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Two's company, three (or more) is a simplex

Algebraic-topological tools for understanding higher-order structure in neural data

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Abstract The language of graph theory, or network science, has proven to be an exceptional tool for addressing myriad problems in neuroscience. Yet, the use of networks is predicated on a critical simplifying assumption: that the quintessential unit of interest in a brain is a dyad – two nodes (neurons or brain regions) connected by an edge. While rarely mentioned, this fundamental assumption inherently limits the types of neural structure and function that graphs can be used to model. Here, we describe a generalization of graphs that overcomes these limitations, thereby offering a broad range of new possibilities in terms of modeling and measuring neural phenomena. Specifically, we explore the use of *simplicial complexes*: a structure developed in the field of mathematics known as algebraic topology, of increasing applicability to real data due to a rapidly growing computational toolset. We review the underlying mathematical formalism as well as the budding literature applying simplicial complexes to neural data, from electrophysiological recordings in animal models to hemodynamic fluctuations in humans. Based on the exceptional flexibility of the tools and recent ground-breaking insights into neural function, we posit that this framework has the potential to eclipse graph theory in unraveling the fundamental mysteries of cognition.

Keywords Networks · Topology · Simplicial complex · Filtration

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The recent development of novel imaging techniques and the acquisition of massive collections of neural data make finding new approaches to understanding neural structure a vital undertaking. Network science is rapidly becoming an ubiquitous tool for understanding the structure of complex neural systems. Encoding relationships between objects of interest using graphs (Figs. 1a–b, 4a) enables the use of a bevy of well-developed tools for structural characterization as well as inference of dynamic behavior. Over the last decade, network models have demonstrated broad utility in uncovering fundamental architectural principles (Bassett and Bullmore 2006; Bullmore and Bassett 2011) and their implications for cognition (Medaglia et al. 2015) and disease (Stam 2014). Their use has led to the development of novel diagnostic biomarkers (Stam 2014) and conceptual cognitive frameworks (Sporns 2014) that illustrate a paradigm shift in systems, cognitive, and clinical neuroscience: namely, that brain function and alteration are inherently networked phenomena.

All graph-based models consist of a choice of *vertices*, which represent the objects of study, and a collection of *edges*, which encode the existence of a relationship between pairs of objects (Figs. 1a–b, 4a). However, in many real systems, such *dyadic* relationships fail to accurately capture the rich nature of the system's organization; indeed, even when the underlying structure of a system is known to be