between two or more nodes and are necessary to describe dynamical processes depending on many-body interactions. In recent years this research field has boomed and important new progress has been made to uncover the interplay between higher-order structure and dynamics. In this work we aim to provide a brief introduction to the subject that could be useful for graduate students and for researchers to jump start into this lively research field.

1.2 Simplicial Complexes and Hypergraphs

When faced with the problem of capturing higher-order interactions existing in a dataset, two generalized network structures are potentially useful for the researcher: simplicial complexes and hypergraphs.

Both simplicial complexes and hypergraphs capture higher-order interactions and are formed by a set of nodes \( v_2 \in \{1,2,3\ldots,N\} \) and a set of many-body interactions including two or more nodes, such as

\[
\alpha = [v_0, v_1, \ldots, v_d],
\]

with \( d \geq 1 \). These many-body interactions are called *simplices* of a simplicial complex or *hyperedges* of a hypergraph. These higher-order interactions induce a very rich combinatorial structure for higher-order networks [12] that can also have very relevant consequences for higher-order dynamics, including synchronization and contagion processes [13, 14]. As both simplicial complexes and hypergraphs capture the many-body interactions in a complex system, the vast majority of many-body phenomena obtained in one framework can be directly translated into the other framework.

The only difference between simplicial complexes and hypergraphs is a subtle one: the set of simplices of a simplicial complex is closed under the inclusion of subsets of the simplices in the set while no such constraint exists for a hypergraph. This means that in a simplicial complex, if the simplex \( \alpha \) given by

\[
[v_0, v_1, v_2],
\]

belongs to the simplicial complex, then the simplices...
must also belong to the simplicial complex. In other words, if we consider a collaboration network in which three authors have written a paper together, then we should include in the simplicial complex also the three pairwise interactions between the authors and the set of the three isolated nodes. This might look like an artificial constraint, but actually it comes with the great advantage that simplicial complexes are natural topological spaces for which important topological results exist. This widely developed branch of mathematics provides a powerful resource for extracting information and revealing the interplay between topological and geometrical properties of higher-order networks and their dynamics.

The scientific research on higher-order networks is currently growing and many important results have been recently obtained in this field. In this Element, our goal is to provide a self-contained, coherent and uniform account of the results on higher-order networks. For space limitations we have chosen to focus mostly on simplicial complexes. However, on a number of occasions we will refer to results exclusively applying to hypergraphs.

1.3 A Topological Approach to Complex Interacting Systems

A simplex characterizes an interaction between two or more nodes. The simplices of a simplicial complex are glued to one another by sharing a subset of their nodes, resulting in topological spaces. Topological spaces have a number of features, for instance they can be characterized not only by the number of their connected components, like networks, but also by the number of their higher-order cavities or holes indicated by their Betti numbers. Applied topology [8, 15–19] studies the underlying topology (including the Betti numbers) of simplicial complexes coming from real data. This field has been flourishing in the last decades and was initially applied to extract information from data-clouds coming from different sources of data including, for instance, gene-expression. An important framework that has been developed in applied topology is called persistent homology and is based on an operation called filtration that aims at coarse-graining the data with different resolution characterizing how long topological features persist. Only recently [20, 21] has this approach been applied to real networked data and in particular to brain functional networks, which are weighted networks in which the filtration procedure is not simple coarse-graining, rather it is substituted with a change of threshold in the weights of the links. Persistence homology of complex networks is a powerful topological tool that makes extensive use of the simplicial representation of data and has shown to reveal differences not accounted for by
other more traditional Network Science measures. However the possibility of using persistence homology is by no means the only benefit of using topology to analyze higher-order networks. In neuroscience [8, 22] the use of simplicial complexes has been booming in recent years and novel results show the rich interplay between topology and dynamics in the framework of the in-silico reconstruction of rat brain cortex [23]. Moreover, simplicial topology can be also used to investigate the local [24] and the meso-scale structure [25, 26] of network data.

Departing from the benefit that topology can bring to higher-order data analysis, recently it has been shown that topology, and specifically Hodge theory, can be exploited by higher-order networks for sustaining and synchronizing higher-order topological signals, i.e. dynamical variables that are not only defined on the nodes of the network, but rather like fluxes they can be defined on links or even on higher-order structures like triangles or tetrahedra [27]. Interestingly topological signals are also attracting increasing attention from the signal processing perspective [28].

This multifaceted research field clearly shows that topology is a fundamental tool to investigate higher-order network structure and dynamics.

1.4 A Geometrical Approach to Higher-Order Networks

If the links of a simplicial complex are assigned a distance, simplices have an automatic interpretation as geometrical objects, and can be understood as nodes, links, triangles, tetrahedra, etc. In particular, in absence of other data that can be used to assign a distance to each link, the network scientist can always choose to assign the same distance to each link.

Since simplicial complexes describe discrete simplicial geometries, modeling simplicial complexes opens the possibility to reveal the fundamental mechanisms of emergent simplicial geometry.

The long-standing mathematical problem of emergent geometry originates in the field of quantum gravity, but this field is also very significant for complex systems such as brain networks. Emergent simplicial geometry refers to the ability of non-equilibrium or equilibrium models to generate simplicial complexes with notable geometric properties by using purely combinatorial rules that make no explicit reference to the network geometry. For instance emergent geometry models should be independent of any possible simplicial complex embedding.

Recently a series of works [29–31] has proposed a theoretical framework called Network Geometry with Flavor that captures the fundamental mechanism of emergent hyperbolic geometry. This framework opens a new perspective into the long-standing problem of emergent geometry and has possible
implications ranging from quantum gravity to complex systems. Additionally, this framework generates simplicial networks whose underlying network structure displays all the statistical properties of complex networks including scale-free degree distribution, high clustering coefficient, small-world diameter and significant community structure. The resulting simplicial complexes can reveal distinct geometrical features including a finite spectral dimension [32, 33]. The spectral dimension [34] characterizes the slow relaxation of diffusion processes to their equilibrium steady-state distribution, similarly to what happens for finite-dimensional Euclidean networks. However, higher-order networks with finite spectral dimensions might dramatically differ from Euclidean networks. In fact a finite spectral dimension can co-exist with small-world properties (including an infinite Hausdorff dimension) and a non-trivial community structure. The intrinsic geometrical nature of simplicial complexes with finite spectral dimensions can have a profound effect on dynamical processes such as diffusion and synchronization [35, 36]. In particular, if the spectral dimension $d_S$ is smaller than four, $d_S \leq 4$, it is not possible to observe a synchronized phase of the Kuramoto dynamics and strong spatio-temporal fluctuations are observed instead.

Hyperbolic simplicial geometry also has an important effect on percolation processes. Indeed, percolation on hyperbolic simplicial complexes can display more than one transition and critical behavior at the emergence of the extensive component that deviates from the standard second-order continuous transition. Indeed discontinuous transitions or continuous transitions with non-trivial critical behavior can be found, depending on the geometry of the higher-order network [37].

1.5 The Advantages of Using Simplicial Complexes and the Outline of the Element Structure

Beside allowing a full topological analysis of higher-order networks, simplicial complexes have the following two advantages: they capture the many-body interactions of a complex system and they allow us to uncover the important role that simplicial topology and simplicial geometry have in dynamics. So far our understanding of the interaction between structure and dynamics has focused on the combinatorial properties of networks (such as their degree distribution) and some of their spectral properties [3, 5]. Study of the interplay between higher-order networks starts to reveal a much richer picture summarized in the diagram presented in Figure 1 in which discrete simplicial network geometry and topology provides new clues to interpret higher-order dynamics. This very innovative framework is emerging from recent research on higher-order networks and has the potential to significantly change the way in which
The Structure and Dynamics of Complex Networks

Figure 1 The interplay between higher-order structure and dynamics is mediated by the higher-order combinatorial and statistical properties combined with simplicial network topology and geometry.

we investigate the interplay between structure and dynamics in complex systems. In this Element our goal is to provide the fundamental tools to understand the current research in the field and to make the next steps in this wonderful world of higher-order networks. The Element will introduce important aspects of discrete topology and discrete geometry in a pedagogical way accessible to the interdisciplinary audience of PhD students and researchers in network science.

The Element is structured as follows: in Section 2 we will provide the mathematical definitions of simplicial complexes and discuss their combinatorial and statistical properties, covering generalized degrees and the maximum entropy models of simplicial complexes; Section 3 will cover the basic elements of simplicial network topology, ranging from Topological Data Analysis (TDA) of simplicial complexes, to properties of the higher-order Laplacians; Section 4 is devoted to simplicial network geometry; Section 5 discusses models of emergent geometry including Network Geometry with Flavor; Sections 6, 7, 8 discuss higher-order dynamics including synchronization, percolation and contagion models; finally in Section 9 we provide concluding remarks. The Appendices provide further useful details on the material presented in the main body of this work.
Due to space limitations we have adopted a style that favors coherence of narrative over providing an exhaustive review of all the papers on the subject. Therefore we regret that we have not been able to cover all the growing literature on the subject.

2 Combinatorial and Statistical Properties of Simplicial Complexes

2.1 Mathematical Definitions

2.1.1 Basic Properties of Simplicial Complexes and Hypergraphs

A network is a graph $G = (V, E)$ formed by a set of nodes $V$ and a set of links $E$ that represent the elements of a complex system and their interactions, respectively. Networks are ubiquitous and include systems as different as the WWW (web graphs), infrastructures (such as airport networks or road networks) and biological networks (such as the brain or the protein interaction network in the cell). Networks are pivotal to capturing the architecture of complex systems; however, they have the important limitation that they cannot be used to capture the higher-order interactions. In order to encode for the many-body interactions between the elements of a complex system, higher-order networks need to be used. A powerful mathematical framework to describe higher-order networks is provided by simplicial complexes. Simplicial complexes are formed by a set of simplices. The simplices indicate the interactions existing between two or more nodes and are defined as follows:

**Simplices**

A $d$-dimensional simplex $\alpha$ (also indicated as a $d$-simplex $\alpha$) is formed by a set of $(d + 1)$ interacting nodes

$$\alpha = [v_0, v_1, v_2, \ldots, v_d].$$

It describes a many-body interaction between the nodes. It allows for a topological and a geometrical interpretation of the simplex.

For instance, a node is a 0-simplex, a link is a 1-simplex, a triangle is a 2-simplex a tetrahedron is a 3-simplex and so on (see Figure 2).

**Faces**

A face of a $d$-dimensional simplex $\alpha$ is a simplex $\alpha'$ formed by a proper subset of nodes of the simplex, i.e. $\alpha' \subset \alpha$. 
A simplicial complex $K$ is formed by a set of simplices that is closed under the inclusion of the faces of each simplex. The dimension $d$ of a simplicial complex is the largest dimension of its simplices.

Simplicial complexes represent higher-order networks, which include interactions between two or more nodes, described by simplices. In more stringent mathematical terms a simplicial complex $K$ is a set of simplices that satisfy the following two conditions:

1. A simplicial complex $K$ is formed by a set of simplices that is closed under the inclusion of the faces of each simplex.
2. The dimension $d$ of a simplicial complex is the largest dimension of its simplices.
(a) if a simplex $\alpha$ belongs to the simplicial complex, i.e. $\alpha \in \mathcal{K}$, then any face $\alpha'$ of the simplex $\alpha$ is also included in the simplicial complex, i.e. if $\alpha' \subset \alpha$ then $\alpha' \in \mathcal{K}$;

(b) given two simplices of the simplicial complex $\alpha \in \mathcal{K}$ and $\alpha' \in \mathcal{K}$ then either their intersection belongs to the simplicial complex, i.e. $\alpha \cap \alpha' \in \mathcal{K}$, or their intersection is null, i.e. $\alpha \cap \alpha' = \emptyset$.

Here and in the future we will indicate with $N$ the total number of nodes in the simplicial complex and we will indicate with $N_{[m]}$ the total number of $m$-dimensional simplices in the simplicial complex (note that $N_{[0]} = N$). Furthermore we will indicate with $Q_m(N)$ the set of all possible and distinct $m$-dimensional simplices that can be present in a simplicial complex $\mathcal{K}$ including $N$ nodes. With $S_m(\mathcal{K})$ we will indicate instead the set of all $m$-dimensional simplices present in $\mathcal{K}$.

Among the simplices of a simplicial complex, the facets play a very relevant role.

### FACET
A facet is a simplex of a simplicial complex that is not a face of any other simplex. Therefore a simplicial complex is fully determined by the sequence of its facets.

A very interesting class of simplicial complexes are pure simplicial complexes.

### PURE SIMPLICIAL COMPLEXES
A pure $d$-dimensional simplicial complex is formed by a set of $d$-dimensional simplices and their faces. Therefore pure $d$-dimensional simplicial complexes admit as facets only $d$-dimensional simplices.

This implies that pure $d$-dimensional simplicial complexes are formed exclusively by gluing $d$-dimensional simplices along their faces. In Figure 4 we show an example of simplicial complex that is pure and an example of a simplicial complex that it is not pure.

An interesting question is whether it is possible to convert a simplicial complex into a network and vice versa and how much information is lost/retained
Figure 4 An example of a 2-dimensional simplicial complex that is pure and an example of a 2-dimensional simplicial complex that is not pure.

Hypergraph

A hypergraph $\mathcal{G} = (V, E_H)$ is defined by a set $V$ of $N$ nodes and a set $E_H$ of hyperedges, where an $(m+1)$-hyperedge indicates a set of $m+1$ nodes

$e = [v_0, v_1, v_2, \ldots, v_m].$

with generic values of $1 \leq m < N.$

A hyperedge describes the many-body interaction between the nodes.

As mathematical objects simplicial complexes are distinct from hypergraphs, the difference being that simplicial complexes include all the subsets of a given simplex. From a network science perspective a given dataset including higher-order interactions can be described either as a simplicial complex.