PhD Thesis

HIGHER-ORDER NETWORKS: STRUCTURAL MODELS, RARE EVENTS AND BRAIN FUNCTIONAL ORGANIZATION

by

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To Alberto, Clelia and Federico

Abstract

In many complex systems, interactions occur not just between pairs but among groups involving three or more entities. Higher-order networks are mathematical frameworks that extend traditional network models by capturing these multi-way interactions. Recognizing and modeling higher-order interactions is crucial because they provide a more accurate representation of real-world systems, leading to a deeper understanding of emergent behaviors that cannot be explained by pairwise interactions alone.

In the first part of this thesis, we develop a mathematical framework to analyze networks incorporating higher-order interactions. We introduce an extension of the Hidden Variables formalism tailored for higher-order networks, which allows for the characterization of systems with multi-way interactions. Through this formalism, we explore key structural properties such as hyper-degree distributions, degree correlations, and the overall connectivity of the network, revealing that higher-order interactions significantly influence network topology, particularly in aggregated structures generated by higher-order interactions that accumulate over time. Building upon this methodology, future research can extend the Hidden Variables formalism to a broader class of generative network models based on intrinsic node properties, such as fitness models or embedding space models, while accounting for any order of interactions.

In the second part of this thesis, we examine how higher-order interactions influence the dynamics of random walks on hypergraphs. Specifically, we focus on rare events in which the behavior of the random walk deviates significantly from what is typically expected. By exploring both quenched and annealed scenarios, corresponding respectively to cases where we compute fluctuations over static networks and ensembles of networks, we investigate how higher-order interactions impact dynamical fluctuations in different settings. Our analysis reveals that higher-order interactions can either suppress or amplify fluctuations from the typical behavior depending on the network configuration. The approach proposed in this thesis can be further used in the future to investigate rare events in a wider class of dynamical systems whenever they can be mapped onto Markovian processes opening possibilities for studying dynamical fluctuations beyond random walks on hypergraphs, such as investigating the controllability of epidemic models or other types of spreading processes not exclusively on higher-order structures.

In the final part of this thesis, higher-order network analysis is applied to the study of brain networks in epilepsy patients. A neighborhood-based description of brain connectivity is introduced to identify pathological hubs, which are regions that play a crucial role in the spread of seizures but are not the primary epileptogenic focus (i.e., not the initial source of epileptic activity). By employing higher-order network metrics, the study offers new perspectives on brain network organization. The findings suggest that surgical strategies should account for the higher-order structure of the neighborhoods of these pathological hubs, potentially leading to more effective treatments that reduce seizure recurrence while preserving essential brain functions. This higher-order representation of brain data offers innovative perspectives for investigating neurological disorders beyond epilepsy, such as Alzheimer's disease and schizophrenia.

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Here we are, at the most self-referential and egocentric acknowledgements in history.

As my supervisor told me at the beginning of the PhD: "A PhD is not a sprint, but a marathon". I would add that a PhD is also a journey. Among those who set out on a journey, there are two kinds of people: travelers and wanderers. The traveler is focused on reaching a destination, driven by a specific goal or purpose. The wanderer, however, finds meaning in the journey itself, embracing uncertainty and the unknown. For the wanderer, the act of moving forward, without a fixed end in sight, is where true discovery and fulfillment lie. I hope that everyone reading these acknowledgments can embrace the spirit of the wanderer, finding purpose not in a final destination, but in the richness of the experiences, growth, and learning that come from the path itself. And perhaps, in the end, as the Wizard of Oz teaches us, the real treasure isn't the Physical Review Letters we chase, but the friends we make along the way.

Like many long journeys, my PhD was far from linear. I started not really knowing what a PhD was, and honestly, I wanted to do it for reasons that later didn't seem as important. But from the very beginning, I found a guide in my supervisor, Federico, who believed in me and always encouraged me. I always say that the relationship with your supervisors dramatically affects your PhD experience, and I couldn't have been more fortunate. For this, I thank him for helping me grow academically, for shaping me, and for drawing out more from me than I thought possible. A special thanks also goes to Michele, who, with his exceptional guidance and intelligence in understanding my limits and needs, taught me the tricks of the trade. I owe much of what I've accomplished to their mentorship and even though they may not recognize the reference, I thank them for insisting on a silly Magikarp, bringing out the best in him. I hope one day to be half the scientist they are. And of course, I thank my collaborators Ana, Fernando, and Francesco for their immense patience and perseverance in working with me, as I often take my time and extend projects indefinitely. I have been truly privileged to work with such extraordinary people.

As with any journey, mine began at home. The early years were tough due to Covid, but I was lucky to spend them in Catania, surrounded by friends like Margherita, Branca, Panta, Guido, Ciccio, Riccardo, Jimbo, Omar, and Giovanni. I'm also deeply grateful to the exceptional physicists I met there—Alfredo, Alberto (the ghoster), Alberto, Fabrizio and GGN—who gave me plenty of complexes about what it means to be a real physicist. I'm glad we've kept in touch after all this time.

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After Covid, my academic life took a new direction, leading me to the Netherlands, where I worked on neuroscience and lived with Zio Mollica. Thank you for the bouldering, the cycling, the adventures, and "for unlocking my potential like the wise elder from Namek". *Grazie Zio Mollica*.

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Then came the best period of my PhD: the time when I wasn't actually doing my PhD, working as a bartender in Copenhagen. I'm constantly teased by my friends because this is the story I always tell first when I meet someone new. But I'm truly grateful for that summer, one of the happiest times of my life, which taught me to love what I do and to appreciate the privilege of doing what I love. "*Have I already told you I worked as a bartender in Copenhagen?*" A heartfelt thanks to Nora, Ale, Nico, Davide, Laura, Mina, Thom, Andrea, and all the amazing people from Downtown and Copenhagen who made that time unforgettable.

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Declaration of Authorship

I, the undersigned, Leonardo Di Gaetano, candidate for the PhD degree in Network Science declare herewith that the present thesis is exclusively my own work, based on my research and only such external information as properly credited in notes and bibliography. I declare that no unidentified and illegitimate use was made of the work of others, and no part of the thesis infringes on any person's or institution's copyright. I also declare that no part of the thesis has been submitted in this form to any other institution of higher education for an academic degree.

Vienna, 4th of October, 2024

Signature

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Publications

Ideas, results, and figures appearing in this thesis are based on the publications listed below

[I] **Di Gaetano, L.**, Battiston, F., & Starnini, M. (2024). Percolation and topological properties of temporal higher-order networks. *Physical Review Letters*, 132(3), 037401. [1].

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– La ginestra, Giacomo Leopardi

1 Introduction

1.1 Network representation of complex systems

Complex systems are prevalent across diverse domains, including ecosystems, human societies, and technological infrastructures [10-13]. These systems are characterized by complex, often non-linear interactions among their components, which lead to emergent behaviors that cannot be deduced by examining the individual parts in isolation [14, 15]. For instance, in ecosystems, the interdependencies between species give rise to population dynamics that are inherently complex [16]. Similarly, in human societies, social interactions often result in the spontaneous formation of communities and the spread of ideas, illustrating the intricacies of social dynamics [17].

Network theory has become a fundamental tool for representing and analyzing such systems [18, 19]. By abstracting complex systems into graphs, where nodes represent entities and edges depict interactions between them, networks provide a structured way to capture the relationships within the parts of these systems. This approach has proven invaluable across various fields, as illustrated in Figure 1.1, which highlights the applicability of networks to numerous real-world scenarios. In epidemiology, for example, networks are used to model the spread of diseases by representing individuals as nodes and their contacts as edges, helping to predict and control outbreaks (Figure 1.1 (c)) [20, 21]. In ecology, networks model the complex interactions within ecosystems, where nodes represent different species and edges represent interactions such as predation or symbiosis, providing insights into the balance and stability of ecosystems (Figure 1.1 (d)) [22]. In social sciences, networks provide insights into the structure and dynamics of social groups, including the spread of information and influence, the formation of social capital, and the dynamics of collaboration (Figure 1.1 (b)) [23]. For instance, the study of online social networks has revealed how information and behaviors spread through populations, leading to phenomena like viral marketing and the rapid adoption of innovations [17].

However, while traditional network models focus predominantly on pairwise interactions, these models often fail to capture the true complexity of real-world systems. As illustrated in Figure 1.1, the examples provided are pairwise representations of real-world phenomena that, in reality, often exhibit group interactions. In nature, interactions not always occur solely between two entities; instead, they frequently involve groups, where three or more components engage simultaneously. In reality, complex systems are often composed of parts that interact in groups, and and in most of the cases, reducing the system to pairwise interactions obscures the true dynamics that are driven by these group-level relationships. Furthermore, many of the dynamics observed in complex systems are driven by group mechanisms, which are the underlying processes that cause the observed emergent behaviors. Understanding a mechanism can explains how the global effect of the interactions of a



Figure 1.1: Illustration of network representation of complex systems. (a) A simple network as a mathematical entity, consisting of nodes and edges, models pairwise interactions. (b) Social Networks: Nodes represent individuals and their connections, illustrating social interactions within a community. (c) Epidemiology: Networks model the spread of diseases, where nodes represent individuals, and edges represent potential transmission pathways. (d) Ecological Networks: Nodes represent different species, and edges represent interactions such as predation, illustrating the complexity of ecological systems.

system leads to a specific collective behaviour, and therefore using the wrong representation of a mechanism, for instance, not taking into account group interactions, can lead to wrong predictions of the emergent property of the system we are studying. In the next subsection, we will explore several real-world examples of group interactions and mechanisms in more detail, illustrating how going beyond pairwise network models are essential for accurately describing the collective behaviors in complex systems.

1.2 Group mechanism and interactions in the real world

Understanding collective behaviors in complex systems requires capturing the group-wise interactions that drive these phenomena. As we have said, many real-world systems exhibit interactions that occur at the group level rather than just between pairs, significantly influencing the overall system dynamics. Below, we explore several real-world examples where group mechanisms play a key role, highlighting the need to move beyond pairwise models.

In social systems, sociological mechanisms such as peer pressure and social influence play a crucial role. Individuals are often influenced by the behaviors and opinions of groups, leading to phenomena like peer pressure and social reinforcement [24, 25]. Collaborations and group decision-making processes in workplaces and project teams also involve multi-way interactions, impacting productivity and outcomes [26–28].

In addition, collaboration and co-authorship networks offer another clear example of group interactions in action. In research, collaboration often involves teams of scientists

working together, with many scientific papers that are the product of large, multi-disciplinary teams, where the contributions of each member are interdependent.

Also in ecological and animal systems, group dynamics such as flocking and schooling are driven by interactions among multiple individuals. The collective movement patterns observed in bird flocks or fish schools emerge from group-level interactions, not just pairwise connections [29]. Predator-prey dynamics also involve complex multi-species interactions, such as coordinated hunting or defense mechanisms [30].

Lastly, neuroscience provides another compelling example, where brain functions result from interactions among groups of neurons. The functional connectivity of the brain cannot be adequately represented by pairwise connections alone; group-level activities are essential for understanding cognitive processes and neurological diseases [31, 32].

1.3 Limitations of Pairwise Models

Whether in social, biological, ecological, or neural networks, the dynamics of these systems are often shaped by interactions involving three or more entities simultaneously. Pairwise models, by reducing all interactions to dyads, overlook critical aspects of these systems, leading to oversimplified or inaccurate conclusions. This section examines the circumstances in which these models fail to capture the complexity of real-world interactions.

In social networks, for instance, group dynamics—such as team collaborations or group discussions—cannot be fully captured by pairwise interactions alone. The influence exerted in a group setting is often the result of multiple individuals acting together, creating effects like social reinforcement or peer pressure that require modeling interactions between more than two members at a time [24, 25]. Pairwise models reduce these dynamics to isolated interactions, which oversimplifies the processes driving phenomena like group decision-making or rumor spreading. For example, group collaborations in co-authorship networks have been shown to significantly increase research impact, with large collaborative teams producing more influential work than smaller, isolated teams [33].

Similarly, complex contagion in social systems demonstrates the limitations of pairwise models. The adoption of behaviors, norms, or innovations often requires reinforcement from multiple contacts, not just one [34]. Rumor spreading and information diffusion provide further evidence that modeling interactions between only two individuals misses key aspects of how information propagates. Such processes are more effective within clusters of interconnected individuals rather than isolated pairs [35, 36].

In biological systems, reducing interactions to pairwise models also falls short. For example, many cellular processes rely on complexes of three or more proteins interacting cooperatively. Pairwise models cannot fully capture the cooperative nature of these multiprotein assemblies, resulting in an incomplete understanding of key biological mechanisms. In areas like signaling pathways and structural biology, considering only pairwise interactions often fails to account for the broader, cooperative interactions necessary for proper cellular function [37, 38].

In ecology, multi-species interactions such as mutualistic networks and predator-prey dynamics also illustrate the inadequacy of pairwise models. The survival or success of one species may depend on the combined influence of others, and these group interactions are crucial to understanding ecosystem stability [39, 40]. For instance, predator-prey relationships that involve multiple species can lead to cascading ecological effects that are not visible in a pairwise framework.

Finally, neuroscience is another domain where pairwise models struggle to capture the full complexity of brain dynamics. Brain functionality arises not from isolated interactions between neuron pairs, but from coordinated activity across multiple brain regions. Cognitive processes such as decision-making and memory retrieval depend on the collective behavior of large groups of neurons. Models based solely on pairwise interactions risk missing the higher-level coordination that drives these complex brain functions [31,41].

In summary, while pairwise models have been instrumental in advancing the study of complex systems, they fail to account for the full range of interactions that occur in the real world. Systems across diverse domains often involve multi-way interactions, where the behavior of the whole cannot be reduced to individual pairwise connections. Understanding these interactions requires moving beyond pairwise models to more comprehensive approaches that capture the true complexity of these systems.

1.4 Limits of traditional representation and loss of information

The reason a pairwise representation of complex systems often falls short in predicting behaviors is that this leads to a loss of crucial information about the system's structure and dynamics. This loss of information is analogous to the projection of temporal data into static representations, which aggregates and obscures the temporal dynamics of interactions. In temporal networks, ignoring the timing of interactions and collapsing them into static snapshots can significantly alter the perceived structure and function of the network [42]. The same issue arises in group interactions when they are reduced to pairwise approximations.

To make this more clear, consider a scenario where three researchers are working together. In one case, they are collaborating on a single paper as a group, and in another case, each pair of researchers is working on separate papers. Traditional pairwise models would represent both scenarios similarly, as sets of pairwise interactions between the researchers. However, these representations fail to capture the distinct nature of the group collaboration versus the separate pairwise collaborations. In the group collaboration, the interactions



Figure 1.2: Schema portraying two different social situations: (a) three distinct conversations among three agents and (b) on group conversation engaing all of them togheter.

are collective, with all three researchers contributing simultaneously and influencing each other's work directly. In contrast, the separate pairwise collaborations do not involve this group dynamic and are instead a series of independent interactions (Fig. 1.2).

1.5 Higher-order networks

Given that collective behaviors are inherent in complex systems, representing such systems using traditional pairwise networks has often been insufficient, especially for describing interactions that involve more than two entities simultaneously.

For this reason, higher-order networks, where nodes can interact in groups beyond the pairwise level, have emerged as an essential framework for understanding the complexity of interactions in many real-world systems. Higher-order network models, such as hyper-graphs and simplicial complexes, address these limitations by allowing for the modeling of multi-way interactions [43, 44]. By extending the analysis beyond pairwise interactions, researchers can explore phenomena that are not observable in traditional models, such as group synchronization, higher-order contagion processes, and the formation of multi-scale structures [43, 45, 46].

Historically, the recognition of higher-order interactions dates back several decades [47], but it is only in recent years that a wave of enthusiasm for these representations has revolutionized our understanding and capability to tackle real-world systems characterized by more than simple dyadic connections. Early works laid the foundation, but contemporary advancements have significantly deepened our comprehension and application of higher-order models. For instance, in epidemiology, higher-order models are used to study the spread of diseases through populations, considering the effects of group gatherings and community-level interactions on disease dynamics [48]. In social sciences, these models help in understanding the spread of behaviors and information through communities, taking into account the influence of group interactions [49, 50].

In conclusion, higher-order networks represent a significant advancement in the study of complex systems. By capturing multi-body interactions, these models provide a more accurate and comprehensive representation of real-world systems. The ability to analyze higher-order interactions opens up new avenues for research and applications, offering deeper insights into the structure and dynamics of complex networks. As the field continues to evolve, higher-order network models are expected to play an increasingly important role in understanding complex systems across various domains.

1.6 Representations of Higher-Order Networks

Here we briefly present the two representations of higher-order networks used in this thesis and necessary to understand the upcoming chapters: hypergraphs and simplicial complexes.

1.6.1 Hypergraphs

A hypergraph, illustrated in Fig. 1.3, is a generalization of a traditional graph where edges, known as hyperedges, can connect any number of nodes. Formally, a hypergraph H is defined as H = (V, E), where V is a set of nodes and E is a set of hyperedges, each of which is a subset of V. This allows hypergraphs to model interactions involving more than two entities, which is essential for representing systems such as social networks, biological networks, and collaboration networks.

1.6.2 Simplicial Complexes

A simplicial complex is a collection of simplices, which are generalizations of points, line segments, triangles, and higher-dimensional polytopes. A k-simplex is a set of k + 1 nodes. For example, a 0-simplex is a node, a 1-simplex is an edge, a 2-simplex is a triangle, and so on [51]. Hence, a simplicial complex K is a collection of simplices that satisfies the



Figure 1.3: Example of a hypergraph plotted with the python package HGX.

condition that any face of a simplex in K is also in K, and the intersection of any two simplices in K is either empty or a common face [52].

1.6.3 Differences between Hypergraphs and Simplicial Complexes

While both hypergraphs and simplicial complexes are used to model higher-order interactions, they differ in how they represent these interactions and their suitability for different types of analyses. Hypergraphs are particularly effective for modeling systems where interactions among any number of entities need to be captured without enforcing a specific topological structure. This flexibility makes hypergraphs suitable for social networks, biological networks, and collaboration networks, where the focus is on the presence and diversity of group interactions rather than their geometric or topological properties [43].

In contrast, simplicial complexes are better suited for situations where the topological structure of interactions is important. By including all faces of each simplex, simplicial complexes inherently capture the hierarchical relationships and topological features of multi-way interactions. This makes them ideal for topological data analysis and for studying systems like neural connectivity, where the geometric configuration of connections provides significant insights, or ecological networks, where interactions often form nested, hierarchical patterns [40, 41]. Therefore, the choice between hypergraphs and simplicial complexes depends on whether the primary interest lies in the general multi-way interactions (favoring hypergraphs) or the detailed topological structure of these interactions (favoring simplicial



Figure 1.4: Illustration comparing hypergraphs (a) and simplicial complexes (d), and their interactions. Panels (b) and (e) show the three-body interactions of respectively (a) and (d) while (c) and (f) the two-body ones.

complexes). In Figure 1.4, we show an example of the same system portrayed with these two representations. The figure illustrates the differences between first and second order interaction that constitute both the hypergraph and simplicial complex representations. As shown in the figure, when broken down into its components, the hypergraph exhibits fewer first-order interactions than the simplicial complex. The hypergraph includes only interactions that are purely first-order (Figure 1.4 (c)), whereas the simplicial complex also incorporates all the first-order interactions that are part of second-order simplices (Figure 1.4 (f)).

1.7 Outline of the thesis

The thesis is structured into three main chapters, each addressing a significant aspect of higher-order networks.

In Chapter 2, we will introduce the Hidden Variables formalism for higher-order networks. The primary objective of this chapter is to provide an analytical tool for solving higher-order generative models. We aim to derive key topological properties such as hyper-degree distributions, hyper-degree correlations, and temporal properties like percolation time of networks generated with these models. By developing this formalism, we can analytically characterize higher-order networks that evolve over time providing insights on what happen if one generate networked structures with higher-order interactions. In particular, we will apply this formalism to solve a temporal and higher-order network model, the higher-order activity-driven (HOAD). The HOAD model extends the traditional activitydriven model, which is commonly used to represent temporal networks where nodes activate over time and form connections. In traditional activity-driven models, nodes have an associated activity rate determining the probability of becoming active and forming links with other nodes. This model is widely used to study dynamic processes such as information diffusion, social contagion, and disease spreading. The HOAD model incorporates higher-order interactions, allowing nodes to participate in group interactions rather than just pairwise connections, providing a more accurate representation of real-world systems, such as social networks, where interactions often occur in groups rather than pairs. Furthermore, we will apply our analytical tool to real-world data, particularly focusing on empirical activity data gathered from a scientific collaboration dataset. We will study the implications of generating models from data using an incorrect order of representation and highlight the potential errors and misinterpretations that may arise. For instance, generating networks based on empirical activity without considering higher-order representations can lead to a significant underestimation of the percolation time of such networks.

In **Chapter 3**, we will present an extensive study on the out-of-equilibrium dynamics of higher-order networks. The primary objective of this chapter is to understand how higher-order interactions influence rare events of dynamic processes on these networks. We will delve into the mathematical formulations and analytical techniques used to study these processes by means of large deviation theory, a theory utilized in out-of-equilibrium thermo-dynamics to study rare events and fluctuations. Among the many dynamical processes on higher-order networks, we will study random walks on hypergraphs. This process has been used for describing diffusion phenomena, such as the spread of information or rumors, in systems where interactions occur in groups. We will explore how random walks on hypergraphs differ from those on traditional networks, particularly in terms of the time that a walker unexpectedly spends on specific nodes over time. In particular, we will apply our theoretical framework to structures generated by a toy model that we propose, allowing us to

combinatorically solve the probability of configurations of such structures. We will validate our theoretical results on more general structures via extensive Monte Carlo simulations, ensuring the robustness of our findings across different network topologies. Lastly, we will extend our results to more general dynamics by introducing the biased random walk on hypergraphs, a more general dynamical process in which random walkers can be positively or negatively biased towards highly connected nodes.

In Chapter 4, we will explore the application of higher-order network representation and topological data analysis (TDA) in understanding the functional organization of brain networks, particularly in the context of epilepsy. The primary objective of this chapter is to uncover topological signatures that identify pathological hubs in the brain, which are crucial for understanding seizure dynamics and improving epilepsy surgery outcomes. We will delve into the methodological framework that integrates TDA with network neuroscience, focusing on how topological features can be used to characterize the functional properties of brain networks. We will apply TDA to magnetoencephalography (MEG) data from a cohort of epilepsy patients, aiming to identify the extended neighbourhoods of brain regions. Extended neighbourhoods provide a mesoscopic description of brain organization, capturing the regional influence of each node. This analysis will show how a higher-order perspective of brain networks can reveal centrality and connectivity patterns of the epileptogenic zone (EZ) and its surrounding areas, providing insights into the emergence and role of pathological hubs. Our findings will show that both the resection area and its neighbourhood are more central in the brain network compared to other regions with respect to several higher-order metrics. These findings will give us predictive power in classifying resected and non-resected areas of the networks build from our data. Regarding the classification of different patients, or equivalently the classification on networks, we will observe that the relative centrality of these regions varies significantly among patients, suggesting the need for personalized approaches in epilepsy surgery and not giving us the same predictive power we have for node classification.

Lastly, in **Chapter 5**, we will present our conclusions and outlook for future research. This final chapter synthesizes the key findings from the previous chapters and discusses their broader implications for the field of network science. We will reflect on how our work advances the understanding of higher-order interactions in complex networks. Specifically, we will highlight how higher-order interactions can drastically alter network topology and influence rare events in dynamical systems. Furthermore, we will outline potential directions for future research. One avenue is extending the Hidden Variables formalism to other established network models, such as spatial, gravity, geometric, and fitness models, to better understand how higher-order interactions affect different types of networks. We will also consider investigating the influence of specific higher-order structural features on dynamical fluctuations and rare events, which could reveal how heterogeneity and community structures impact system behavior. Additionally, we will discuss applying the methodolo-

gies developed to other dynamical processes beyond random walks, such as social contagion and percolation, to explore how higher-order interactions affect the spread of information or diseases. Lastly, we will explore expanding the higher-order network analysis to other neurological disorders beyond epilepsy, such as Alzheimer's disease and schizophrenia, to uncover new insights into their underlying network dynamics. By highlighting these opportunities, we aim to inspire further studies that build upon our contributions and continue to explore the rich complexities of higher-order networks.

La consapevolezza, Che con l'aiuto del tempo, anche un Magikarp è in grado Di diventare Gyarados

– Tetris, Pinguini Tattici Nucleari

2 Analytical Framework for Higher-Order Network Models

As previously discussed, networks allow us to describe and study a wide variety of complex systems. However, scientific interest extends beyond merely describing these systems; it also involves making predictions and anticipating behaviors. To achieve this, theoretical models are employed to simplify and model real-world scenarios, enabling us to predict properties and characteristics of complex systems or to interpret the emergent behaviors observed in these networks. In network science, generative network models are central for these reasons. Based on simple foundational rules, often incorporating random mechanisms, they lead to the emergence of non-trivial structures. The ability to analytically solve these models allows for accurate predictions and deeper understanding of emergent properties in complex systems.

Outline In this chapter, we aim to develop and analyze solvable structural models of higher-order networks. We will begin by reviewing the most well-known generative models for pairwise interactions, to highlight the need for moving beyond traditional frameworks and into higher-order models. Following this historical overview, we will introduce the hidden variables formalism, which allows for the analytical characterization of higher-order networks models. This formalism will be employed to derive key properties such as the hyper-degree distribution and hyper-degree correlations. We will then extend our analysis to temporal systems by introducing the higher-order activity-driven (HOAD) model. This model captures the dynamic nature of interactions within higher-order networks. We will investigate the topological properties of the HOAD model, including the distribution and correlation of hyper-degrees over time. Furthermore, we will explore temporal percolation in hypergraphs, providing analytical estimates for the percolation times in both uncorrelated and correlated hypergraphs. Finally, we will apply our theoretical framework to empirical data, quantifying the difference in computing the percolation time between generating networked structures with higher-order or first-order activity distributions observed in realworld datasets. Through these analyses, we aim to provide a comprehensive understanding of the structural and dynamical properties of higher-order networks and which mistakes can arise if one neglects the intrinsic higher-order nature of data.

2.1 Random Network models

Review on Random models One of the foundational approaches in network science is the use of random network models. These models serve as null hypotheses or baseline scenarios against which the structure and dynamics of real-world networks can be compared. By

applying simple probabilistic rules to the formation of networks, random models help us understand the essential properties that emerge in complex systems. These models have proven powerful, revealing key insights into the nature of connectivity, robustness, and the spread of information within networks [19, 53, 54].

The simplest random network model is the Erdős-Rényi (ER) model. In this model, each pair of nodes is connected with a fixed probability. This model has been widely used in epidemiology and communication networks to understand how connectivity and robustness manifest in random structures [53, 55]. Despite its simplicity, the ER model reveals important emergent properties, such as the percolation threshold, where a giant connected component suddenly forms as the average degree increases, marking a phase transition in network connectivity [54]. Another notable property that emerges from the ER model is disassortativity—a tendency for high-degree nodes to connect with low-degree nodes. This is not a property explicitly encoded in the model but arises naturally from the random connection process [56].

Following the ER model, we look at the Barabási-Albert (BA) model, which offers a more refined approach by incorporating growth and preferential attachment into the network formation process. Unlike the ER model, where connections are made randomly, the BA model assumes that new nodes are more likely to attach to existing nodes with higher degrees. This mechanism, often referred to as the "rich-get-richer" phenomenon, leads to the emergence of scale-free networks characterized by a power-law degree distribution [57].

While the BA model focuses on the preferential attachment mechanism, spatial network models introduce the concept of physical space into network formation. In spatial networks, nodes are placed in a geometric space, and the probability of a connection between two nodes decreases with the distance between them. This reflects the intuitive notion that connections are more likely to form between geographically proximate entities [58]. Despite the constraints imposed by spatial separation, these networks often exhibit small-world properties, characterized by short average path lengths and high clustering [58, 59].

Building on spatial models, the gravity model refines the spatial approach by incorporating the concept of node "mass," which can represent factors like population size, economic strength, or other measures of importance [60]. In this model, the probability of interaction between two nodes is proportional to their masses and inversely proportional to the distance between them [61]. The gravity model is widely used in trade networks, where larger economies engage in more trade with each other, and in urban planning, where the connectivity of cities depends on both their size and proximity. By capturing these real-world dynamics, the gravity model provides insights into how large, influential nodes dominate interactions within a network, while still respecting spatial constraints [62].

The geometric model extends these ideas into more abstract or higher-dimensional spaces. Nodes are placed in a geometric space, and connections are established based on distance thresholds or more complex geometric relationships [63]. This model is particularly useful for studying networks where connections depend on multiple factors beyond mere physical distance. For instance, in wireless sensor networks, connectivity might depend on both the physical proximity of sensors and their functional compatibility [64]. Similarly, in biological networks, interactions might depend on spatial positioning within a cellular environment as well as other biochemical factors.

Further extending the concept of geometric embedding, hyperbolic models place networks in hyperbolic space, a non-Euclidean space that combines geometric proximity with scale-free degree distributions [65]. For example, the internet can be modeled in hyperbolic space, where the hierarchical organization of domain names and the clustering of websites are naturally represented [66]. Hyperbolic models also help explain the small-world phenomena observed in many networks, where short paths exist between any two nodes despite the network's large size. This is crucial for understanding how information or diseases spread efficiently in these networks, balancing the need for local clustering with global connectivity [67].

The fitness model introduces another layer by considering the intrinsic "fitness" of each node—a measure of its ability to attract connections independently of its degree [68]. In this model, connections are more likely to form between nodes with higher fitness, allowing for the emergence of super-hubs—nodes that become highly connected due to their inherent properties rather than their position in the network. This model is particularly relevant in contexts where the inherent characteristics of nodes, such as popularity, influence, or productivity, play a significant role in network dynamics. For example, in social networks, individuals with greater social capital or influence can become central nodes, regardless of their initial connectivity. Similarly, in scientific collaboration networks, highly productive researchers are more likely to collaborate with others, leading to the formation of hubs based on fitness [69].

From Nodes' Properties to Global Behaviors Despite the diversity of these models, they share a common foundation: the probability of connections between nodes depends on specific properties of the nodes themselves. Whether these properties are homogeneously distributed (as in the ER model), based on preferential attachment (as in the BA model), influenced by spatial coordinates (as in spatial and geometric models), or determined by intrinsic fitness (as in the fitness model), the connection probabilities are rooted in the local characteristics of the nodes. These models attempt to replicate real-world scenarios by starting from these localized rules or individual behaviors, allowing researchers to explore how complex global patterns emerge from simple, well-defined interactions.

These local rules, though simple, can lead to the emergence of complex global properties, such as scale-free distributions, small-world characteristics, and hierarchical structures. These emergent properties are not explicitly programmed into the models but arise naturally from the interactions defined by the nodes' properties. This principle of emergence has been observed across various domains, from biology (e.g., neural or genetic networks) to sociology (e.g., social influence and community formation) to technology (e.g., the robustness of the internet or power grids) [13]. By understanding these emergent properties, researchers can gain valuable insights into the underlying mechanisms that drive the behavior of complex systems.

Beyond Pairwise Interactions: Higher-Order models While the models discussed so far have focused on interactions at the level of pairs of nodes, recent advances in network science emphasize the importance of considering higher-order interactions.

This shift towards higher-order network models raises an important question: can the principles and local rules that underpin traditional network models be extended to account for higher-order interactions? By exploring this question, we can develop models that not only capture pairwise relationships but also the rich, multi-node interactions inherent in complex systems. Incorporating these higher-order interactions allows for the study of new emergent phenomena, which cannot be explained by pairwise interactions alone [1,43,46]. Additionally, these models can capture the collective dynamics of systems more accurately, making them essential for applications in fields like neuroscience, where group activities are crucial, or in epidemiology, where the spread of diseases often occurs through group interactions rather than simple pairwise contacts.

For these reasons, in the following subsections, we aim to build upon the foundation of traditional network models to develop and analyze solvable structural models of higherorder networks.

2.2 Hidden variables formalism for higher-order networks

Here, we introduce a general approach to analytically characterize higher-order time-varying networks by means of a hidden variables (HV) framework. In pairwise networks, HV were introduced to model the presence of links in networks with structural correlations [70].

Until now, the HV formalism has been employed across a vast spectrum of first-order generative processes, such as to map networks into embedded spaces, including latent [71] and hyperbolic spaces [72], fitness models [69, 73], protein interaction [74] and social distance [75]. Furthermore, the HV formalism has been applied to networks evolving over time [76], networks with inherent correlations [70], and subsequently employed to pinpoint the topological characteristics of activity-driven networks [77–79]. However, the aforementioned works neglected the higher-order organization of the considered social and biological systems.

To this end, we start by developing the HV formalism for higher-order networks. Each node *i* of a network of *N* nodes is endowed with an intrinsic vectorial HV $\vec{h}_i = (h_i^{(1)}, h_i^{(2)}, \dots, h_i^{(m)}, \dots)$, where the HV $h_i^{(m)}$ determines the *m*-order interactions of node *i*. For each order *m*, $h_i^{(m)}$ is drawn from an independent distribution $\rho(h^{(m)})$. The higher-order HV model assumes that the existence of an *m*-order hyperlink (*m*-link) among m+1 nodes depends only on their HV, i.e., a connection probability $\mathbb{P}(h_1^{(m)}, \dots, h_m^{(m)}, h_{m+1}^{(m)})$.

The main idea of the HV approach to solve network models is then to write temporal and structual properties as a function of \mathbb{P} , and therefore the knowledge of the connection probability allows one to approximate network properties.

2.2.1 Hyper-degree distribution

To start, we show how to approximate one of the main topological properties of a higherorder generative model, the hyper-degree distribution. The goal here is to write the *m*-order degree distribution $P(k^{(m)})$ as a function of \mathbb{P} .

As a first step, the *m*-order degree distribution $P(k^{(m)})$ can be written as

$$P(k^{(m)}) = \sum_{h^{(m)}} g(k^{(m)}|h^{(m)})\rho(h^{(m)}), \qquad (2.1)$$

where the propagator $g(k^{(m)}|h^{(m)})$ is the probability that a node with hidden variable $h^{(m)}$ ends with an *m*-order degree equal to $k^{(m)}$, i.e., it has $k^{(m)}$ incident *m*-links. Note that $\sum_{k \in m} g(k^{(m)}|h^{(m)}) = 1$.

As it has been done for pairwise networks [70], we can express the propagator as the

convolution of all possible conditional probabilities that lead to it, namely the partial propagators. For the 2-order case:

$$g(k^{(2)}|h^{(2)}) = \sum_{\substack{k_{11}^{(2)}, k_{12}^{(2)}, \dots, k_{CC}^{(2)}}} \delta_{k_{11}^{(2)} + k_{12}^{(2)} + \dots + k_{CC}^{(2)}}^{k_{CC}^{(h^{(2)})}} g_{11}^{(h^{(2)})}(k_{11}^{(2)}|h_1^{(2)}, h_1^{(2)}) \\ g_{12}^{(h^{(2)})}(k_{12}^{(2)}|h_1^{(2)}, h_2^{(2)}) \dots g_{CC}^{(h^{(2)})}(k_{CC}^{(2)}|h_C^{(2)}, h_C^{(2)}),$$

shortly,

$$g(k^{(2)}|h^{(2)}) = \sum_{\{k_{ij}^{(2)}\}} \delta_{\sum k_{ij}^{(2)}}^{k^{(2)}} \prod_{i \ge j}^{C} g_{ij}^{(h^{(2)})}(k_{ij}^{(2)}|h_i^{(2)}, h_j^{(2)}),$$
(2.2)

where $g_{ij}^{(h^{(2)})}(k_{ij}^{(2)}|h_i^{(2)},h_j^{(2)})$ is the probability that a node (with hidden variable $h^{(2)}$) ends up with a number of 2-order interactions with neighbors of hidden variables $h_i^{(2)}$ and $h_j^{(2)}$ equal to $k_{ij}^{(2)}$. In the convolution, we take into account all the possible pairs of classes of hidden variables excluding permutations $(i \ge j)$, being $h_C^{(2)}$ the maximum value of $h^{(2)}$ and we sum over the set of all possible 2-degree values $\{k_{ij}^{(2)}\} = \{k_{11}^{(2)}, k_{12}^{(2)} \dots k_{CC}^{(2)}\}$. Note that the number of all possible partial propagators is equal to the number of multisets of cardinality 2 among C elements, $\binom{C}{2} = \binom{C+2-1}{2}$. The term $\delta_{\sum k_{ij}}^{k^{(2)}}$ constraints the sum of partial degrees to be equal to $k^{(2)}$. For simplicity, from now on we omit the explicit dependence of $h^{(m)}$ in m without losing generality in the discussion.

For the *m*-order case, one has to consider that an *m*-order interaction between the node with hidden variable h and other *m* nodes involves *m* (not necessarily different) hidden variable classes, $h_{i_1}, h_{i_2}, \ldots, h_{i_m}$. Notice that we have dropped the explicit dependence of h on *m* to have a lighter notation, $h = h^{(m)}$. The propagator thus reads

$$g(k^{(m)}|h) = \sum_{\{k_{i_1i_2\dots i_m}\}} \delta^{k^{(m)}}_{\sum k_{i_1i_2\dots i_m}} \prod_{i_1 \ge i_2 \ge \dots \ge i_m}^C g^{(h)}_{i_1i_2\dots i_m}(k_{i_1i_2\dots i_m}|h_{i_1}, h_{i_2}, \dots, h_{i_m}), \quad (2.3)$$

As in the m = 2 case, $g_{i_1 i_2 \dots i_m}^{(h)}(k_{i_1 i_2 \dots i_m} | h_{i_1}, h_{i_2}, \dots, h_{i_m})$ is the probability that a node with hidden variable h has exactly $k_{i_1 i_2 \dots i_m}$ m-order interactions with neighbours of hidden variables $h_{i_1}, h_{i_2}, \dots, h_{i_m}$. In this case, the convolution is done again considering $i_1 \ge i_2 \ge \dots \ge i_m$ in order to avoid all repetitions given by the permutation of the indexes. As for the second-order case, C is the number of hidden variable classes. The number of partial propagators in the convolution is $\binom{C}{m} = \binom{C+m-1}{m}$, namely the number of

multisets with m possibly repeated items, chosen from a set of C distinct elements. The term $\delta_{\sum k_{i_1i_2...i_m}}^{k^{(m)}}$ constraints the sum of partial degrees to be equal to $k^{(m)}$, and $\{k_{i_1i_2...i_m}\}$ is again the set of all possible values of m-degree.

For the purpose of solving the convolution in Eq. (2.3), we resort to the properties of generating functions. The generating function of the propagator is defined as

$$\hat{g}(z|h) = \sum_{k} z^{k} g(k|h), \qquad (2.4)$$

where we omit the *m* index on the hyper-degree $k^{(m)}$. Since the propagator is given by a convolution of Eq. (2.3), we can write its generating function as the product of the generating functions of the partial propagators. For a general order *m* we have

$$\hat{g}(z|h) = \prod_{i_1 \ge i_2 \ge \dots \ge i_m} \hat{g}_{i_1, i_2, \dots, i_m}^{(h)}(k_{i_1, i_2, \dots, i_m}|h_{i_1}, h_{i_2}, \dots, h_{i_m}).$$
(2.5)

Since the *m*-links between vertices with hidden variables $h, h_{i_1}, h_{i_2}, \ldots, h_{i_m}$ are independently drawn with probability $\mathbb{P}(h, h_{i_1}, h_{i_2}, \ldots, h_{i_m})$, the partial propagator

 $g_{i_1,i_2,\ldots,i_m}^{(h)}(k_{i_1,i_2,\ldots,i_m}|h_{i_1},h_{i_2},\ldots,h_{i_m})$ is simply given by a binomial distribution, as in the first order case. Consequently, its generating function reads

$$\hat{g}^{(h)}(z|h_{i_1}, h_{i_2}, \dots, h_{i_m}) = \left[1 - (1 - z) \mathbf{\mathbb{P}}(h, h_{i_1}, h_{i_2}, \dots, h_{i_m})\right]^{N_{i_1 i_2 \dots i_m}},$$
(2.6)

where $N_{i_1,i_2...i_m}$ is the number of possible sets with nodes of hidden variables $h_{i_1}, h_{i_2}, ..., h_{i_m}$, that can be written as $N_{i_1i_2...i_m} = N_{i_1}N_{i_2}...N_{i_m}$, where $N_{i_1} = N\rho(h_{i_1})$ is the number of nodes with hidden variable h_{i_1} .

By taking the logarithm of the full propagator, one obtains

$$\ln \hat{g}(z|h) = N^m \sum_{i_1 \ge i_2 \ge \dots \ge i_m} \rho(h_{i_1}) \rho(h_{i_2}) \dots \rho(h_{i_m}) \ln[1 - (1 - z) \mathbb{P}(h, h_{i_1}, h_{i_2}, \dots, h_{i_m})].$$
(2.7)

In the limit $C \gg m$, the number of elements in the summation, equal to the number of multisets $\binom{C}{m}$, is equal to $\frac{C^m}{m!}$. We can thus sum over m independent indexes $i_1, i_2 \dots i_m = 1, 2, \dots C$, and divide by m!. At this point, since Eq. (2.7) does not depend anymore on the specific indexes $i_1, i_2 \dots, i_m$, we can simplify the notation and directly sum over different hidden variable classes $h_1, h_2 \dots, h_m$,

$$\ln \hat{g}(z|h) = \frac{N^m}{m!} \sum_{h_1, h_2, \dots, h_m} \rho(h_1) \rho(h_2) \dots \rho(h_m) \ln[1 - (1 - z) \mathbb{P}(h, h_1, h_2, \dots, h_m)].$$
(2.8)
We now consider the limit of sparse networks $N \gg 1$ and small connection probability $\mathbb{P}(h, h_1, h_2, \dots, h_m) \ll 1$, which allows us to write $\hat{g}(z|h)$ as a pure exponential generating function, as in the first order case. Consequently, the propagator takes the form of a Poisson distribution

$$g(k^{(m)}|h) \simeq \frac{e^{-\overline{k^{(m)}}(h)}\overline{k^{(m)}}(h)^{k^{(m)}}}{k^{(m)}!},$$
(2.9)

where $\overline{k^{(m)}}(h)$ is the expected *m*-degree of a node of hidden variable *h*, that can be obtained by taking the first derivative of $\hat{g}(z|h)$ evaluated at z = 1,

$$\overline{k^{(m)}}(h) = \frac{N^m}{m!} \sum_{h_1,\dots,h_m} \rho(h_1) \dots \rho(h_m) \mathbb{P}(h, h_1,\dots,h_m).$$
(2.10)

By inserting the form of the propagator Eq. (2.9) and its mean Eq. (2.10) into the general Eq. (2.1), one can obtain the *m*-degree distribution as a function of the hidden variable distribution. The form of the propagator is exponential (as in the first order case) and the value of its mean depends explicitly on the connection probability. Remarkably, the problem-specific piece of information that allows us to treat different models is contained in Eq. (2.10) through the connection probability $\mathbb{P}(h, h_1, \ldots, h_m)$, which is the key ingredient to find the hyper-degree distribution, given by Eq. (2.1). In the following parts, we will discuss how to find $\mathbb{P}(h, h_1, \ldots, h_m)$ in the case of a higher-order activity-driven model.

2.2.2 Hyper-degree correlations

As well as hyper-degree distribution, hyper-degree correlation plays an important role in understanding the structural dependencies within higher-order networks. This correlation describes how the hyper-degrees of neighboring nodes are related, shedding light on the network's tendency to form group connections among nodes with similar or dissimilar hyperdegrees. Here we show how to obtain general analytical expressions for the hyper-degree correlations.

We start by writing $\overline{k_{nn}^{(m)}}(h)$, namely the average *m*-degree of the nearest neighbors of a node with hidden variable *h*. For m = 2, one has to average over all possible hidden variables h_i and h_j of the two neighbors *i* and *j* in the 2-link,

$$\overline{k_{nn}^{(2)}}(h) = \sum_{h_i, h_j} \left(\frac{\overline{k^{(2)}}(h_i) + \overline{k^{(2)}}(h_j)}{2} \right) p(h_i, h_j | h),$$
(2.11)

where $p(h_i, h_j | h)$ is the conditional probability that a node with hidden variable h is connected to nodes with hidden variables h_i, h_j . Such conditional probability can be written as

$$p(h_i, h_j | h) = \frac{N^2 \rho(h_i) \rho(h_j) \mathbf{P}(h, h_i, h_j)}{2 \,\overline{k^{(2)}}(h)}, \tag{2.12}$$

where $N^2 \rho(h_i) \rho(h_j)$ is the total number of all possible pairs made up of one node with hidden variable h_i and one with h_j , $N^2 \rho(h_i) \rho(h_j) \mathbb{P}(h, h_i, h_j)$ represents the expected number of 2-links that a node with hidden variable h shares with this type of pair, and the factor 2 at the denominator ensures that the probability is correctly normalized when we sum over independent indexes, $\sum_{h_i,h_j} p(h_i, h_j | h) = 1$.

For general m, the average m-degree of neighbors of a node with hidden variable h reads

$$\overline{k_{nn}^{(m)}}(h) = \sum_{h_1, h_2 \dots h_m} \left(\frac{\overline{k^{(m)}}(h_1) + \overline{k^{(m)}}(h_2) \dots + \overline{k^{(m)}}(h_m)}{m} \right) p(h_1, h_2 \dots h_m | h), \quad (2.13)$$

where $p(h_1, h_2 \dots h_m | h)$ is the conditional probability that a node with hidden variable h is connected in an *m*-links with neighbours $h_1, h_2 \dots h_m$, which reads

$$p(h_1, h_2..., h_m | h) = \frac{N^m \rho(h_1) \rho(h_2) \dots \rho(h_m) \mathbf{P}(h, h_1, h_2..., h_m)}{m! \, \overline{k^{(m)}}(h)},$$
(2.14)

where, again, the correct normalization over independent indexes is ensured by the term m! leading to $\sum_{h_1,h_2...h_m} p(h_1,h_2...,h_m|h) = 1.$

The average *m*-degree of the nearest neighbors of a node with degree k^m can be obtained by following Ref. [70],

$$\overline{k_{nn}^{(m)}}(k^{(m)}) = 1 + \frac{1}{P(k^{(m)})} \sum_{h} g(k^{(m)}|h)\rho(h)\overline{k_{nn}^{(m)}}(h).$$
(2.15)

equivalently to the first-order case.

At this point, knowing the relations between $P(k^{(m)})$, $g(k^{(m)}|h)$ and \mathbb{P} found in previous subsection, one is able to explicitly write $\overline{k_{nn}^{(m)}}$ as a function of h.

2.3 The activity-driven model

As an example of HV's possible applications, in this section, we propose the activity-driven model as a representative network model that can be analytically solved using such a technique.

The activity-driven (AD) model has been instrumental in capturing the temporal aspects of network interactions and is particularly useful for representing systems where the interactions between entities are not static but change over time, such as social networks, communication networks, and epidemiological networks [80]. This model has been widely studied and applied in various contexts. For instance, it has been used to model contagion dynamics in time-varying metapopulation networks [81], analyze random walks and search strategies in time-varying networks [82], and control contagion processes [83]. Furthermore, the AD model has been extended to account for heterogeneous activity and tie allocation in social networks [84], and to study the impact of committed activists on social consensus [85]. Applications in epidemiology include modeling the effects of self-initiated behavioral changes on disease dynamics [86], and understanding phase transitions in information spreading on structured populations [87]. Additionally, the model has been used to explore the effects of attractiveness on random walks [88], and to develop frameworks for the study of epidemic models [89].

In the AD model, each node is assigned an activity rate a_i , drawn from a distribution F(a), which determines the probability of the node becoming active at each time step. When a node becomes active, it creates edges with a fixed number of randomly selected nodes. This simple yet powerful mechanism allows the model to capture the dynamic formation and dissolution of connections, which is characteristic of many real-world networks. The model has been used to study various phenomena, including the spread of information, disease dynamics, and synchronization processes.

Formally, the AD model operates as follows: at each discrete time step t, the network G_t starts with N disconnected nodes. Each node i becomes active with probability $a_i \Delta t$ and creates m links to m other randomly selected nodes. Over a given time window T, the aggregated network G_T is formed by the union of all the edges created during this period, allowing for the analysis of cumulative interaction patterns.

Note that the activity-driven model is a temporal network model, but our framework is not explicitly meant to solve temporal models. We will show how we are able to predict topological information over time by studying the aggregated networks at every T by expressing the probability that two nodes are connected as a function of T, while the aggregated structure gets more and more connected.

2.3.1 Higher-order activity-driven model

Simplicial activity-driven model To extend the AD model to account for higher-order interactions, Petri et al. introduced the Simplicial Activity-Driven (SAD) model [46]. In many biological and social systems, interactions involve more than two entities, making simplicial complexes a more suitable representation. The SAD model generalizes the AD model by allowing interactions to involve multiple nodes simultaneously, forming simplices instead of simple edges. This approach captures the complex nature of group interactions, such as collaborations in scientific research or multi-agent interactions in social networks.

The SAD model operates similarly to the AD model but with a crucial difference: when a node becomes active, it creates a simplex involving m other nodes, forming a higherorder structure that represents a group interaction. This results in a network composed of simplices, which can be aggregated over time to study the cumulative interaction patterns. The model has been shown to capture important structural differences and dynamics that are not evident in pairwise interaction models, making it valuable for studying processes such as disease propagation and social contagion.

HOAD model In this thesis, we make use of a similar extended model called the Higher-Order Activity-Driven (HOAD) model, which focuses on generating hypergraphs instead of simplicial complexes. While the underlying principles are similar to the SAD model, the HOAD model uses hyperedges to represent many-body interactions. This approach provides a more flexible framework for modeling higher-order interactions in various systems.

Formally, the higher-order activity-driven model (HOAD model) is defined as follows. Each agent *i* in a population of size *N* is endowed with a higher-order activity potential $\mathbf{a}_i = (a_i^{(1)}, a_i^{(2)}, ..., a_i^{(m)})$ for every interaction order *m*.

The activities of the agents are random variables, extracted from distributions

$$\rho(\mathbf{a}) = (\rho(a^{(1)}), \rho(a^{(2)}), ..., \rho(a^{(m)})),$$

which we assume independent. The activity of node *i* at order *m*, $a_i^{(m)}$, represents the probability that they engage in an interaction with *m* other nodes in a certain time-interval Δt .

The activity potentials can be measured in empirical data by considering that the activity $a_i^{(m)}$ is proportional to $n_i^{(m)}$, the number of interactions of order m involving node i in Δt . The proper normalization of $a_i^{(m)}$, $\sum_{i,m} a_i^{(m)} = 1$, implies that $a_i^{(m)}$ is equal to the number of interactions of order m involving node i in Δt , divided by the total number of interactions of any order all nodes are involved in Δt , $a_i^{(m)} = n_i^{(m)} / \sum_{i,m} n_i^{(m)}$.



Figure 2.1: Illustration of a hypergraph generated via HOAD model growing over time.

The HOAD model generates temporal hypergraphs starting by N initially disconnected nodes. At every time step, each node *i* generates one hyperlink of order *m* towards randomly selected nodes, with probability proportional to their activity $a_i^{(m)}$. At the following time step, the existent higher-order interactions are erased and the process continues. The temporal hypergraph is defined by the sequence of instantaneous, sparse hypergraphs generated at each time step. One can obtain a static hypergraph by integrating all instantaneous hypergraphs up to a certain time *T*, where two nodes *i* and *j* will be connected if any hyperedge between them exists in any instantaneous hypergraph in $t \in [1, T]$, Figure 2.1.

Mapping HOAD model into HV formalism A node *i* of the HOAD network with activity \mathbf{a}_i can be mapped as $\mathbf{a}_i \to \vec{h}_i$. Since hyperlinks of different orders are generated independently, we can treat all orders separately by means of *m* distinct scalar hidden variables. For every *m* we can write $a_i^{(m)} \to h_i$.

2.4 Topological properties in the HOAD model

In this section, we utilize the mapping from hidden variables to activity potentials to translate the general formulas previously derived into the specific context of the HOAD model. This allows us to analytically determine the topological properties, such as hyper-degree distribution and hyper-degree correlations, within this model framework.

2.4.1 Hyper-degree distribution

We now derive the analytical form of the distribution $P(k^{(m)})$ by means of the hidden variables formalism. For the sake of simplicity, we first focus on the second-order case and compute the $\mathbb{P}_T(a_i, a_j, a_k)$ that three nodes i, j, k with hidden variables, a_i, a_j , and a_k are connected by at least one 2-link in the aggregated HOAD network at time T. By following [77], we start from the probability that these nodes are not connected, $\mathcal{Q}_T(a_i, a_j, a_k) =$ $1 - \mathbb{P}_T(a_i, a_j, a_k)$. Let n_i, n_j, n_k be the number of activations of the three nodes until time T. Since every time a node is active it selects two random neighbors, we have

$$\mathcal{Q}_{T}(a_{i}, a_{j}, a_{k}) = \sum_{n_{i}, n_{j}, n_{k}} \rho_{T}(n_{i}) \rho_{T}(n_{j}) \rho_{T}(n_{k}) \left(1 - \frac{1}{\binom{N}{2}}\right)^{n_{i}} \left(1 - \frac{1}{\binom{N}{2}}\right)^{n_{j}} \left(1 - \frac{1}{\binom{N}{2}}\right)^{n_{k}},$$
(2.16)

where $\rho_T(n_i)$ is the probability that node *i* has been activated n_i times at time *T*, given by a binomial distribution

$$\rho_T(n_i) = \binom{TN}{n_i} \left(\frac{a_i}{N}\right)^{n_i} \left(1 - \frac{a_i}{N}\right)^{TN - n_i}.$$
(2.17)

Substituting $\rho(n_i)$ into $Q_T(a_i, a_j, a_k)$, and using the binomial theorem to solve the sum in equation (2.16), we find

$$\mathcal{Q}_T(a_i, a_j, a_k) = \left[\left(1 - \frac{a_i}{N\binom{N}{2}} \right) \left(1 - \frac{a_j}{N\binom{N}{2}} \right) \left(1 - \frac{a_k}{N\binom{N}{2}} \right) \right]^{TN} \simeq e^{-\frac{T}{\binom{N}{2}}(a_i + a_j + a_k)}$$

where the last equivalence holds for $\binom{N}{2} \gg T$. Therefore, $\mathbb{P}_T(a, a_i, a_j)$ reads as

$$\mathbf{P}_T(a_i, a_j, a_k) \simeq 1 - e^{-\frac{T}{\binom{N}{2}}(a_i + a_j + a_k)} \simeq \frac{2T}{N^2}(a_i + a_j + a_k),$$
(2.18)

where we have approximated $\binom{N}{2} \simeq \frac{N^2}{2}$.

Following analogous steps, the probability $\mathbb{P}_T(a, a_1, a_2, \ldots, a_m)$ that m + 1 nodes with hidden variables a, a_1, a_2, \ldots, a_m are connected by at least one *m*-link in the aggregated HOAD network at time *T* is

$$\mathbf{P}_T(a, a_1, a_2, \dots, a_m) \simeq 1 - e^{-\frac{T}{\binom{N}{m}}(a+a_1+a_2+\dots, a_m)} \simeq \frac{m!}{N^m}(a+a_1+a_2+\dots, a_m)T.$$
(2.19)

From Eq. (2.10), the expected degree is thus

$$\overline{k^{(m)}}(a) = (a + m\langle a \rangle)T.$$
(2.20)

This means that, on average, the *m*-order degree of a node with activity *a* at time *T* is given by Ta outgoing *m*-links plus $mT\langle a \rangle$ received from random neighbors.

Inserting this expression into Eq. (2.9), we finally get

$$g(k|a) = e^{-T(a+m\langle a \rangle)} \frac{[T(a+m\langle a \rangle)]^{k^{(m)}}}{\Gamma(k+1)}.$$
(2.21)

The propagator of the order m is thus functionally equivalent to the first-order one [77], but with a different mean. Again following [77], one can now find the explicit expression of the m-degree distribution of the aggregated network until time T, $P_T(k^{(m)})$. Inserting Eq. (2.21) into Eq. (2.1) and taking the continuum limit of latter, for $T^2 \gg k^{(m)} \gg 1$, performing a steepest descent approximation we find the asymptotic form of the degree distribution

$$P_T(k^{(m)}) \simeq \frac{1}{T} \rho(k^{(m)}/T - m\langle a \rangle).$$
(2.22)

We recall that in the approximation above we have considered a sparse hypergraph. Hence, the goodness of the approximation above depends on time T, which regulates the density of the higher-order network. Indeed, the HOAD model starts from disconnected nodes, which over time are connected by m-links, eventually percolating the network. From Eq. (2.19), such hypergraph sparsity condition for a HOAD model for general order m is fulfilled when $T \ll \frac{N^m}{m!}$.

Figure 2.2 shows the hyper-degree distribution $P_T(k^{(m)})$ of HOAD networks integrated at time T, as obtained by numerical simulations. We arbitrarily select a power-law activity distribution, yet Eq. (2.22) is general for any distribution ρ . The model is implemented as part of the library HGX [4]. One can see a good agreement with the asymptotic behavior indicated by Eq. (2.22).

2.4.2 Hyper-degree correlation

We start by computing $p(a_1, a_2, ..., a_m | a)$, the probability of randomly choosing an *m*-link made of neighbours with activities $a_1, a_2, ..., a_m$ among all *m*-links of *a*, which is given by Eq. (2.14)

$$p(a_1, a_2..., a_m | a) = \frac{N^m \rho(a_1) \rho(a_2) \dots \rho(a_m)}{m! \,\overline{k^{(m)}(a)}} \mathbf{P}_T(a, a_1, a_2...a_m).$$
(2.23)

By inserting the approximation for \mathbb{P}_T (Eq. (2.19)) and $k^{(m)}$ (Eq. (2.20)), for small T we find

$$p(a_1, a_2..., a_m | a) \simeq \frac{\rho(a_1)\rho(a_2)...\rho(a_m)(a + a_1 + a_2...a_m)}{(a + m\langle a \rangle)}.$$
 (2.24)



Figure 2.2: Hyper-degree distribution $P_T(k^{(m)})$, Eq. (2.22) shown as a dashed line. Network size $N = 10^6$, orders m = 1, 2, 5, integration time $T = 10^3$. The activity distributions $\rho(a)$ of order m have power-law form for every order with exponent $\gamma = 2.25$.

Inserting Eq. (2.24) into Eq. (2.13) we finally get

$$\overline{k_{nn,T}^{(m)}}(a) = \frac{T}{a+m\langle a\rangle} \bigg[\langle a^2 \rangle + (m+1)\langle a \rangle a + (m^2+m-1)\langle a \rangle^2 \bigg].$$
(2.25)

Eq. (2.15) relates $\overline{k_{nn}^{(m)}}(k)$ with $\overline{k_{nn}^{(m)}}(a)$. Inserting Eq. (2.25) into Eq. (2.15), and following equivalent steps done in [77], in the limit of $k^{(m)} \gg 1$ we find that the hyper-degree-degree correlation of order m reads

$$\overline{k_{nn,T}^{(m)}}(k) = 1 + \frac{T^2}{k^{(m)}}\sigma^2 + (m+1)\langle a \rangle T,$$
(2.26)

being $\sigma^2 = \langle a^2 \rangle - \langle a \rangle^2$. One can rewrite the latter expression,

$$\frac{k_{nn,T}^{(m)}(k) - 1}{T} = (m+1)\langle a \rangle + \frac{T}{k^{(m)}}\sigma^2,$$
(2.27)

that gives an asymptotic form of $\overline{k_{nn,T}^{(m)}}(k)$.

The last expression, valid in the limit of $k^{(m)} \gg 1$ and sparse network, gives an asymptotic prediction of $\overline{k}_{nn,T}^{(m)}(k)$ as a function of the first two momenta of the activity distribution



Figure 2.3: Hyper-degree correlations $\overline{k}_{nn,T}^{(m)}(k)$, Eq. (2.27) shown as a dashed line. Network size $N = 10^6$, orders m = 1, 2, 5, integration time $T = 10^3$. The activity distributions $\rho(a)$ of order m have power-law form for every order with exponent $\gamma = 2.25$. See Figure 2.5 for additional plots in the case of m = 1, 3, & 4.

of order m. Figure 2.3 shows the correlations minus its first moment of HOAD networks integrated at time T, as obtained by numerical simulations. As for the degree distribution, we plot the rescaled hyper-degree correlations, the differences between the correlations and their leading approximation in order to show how it decays with $T/k^{(m)}$ and the collapse of the curves for three different orders m = 1, 2, 5. One can see that the disassortative behavior proportional to $(k^{(m)})^{-1}$ and governed by σ^2 , as predicted by Eq. (2.27), is confirmed by numerical simulations. See Figure 2.4 for additional plots in the case of m = 1, 3, & 4.

2.5 Temporal percolation HOAD networks

The connectivity properties of the time-integrated HOAD networks allow us to characterize the temporal percolation, i.e., the time T_p marking the onset of a giant connected component in the integrated network. The percolation time T_p corresponds to the time at which the system reaches the structural percolation threshold. This threshold marks the point at which long-range connectivity appears for the first time. Below this threshold, the system remains fragmented, and any dynamic process (like information spreading, epidemic transmission, etc.) will not reach all nodes because the network is insufficiently connected. The percolation threshold essentially sets a lower bound on dynamic processes like spreading or



Figure 2.4: Hyper-degree distribution $P_T(k^{(m)})$, Eq. (2.22) shown as a dashed line. Network size $N = 10^6$, orders m = 1, 3, 4, integration time $T = 10^3$. The activity distributions $\rho(a)$ of order m have power-law form for every order with exponent $\gamma = 2.25$.

diffusion. For a process to fully propagate through a network, the network must be above its percolation threshold. Below this critical point, the process might only affect small, disconnected clusters, not the entire system [90].

For instance, in Fig. 2.6 we illustrate how the same spreading process can behave differently depending on the network's structure. In temporal networks that have not yet percolated, the process cannot reach the entire network because it is not fully connected, making the network's structure a bottleneck for the dynamics. On the contrary, if the structure already contains a giant component, the network no longer restricts the dynamics, allowing the spreading process to reach the entire system.

For this reason, being able to predict the percolation time of a system that increases its interactions over time tells us what is the minimum time scale that a process must have to being able to propagate entirely over such evolving structure.

Here, we discuss temporal percolation for uncorrelated and correlated hypergraphs. We consider hypergraphs formed by hyperlinks of the same order m. Before discussing temporal percolation, we shortly introduce higher-order percolation in static hypergraphs. We consider arbitrary hypergraphs whose nodes may be removed with probability 1 - p: when p = 0, no node remains from the original higher-order network; by contrast, when p = 1 all nodes are retained. With an approach inspired by [91], we consider the probability x_k that, if an *m*-order hyperlink (connecting m + 1 nodes) is attached on one side to a node with



Figure 2.5: Hyper-degree correlations $\overline{k}_{nn,T}^{(m)}(k)$, Eq. (2.27) shown as a dashed line. Network size $N = 10^6$, orders m = 1, 3, 4, integration time $T = 10^3$. The activity distributions $\rho(a)$ of order m have power-law form for every order with exponent $\gamma = 2.25$.

hyper-degree k (where we omit the dependency in m of the hyper-degree), then, following the hyperlink to its other m ends, we will not end in a giant connected component. To this end, one needs to impose that none of the m nodes (with hyper-degree k') leads (through any of its remaining k' - 1 hyperlinks) to the giant component, thus we write:

$$x_{k} = \left[1 - p + p \sum_{k'} P(k'|k) x_{k'}^{k'-1}\right]^{m},$$
(2.28)

where we assume that the probability $x_{k'}$ of each of the *m* nodes to be connected to the giant component is independent of each other, so exponentiate the same probability to the *m*. P(k'|k) is the probability that a node with *m*-degree *k* is connected with a node of *m*-degree *k'*. Close to the percolation threshold, $x_k \leq 1$, hence defining $y_k = 1 - x_k \gtrsim 0$ we write

$$1 - y_k = \left[1 - p + p \sum_{k'} P(k'|k) (1 - y_{k'})^{k'-1}\right]^m.$$
 (2.29)

We then expand at the first order $(1 - y_k)^{k-1}$ as $(1 - y_k)^{(k-1)} \simeq 1 - (k-1)y_k$, and we write



Figure 2.6: Illustration of a spreading process on two fixed hypergraph structures: one without a giant connected component (a) and one with a giant component (b). Both panels show the same spreading process, with the same diffusion rate of two nodes at every time step. In (a), the spreading halts, confined to a small, disconnected part of the network, while in (b), the process propagates across the entire network as it benefits from the global connectivity provided by the giant component.

$$y_k = mp \sum_{k'} \mathbf{B}_{kk'}^{(m)} y_{k'},$$
 (2.30)

where we have defined the *m*-order branching matrix as $\sum_{k'} \mathbf{B}_{kk'}^{(m)} y_{k'} = \sum_{k'} P(k'|k)(k'-1)y_{k'}$

and have expanded $(1 - p \sum_{k'} \mathbf{B}_{kk'}^{(m)} y_{k'})^m$. Moreover, following the procedure defined in [78],

we can easily prove that for every order m the corresponding branching matrix $\mathbf{B}_{kk'}^{(m)}$ has the same element-wise form of the first-order case:

$$\mathbf{B}_{kk'}^{(m)} = (k'-1) \left[\rho(k'-1) + \frac{\rho(k-1)}{k\rho(k)} (k'\rho(k') - \langle k \rangle \rho(k'-1)) \right].$$
(2.31)

Hence, we can solve Eq. (2.30) as for the first-order case by considering the associated dominant eigenvalue (λ_1) equation of the branching matrix:

$$\lambda_1^2 - \langle k \rangle \lambda_1 - \langle k^2 \rangle + \langle k \rangle^2 + \langle k \rangle = 0.$$
(2.32)

Notice that the last equation holds for every order and that the differences in terms of percolation time are implicitly contained in the hyper-degree momenta.

One can also release the condition of *m*-degree correlation and by means of an analogous approach can find the percolation threshold for uncorrelated hypergraphs:

$$x = \left[1 - p + p \sum_{k'} \frac{k' \rho(k')}{\langle k \rangle} x^{k'-1}\right]^m,$$
(2.33)

where the probability $x_k = x$ does not depend on k anymore. Defining x = 1 - y and developing till the first order we find the m-order Molloy-Reed criterion:

$$y = m p \frac{\langle k^2 \rangle - \langle k \rangle}{\langle k \rangle} y, \qquad (2.34)$$

and for p = 1, last expression has non-trivial solution in x for:

$$\frac{\langle k^2 \rangle - \langle k \rangle}{\langle k \rangle} > \frac{1}{m} \tag{2.35}$$

In the uncorrelated case, we found that the results were consistent with those by Sun et al [92].

2.5.1 Temporal percolation in the HOAD model

We now consider the related problem of temporal percolation in the HOAD model. To this end, we utilized calculations equivalent to those presented by Starnini et al. [78], but we report them here for clarity. To find the percolation time we need to express the hyperdegree momenta as a function of the activity variable momenta. We can write the hyperdegree momenta $\langle k^n \rangle_T$ at a time T with respect to the time-dependent propagator $g_T(k|a)$ as

$$\langle k^n \rangle_T = \sum_a \rho(a) \sum_k k^n g_T(k|a).$$
(2.36)

Since the propagator has the form of a Poisson distribution, the momenta of the degree distribution simply read as

$$\langle k^n \rangle_T = \sum_{i=1}^n \left\{ {n \atop i} \right\} T^i \kappa_i, \tag{2.37}$$

where $\binom{n}{i}$ are the Stirling numbers of the second kind and

$$\kappa_i = \sum_a \rho(a)(a+m\langle a\rangle)^i = \sum_{j=0}^i \binom{i}{j} \langle a^j \rangle (m\langle a \rangle)^{i-j}.$$
(2.38)

Explicitly, $\langle k\rangle_T$ and $\langle k^2\rangle_T$ can be written as a function of the first two activity momenta as

$$\langle k \rangle_T = T\kappa_1 = T(m+1)\langle a \rangle, \tag{2.39}$$

$$\langle k^2 \rangle_T = T\kappa_1 + T^2\kappa_2 = T(m+1)\langle a \rangle + [\langle a^2 \rangle + (m^2 + 2m)\langle a \rangle^2]T^2.$$
 (2.40)

Using the last expressions we can find an analytical approximation for the percolation time of hypergraphs with no hyper-degree correlations as a function of the different orders of interactions present in the hypergraphs. For instance, we can solve Eq. (2.32) by means of Eqs. (2.36) (2.37) (2.38), leading to the following formula for the percolation time of correlated hypergraphs for any order m:

$$T_{c}^{(m)} = \frac{2}{(m+1)\langle a \rangle + \sqrt{(m^{2}+2m-3)\langle a \rangle^{2}+4\langle a^{2} \rangle}}.$$
 (2.41)

Notice that the last equation holds for every order and that the differences in terms of percolation time are implicitly contained in the hyper-degree momenta.

We test the validity of the prediction given by Eq. (2.41) by running extensive numerical simulations.

Figure 2.7 shows the growth of the giant component size S over time and the peak of its variance, $\sigma(S)^2$, indicating the estimated percolation time, for several orders m. The percolation time predicted by Eq. (2.41) has a decent agreement with numerical results, yet they do not exactly coincide. We thus run a finite-size scaling analysis, by assuming that the relative difference between the actual percolation time $T_c^{(m)}$ in the thermodynamic limit and the one found in a network of size N, $T^{(m)}(N)$, follows a scaling law of the form $(T^{(m)}(N) - T_c^{(m)})/T_c^{(m)} \sim N^{-\nu}$ for every m. Figure 2.8 shows that the finite-size hypothesis holds, the percolation time estimated by the peak over time of the variance of the giant component size actually approaches $T_c^{(m)}$ for any order m in the thermodynamic limit $N \to \infty$.

Equivalently, for uncorrelated hypergraphs, exploiting again the relation between the momenta $\langle (k^{(m)})^n \rangle$ and $\langle a^n \rangle$ (Eqs. (2.36),(2.37),(2.38)), we find a general prediction of the



Figure 2.7: Giant component size S/N (continuous line) and the peak of its variance $\sigma(S)^2$ (dashed line) over time. The theoretical prediction given by Eq. (2.41) is indicated as a vertical line. Results are averaged over 10^2 runs. Orders m = 1, 2, 5.



Figure 2.8: Finite-size scaling analysis of the relative difference $(T^{(m)}(N) - T_c^{(m)})/T_c^{(m)}$ (circles) and corresponding scaling law $N^{-\nu}$ (dashed line). Results are averaged over 10^2 runs. Orders m = 1, 2, 5.

percolation time for uncorrelated temporal higher-order networks:

$$T_{unc}^{(m)} = \frac{(m+1)\langle a\rangle}{m\left[(m+2)\langle a\rangle^2 + \langle a^2\rangle\right]}.$$
(2.42)

2.5.2 Hyper-degree correlation's effects on percolation time

We now compare the analytical prediction of percolation time for uncorrelated and correlated hypergraphs by plotting the ratio $T_{unc}^{(m)}/T_c^{(m)}$ (Eq. (2.43)) for different orders m and different power-law exponents γ of the activity distribution:

$$\frac{T_{unc}^{(m)}}{T_c^{(m)}} = \frac{(m+1)\langle a\rangle\left((m+1)\langle a\rangle + \sqrt{(m^2+2m-3)\langle a\rangle^2 + 4\langle a^2\rangle}\right)}{2m\left[(m+2)\langle a\rangle^2 + \langle a^2\rangle\right]}.$$
(2.43)

Figures 2.9 and 2.10 present the results of these comparisons visually. In Figure 2.9, we plot the ratio $T_{unc}^{(m)}/T_c^{(m)}$ as a function of γ for various values of m. It is evident that for lower values of γ , particularly around $\gamma = 2$, the disparity between $T_{unc}^{(m)}$ and $T_c^{(m)}$ is more pronounced, indicating a significant underestimation of the percolation time by the uncorrelated model. As γ increases, the ratio approaches unity, suggesting that the difference between the uncorrelated and correlated percolation times diminishes.

This highlights the importance of considering correlation when computing the percolation time, especially for systems with strong heterogeneity in activity distribution (low γ) or lower-order interactions (small m).

Similarly, Figure 2.10 illustrates the ratio $T_{unc}^{(m)}/T_c^{(m)}$ as a function of m. Here, we observe that for small values of m, the uncorrelated percolation time significantly underestimates the correlated one. However, as m increases, the ratio approaches unity, indicating that for higher-order interactions, the difference between uncorrelated and correlated models becomes negligible.



Figure 2.9: $\frac{T_{unc}}{T_c}$ as a function of γ . Network size $N = 10^6$, orders m = [1, 2, 5, 10] and $\gamma \in [2, 4]$. The activity distributions $\rho(a)$ are power-law distributions with $\epsilon = 10^{-3}$.



Figure 2.10: $\frac{T_{unc}}{T_c}$ as a function of m. Network size $N = 10^6$, orders $m = [1, \ldots, 20]$. The activity distributions $\rho(a)$ have the same power-law form for every order with exponent $\gamma = 2.25$, with $\epsilon = 10^{-3}$.

2.6 Temporal percolation on empirical Data

In network science, random models often rely on empirical parameters to simulate and analyze network behavior. For instance, null models of temporal networks frequently use activity-driven frameworks based on observed activity rates. However, empirical data are often interpreted as first-order interactions and subsequently represented as simple networks, despite their inherent higher-order nature. This simplification can lead to significant inaccuracies in understanding network dynamics.

In this section, we explore the consequences of this common misassumption. Specifically, we compare the outcomes of using a first-order activity-driven model versus a higherorder activity-driven model to create random null models. For the former case, we project all interactions into the first order, thus representing higher-order data as a simple network, losing part of the information contained therein.

In particular, we consider two data sets of scientific collaboration networks in the fields of Geology and History, collected by the Microsoft Academic Graph. We inform first-order and higher-order activity-driven models with empirical activities extracted from the dataset, and compare the first-order $(T^{(1)})$ and *m*-order $(T^{(m)})$ percolation times of the networks. The percolation points are obtained by calculating the time for which the variance of the component sizes distribution is maximum.

2.6.1 Data Description

The two datasets we utilized two datasets, *coauth-mag-geology* and *coauth-mag-history*, were obtained from the data repository of XGI [93]. These datasets consist of timestamped higher-order interactions, where each interaction is represented as a set of nodes. Specifically, the *coauth-mag-geology* dataset includes publications tagged with Geology in the Microsoft Academic Graph, while the *coauth-mag-history* dataset includes publications tagged with Geology at the timestamps indicate the year of publication. The projected graphs are weighted undirected networks, where the weights reflect the frequency of co-authorship within the higher-order interactions. In Table 2.1 we report the general properties of the two datasets.

Even if the two datasets contained interactions up to the 25th order, for our analysis, we focused on interactions involving up to 11 nodes (10th order).

2.6.2 Quantifying higher-order and first-order activity distributions

The higher-order activity potential of individuals has been extracted from data as detailed in the definition of the HOAD model. Specifically, we counted the number of interactions



Figure 2.11: Comparison of temporal networks generated using higher-order activities (a) and first-order activities (b), preserving the same number of links when projecting the higher-order case.

each node participated in for different orders and divided by the total number of interactions across all orders. The first-order activity potential of individuals has been extracted from data as detailed in the definition of the activity-driven model [80].

We then directly compare the higher-order percolation threshold with the first-order one. To this aim, we project all interactions into the first order, thus representing higher-order data as a simple network, and measure the activity potential in this case. We note that, in order to meaningfully compare the two cases, the first-order activities of nodes must be multiplied by the factor $\binom{m+1}{2}$, indicating the number of equivalent links included in an *m*-order interaction. In this way, we ensure that, at any given time *T*, the simple activity-driven network and the higher-order activity-driven network projected to the first-order have the same number of links (Fig. 2.11).

Statistic	coauth-MAG-History	coauth-MAG-Geology
Number of nodes	1,014,734	1,256,385
Number of timestamped hyperedges	1,812,511	1,590,335
Number of unique hyperedges	895,668	1,207,390

Table 2.1: Statistics of *coauth-MAG-History* and *coauth-MAG-Geology* Datasets

2.6.3 Effects of neglecting higher-order interactions on percolation time

Figure 2.12 shows that the *m*-order percolation time $T^{(m)}$ estimated by numerical simulations of the HOAD model informed by empirical data is in good agreement with the theoretical prediction $T_c^{(m)}$ given by Eq. (2.41), for every order *m*. Moreover, Figure 2.12 shows that the first-order percolation time $T^{(1)}$ is much smaller than the actual *m*-order one $T^{(m)}$, and such a difference increases with the order *m*.



Figure 2.12: Percolation times in empirical data. Scientific Geology (stars) and History (circles) collaboration networks. Blue points: Ratios between the first-order $(T^{(1)})$ and *m*-order $(T^{(m)})$ percolation times of networks informed by empirical activities, estimated from numerical simulations. Yellow points: Ratios between the theoretical prediction from Eq. (2.41), $T_c^{(m)}$, and the percolation times of networks informed by empirical activities estimated from numerical simulations, $T^{(m)}$.

Therefore, an incorrect representation of higher-order data as classic, dyadic interactions leads to a substantial underestimation of the true, higher-order percolation times, up to 50% already for m = 5, that is, small groups of 6 people.

2.7 Conclusions

In this chapter, we showed that the topological and percolation properties of temporal higherorder networks can be obtained by mapping such networks to a higher-order HV formalism. We illustrate the potential of our theoretical framework by quantitatively showing how much the percolation times of higher-order empirical social networks are underestimated if higherorder interactions are neglected. This result is particularly interesting within the framework of epidemic processes: a disease spreading with a short timescale is expected to percolate when the underlying contact network is assumed to be formed by dyadic interactions, but it would not percolate in the corresponding higher-order network representation. Note, however, that our finding holds within the specific activity-driven modeling framework. Further research should be devoted to addressing this setting in different modeling frameworks and on real contact networks.

The higher-order HV framework we developed holds potential for future applications across a wide array of higher-order and temporal generative models. For instance, it could be applied to higher-order fitness models [69] or social dynamics models including higher-order interactions mapped into latent spaces [75]. Likewise, it could be extended to describe network models incorporating Non-Markovian dynamics [79], which has shown to have a deep impact on epidemic processes.

Future research could quantify and model the presence of correlations between different interaction orders, as well as their effects on the connectivity and percolation properties of time-integrated networks. We hope that our work will stimulate further research to apply the higher-order HV framework to other empirical, time-varying complex systems.

Hito no yume wa owaranai!

– Marshall D. Teach, One Piece

3 Large deviations theory for dynamical processes on higherorder networks

The study of dynamical processes on networks [94, 95] has been a cornerstone of understanding complex systems, where the interactions between components can lead to emergent behavior. For instance in epidemiology, modeling the spread of diseases through networks helps in devising strategies for containment and vaccination [20, 96–98]. More in general, dynamical processes on networks are fundamental to understanding how systems evolve over time and the study of these processes encompasses both equilibrium and nonequilibrium dynamics, each offering unique insights and challenges [99, 100].

Outline Despite many efforts in studying higher-order dynamical models, all the works primarily focus on the equilibrium state of such processes. In this chapter, we propose the first study of rare events on the dynamics of higher-order processes, highlighting the importance of understanding fluctuations and rare events in higher-order networks to predict the behavior of real-world systems. We begin by providing a brief overview of rare events and out-of-equilibrium dynamics, highlighting their significance and relevance to the study of dynamical processes on networks. This is followed by a general, non-technical introduction to large deviations theory, which forms the foundation of the analytical approach used in this study. Then, we explore the application of large deviations theory to out-of-equilibrium dynamics on higher-order networks, focusing on the effect that group interactions have on dynamical fluctuations. Subsequently, we delve into how this theoretical framework is applied to study random walks on higher-order networks, highlighting how higher-order interactions affect out-of-equilibrium dynamics.

3.1 Large deviations and rare events

Typical and Atypical Behaviors In physics and stochastic processes, the primary focus is often on typical behaviors—those outcomes we expect to observe most frequently. These typical outcomes correspond to the average or most probable results of a system. However, there are instances where understanding atypical behaviors, which are not impossible but simply less likely by definition, becomes equally important. Atypical behaviors allow us to explore the full range of potential outcomes of a process, including catastrophic or unexpected events that could have significant consequences. Studying these less probable events helps us control and predict the distribution of all possible outcomes, which is crucial for assessing risks in various systems.

For example, in statistical physics, one often examines the equilibrium distribution of particles in a system using ensemble theory. In a canonical ensemble, for instance, the

typical behavior corresponds to the most probable configuration of particles at a given temperature, such as particles evenly distributed in a box. However, it is also possible, though less likely, for the system to fluctuate into configurations far from this typical state, like a temporary clustering of particles in one corner of the box. These rare configurations, while improbable, are still part of the ensemble's distribution and contribute to our understanding of fluctuations and stability in physical systems.

In stochastic processes, a classic example is the flipping of a fair coin N times. The typical or expected outcome would be to get tails approximately N/2 times. However, the process is stochastic, meaning that the actual outcome might deviate from this expectation. One might be interested in understanding the probability of getting tails significantly more or less than N/2 times, which, though rare, is entirely possible.

Similarly, in dynamical systems on networks, many processes, such as random walks, are inherently stochastic. In a random walk, a walker moves from one node to a neighboring node chosen at random. A typical question in this context is determining the fraction of time the walker spends at a particular node, a result that is well-known to be linked to the spectral properties of the network's adjacency matrix. However, studying atypical behaviors in this scenario involves asking about the chances that the walker behaves in an unexpected way, such as spending significantly more or less time on a given node than predicted. While such outcomes are less likely, they are not forbidden by the stochastic nature of the process and provide valuable insights into the underlying dynamics of the network.

Large deviations To rigorously analyze these behaviours, large deviations theory offers a powerful mathematical framework [101-104]. This theory focuses on the probabilities of rare events that deviate significantly from the average behavior, providing insights into the stability and variability of complex systems [105]. By applying large deviations theory to dynamical processes on networks, we can quantify the likelihood of rare events and understand their impact on the overall system behavior.

The theory of large deviations is fundamentally concerned with the study of rare events in stochastic systems, specifically focusing on the exponential decay of probabilities associated with these events [105]. Originating from statistical mechanics [106], large deviations theory provides a framework for understanding the probabilities of deviations from typical behavior in random processes [107–111]. It refines and generalizes classical results such as the law of large numbers and the central limit theorem by providing a more detailed description of the tail behavior of probability distributions. The cornerstone of large deviations theory is the large deviations principle (LDP), which quantifies the exponential rate at which probabilities of rare events decay as a function of system size . This is typically expressed through a rate function, which encapsulates the cost of deviations from the mean behavior [101].

3 LARGE DEVIATIONS THEORY FOR DYNAMICAL PROCESSES ON HIGHER-ORDER NETWORKS

Going beyond thermodynamics, large deviations theory provides also a powerful framework for understanding the probabilistic structure of rare events in stochastic systems, particularly in the context of dynamical processes on networks [5, 112–114]. When applied to random walks on complex networks, large deviations theory enables the quantification of the probabilities of significant deviations from typical behavior. Specifically, it focuses on the time-integrated functionals or observables of a random walk, such as the degree of nodes visited or the trajectory entropy, and examines their fluctuations over time. For instance, considering an unbiased random walk on a graph, large deviations theory can be used to study the rare fluctuations of the mean degree of nodes visited by the walker [112].

In practice, the application of large deviations theory to networked systems has revealed intricate behaviors such as dynamical phase transitions and localization phenomena. For example, the study of the mean degree of nodes visited by a random walk on Erdős-Rényi graphs demonstrates how high or low degree fluctuations can be linked to localized regions within the network [112]. Similarly, examining the trajectory entropy provides insights into the maximum entropy random walk, which maximizes the entropy rate and represents a uniform distribution over all paths in the network [5]. These analyses highlight the utility of large deviations theory in capturing the complex interplay between network structure and dynamical processes, offering a comprehensive tool for studying rare events and their implications in various applications, including communication networks, epidemiology, and transport systems.

Dynamical Processes in Higher-Order Networks Higher-order networks models consider the collective influence of groups rather than just individual pairs, offering new insights into dynamical processes. Higher-order models account for complex interactions by considering structures such as hypergraphs and simplicial complexes, which better represent real-world systems like social and biological networks. For instance, simplicial contagion models [49], illustrate how group interactions can accelerate the spread of information or diseases compared to traditional models, effectively portraying social influence and the spread of information over groups. In social networks, the presence of higher-order interactions can enhance the diffusion of information, making it faster and more robust than diffusion processes limited to pairwise interactions [115]. Random walks on hypergraphs also reveal that higher-order structures can significantly impact diffusion processes, often leading to more intricate spreading patterns and varying timescales, which portrays the diffusion of ideas or rumors, generally enhanced by group interactions [116]. Additionally, in synchronization phenomena, such as those seen in neural networks, higher-order interactions can profoundly influence the dynamics [117-119]. The traditional Kuramoto model, extended to include higher-order coupling terms, leads to more complex synchronization patterns, where higher-order interactions can stabilize or destabilize synchronous states depending on the nature and strength of the coupling, thus portraying complex coordination in

biological systems. Moreover, in the context of evolutionary dynamics, higher-order interactions in evolutionary games reveal different equilibria compared to pairwise interactions, promoting cooperation under certain conditions and providing insights into the evolution of cooperative behavior in social systems, thus portraying collective decision-making processes [120–122].

3.2 Fluctuations of dynamics on networks

The appearance of fluctuations in dynamical processes is central in determining the future evolution of many real-world systems [123]. The emergence of rare events may be bolstered or hindered by the hosting complex environment, often conveniently modeled as a complex network [124–126]. Large fluctuations in complex networks have been studied across a variety of processes, including percolation [112, 127–129], spreading [130, 131], and transport [132–135]. A stream of research has focused on random walks as a versatile model of diffusion in discrete spaces [136–140] and on their rare event properties [141–143]. Large deviations theory has revealed that low-degree nodes are more susceptible than hubs to the appearance of atypical loads, possibly leading to dynamical phase transitions [113, 144–146].

Regarding dynamical systems on networks, despite their success, graphs can only provide a constrained description of real-world systems, as links are inherently limited to model pairwise interactions only [43, 147]. Yet, from social [27, 44, 148, 149] to biological [37, 38, 41, 150] networks, in a wide variety of real-word systems interactions may occur among three or more units at a time. Interestingly, taking into account higher-order interactions has shown to lead to new collective phenomena in a variety of dynamical processes [151], including diffusion [152, 153], contagion [49, 154, 155], synchronization [117, 119, 156–158] and evolutionary games [120, 121, 159]. While such studies have focused on characterising dynamical behavior at the typical state, understanding fluctuations and rare events driven by the presence of higher-order interactions is to this day still an open problem.

To this end, in the next sections of this chapter we propose a study of fluctuations and rare events on higher-order networks using large-deviation theory tools. We focus on random walks on higher-order networks and on a particular time-additive observable that monitors the time the random walker spends in certain regions of the hypergraph. Our study reveals how fluctuations arise in time for a random walk on a fixed hypergraph structure (*quenched* case), and which higher-order structure is optimal to achieve them (*annealed* case). In the quenched case the density of higher-order interactions regulates fluctuations of occupation times, which are hampered around well-connected nodes and enhanced elsewhere. In the annealed case, where the structure of interactions is not *a-priori* fixed, the random walk dynamics select the optimal higher-order structure that maximises fluctuations and rare events are boosted.

3.3 Random walk on hypergraphs

In this section, we provide a detailed characterization of the random walk on hypergraphs, introduced in [116]. In a first-order unbiased random walk, a walker in a node i moves to one of its neighbours j choosing with equal probability among its links. In the case of a higher-order unbiased random walk, we want to define a dynamics in which the walker chooses with equal probability among its hyperlinks and then selects one of the nodes belonging to such a higher-order structure, favouring intrinsically those neighbours that belong to highest-order hyperlinks, Figure 3.1.



Figure 3.1: Illustration of the random walk on hypegraph.

Such a dynamic portrays the diffusion of ideas or the spreading of rumours or misinformation that is generally enhanced by group interactions. In order to write the transition matrix of this process, we start defining the hyper-incidence matrix $e_{i\alpha}$ telling if a node *i* belongs to a hyperlink E_{α} , namely:

$$e_{i\alpha} = \begin{cases} 1 & \text{if } i \in E_{\alpha} \\ 0 & \text{otherwise} \end{cases}$$
(3.1)

From the hyper-incidence matrix one can define the hyperadjacency matrix as follows:

$$A = ee^T, (3.2)$$

where A_{ij} represents the number of hyperlinks containing both nodes *i* and *j*.

Furthermore, one can build the hyperedges matrix, $C_{\alpha\beta}$,

$$C = e^T e, (3.3)$$

whose entry $C_{\alpha\beta}$ counts the number of common nodes between E_{α} and E_{β} ($E_{\alpha} \cap E_{\alpha}$) and $C_{\alpha\alpha}$ is the size of an hyperlink E_{α} , or equivalently its order of interaction plus one, $|E_{\alpha}| = O_{\alpha} + 1$.

By means of C and e, we can construct the weight of the transition matrix of the unbiased random walk, k_{ij}^H , that reads,

$$k_{ij}^{H} = \sum_{\alpha} (C_{\alpha\alpha} - 1) e_{i\alpha} e_{j\alpha} = (e\hat{C}e^{T})_{ij} - A_{ij}, \qquad (3.4)$$

where its entries represent the sum of the orders of all the common hyperlinks between *i* and *j*. For instance if two nodes *i* and *j* share one link, two second-order hyperlinks (three body interactions) and one third-order hyperlink (four body interactions), $k_{ij}^H = 1 \times 1 + 2 \times 2 + 1 \times 3 = 8$.

Summing k_{ij}^{H} over all neighbours of a node *i*, one obtains the order-weighted hyperdegree,

$$k_i^H = \sum_l k_{il}^H, \tag{3.5}$$

namely the sum of the orders of all the hyperlinks belonging to *i*.

Therefore, the transition matrix of the unbiased random walk on hypergraphs reads

$$\Pi_{ij} = \frac{\sum_{\alpha} (C_{\alpha\alpha} - 1) e_{i\alpha} e_{j\alpha}}{\sum_{l} \sum_{\alpha} (C_{\alpha\alpha} - 1) e_{i\alpha} e_{l\alpha}} = \frac{k_{ij}^H}{\sum_{l} k_{il}^H} = \frac{k_{ij}^H}{k_i^H}.$$
(3.6)

Note that in the case of simple graphs, having only first-order interactions, and therefore $C_{\alpha\alpha} = 2$ for every link E_{α} , we obtain the transition matrix of the unbiased random walk on simple graphs:

$$\Pi_{ij} = \frac{\sum_{\alpha} (C_{\alpha\alpha} - 1) e_{i\alpha} e_{j\alpha}}{\sum_{l} \sum_{\alpha} (C_{\alpha\alpha} - 1) e_{i\alpha} e_{l\alpha}} = \frac{2 \sum_{\alpha} e_{i\alpha} e_{j\alpha} - A_{ij}}{2 \sum_{l} \sum_{\alpha} e_{i\alpha} e_{l\alpha} - k_i} = \frac{A_{ij}}{k_i}.$$
(3.7)

3.4 Dynamical fluctuations of random walks in higher-order networks

In this section, we outline the core methodology of our approach. We begin by defining a higher-order network model whose configuration probabilities can be analytically computed, enabling us to determine the rate functions without resorting to Monte Carlo simulations. We then delve into the study of dynamical fluctuations of a random walk on this structure.

3.4.1 Model

We consider a hypergraph G = (V, E), where V represents the set of nodes, and $E = \{E_1, E_2, \dots, E_M\}$ the set of hyperedges, i.e., E_m is an unordered collection of nodes belonging to the same hyperedge m. We focus in particular on an illustrative structure consisting of a *core* node, labelled 0, connected with *peripheral* nodes through a varying number of higher-order connections, labelled by $i \in \{1, \dots, N-1\}$. As shown in Fig. 3.2,

the graph is composed by |V| = N nodes, a fully connected pairwise structure, i.e. (

binary edges $E_{i(2N-i-1)/2+j} = \{i, j\}$ for $(i, j) \in [0, N-1]^2$ and i < j, and a number η drawn from a binomial distribution of parameter $p \in [0, 1]$ of three-body interactions $E_{N(N-1)/2+i} = \{0, i, j\}$ where *i* is an odd node and j - i = 1, i.e., all triangular interactions are centered in 0. Intuitively, the greater the number of higher-order interactions the better connected the core node is with the periphery of the hypergraph. For simplicity, in the following we constrain the higher-order structure so that each peripheral node can participate in at most one three-body interaction. As we will show, for this symmetric model, non-pairwise interactions affect the statistics of the core occupation time only through their total number η . In particular, the probability of drawing a hypergraph with a number of three-body interactions $H = \eta$ is given by

$$\mathbb{P}(\eta) \coloneqq \mathbb{P}(H = \eta) = \binom{N_{\triangle}}{\eta} p^{\eta} (1 - p)^{N_{\triangle} - \eta} \quad , \tag{3.8}$$

where $N_{\triangle} = \operatorname{ceil} \left[(N-2)/2 \right]$ is the maximum number of possible three-body interactions that the hypergraph can have.

In summary, for the model we consider here, G comes as an instance of an ensemble of hypergraphs whose higher-order structure is fully described by two parameters only, namely N and p. We consider on G an n-step discrete-time random walk $X = \{X_l\}_{l=1}^n$, where X_l denotes the node where the random walk sits at time l [153]. The random walk is characterized by an unbiased dynamics given by the transition matrix $\Pi = \{\pi_{ij}\}$ whose entries are

$$\pi_{ij} = \frac{k_{ij}^H}{\sum_{l=1}^N k_{il}^H} , \qquad (3.9)$$



Figure 3.2: Illustration of our model. Dashed lines represent pairwise interactions that form the underlying complete graph. In pink, two higher-order interactions connect the core node 0 with the peripheral nodes (1, 2), and (3, 4). The random walk's dynamics are represented by arrows departing from certain nodes and pointing towards others, where different thicknesses refer to different jump probabilities.

where k_{ij}^H represents the hyper-degree, i.e., the number of nodes, excluding *i*, that are present in the hyperedges that are common to *i* and *j*. As the random walk explores the graph, it collects information in the form of the time-additive observable

$$T_n = \frac{1}{n} \sum_{l=1}^n \delta_{X_{l,0}} , \qquad (3.10)$$

which measures the fraction of time the random walk has spent on the core node 0 up to time n. In the limit of $n \to \infty$, the typical fraction of time $T_{\eta,\text{typ}}$ the walker spends in 0 for a number $H = \eta$ of three-body interactions reads [153]

$$T_{\eta,\text{typ}} = \frac{4\eta + N - 1}{8\eta + (N - 1)^2} \,. \tag{3.11}$$

The higher the number of triangular interactions, the better connected the core with the periphery of the graph, and the longer the time the random walk will spend in 0. Having delineated the typical behavior of the dynamical process, we now focus on its finite-time fluctuations. We consider dynamical fluctuations in two different physical scenarios. First, we study the mean behavior of rare events of T_n over the ensemble of possible hypergraphs of our model (quenched case). Then, at the expense of an entropic cost associated with the logarithm of $P(\eta)$ in (3.8), we let the random walk choose the optimal hypergraph that

generates a particular atypical fluctuation of T_n (annealed case). Results for more complex higher-order topologies, and for more general dynamics considering random walks biased on the higher-order structure, are qualitatively consistent and illustrated in following sections.

3.4.2 Quenched and annealed scenarios

The properties of the time-additive observable we have defined in the previous subsection can be computed in two different key scenarios often considered in statistical mechanics: quenched and annealed. In the quenched scenario, the structure of the hypergraph is assumed to be fixed, allowing us to analyze dynamics on a static network where only the state of the system evolves over time. In contrast, the annealed scenario introduces an ensemble of possible structures, where each configuration is sampled at each time step, leading to a dynamic interpretation of both the structure and the observable being measured. These differing approaches provide distinct insights into system behavior, with the quenched case emphasizing stability and path-dependence, and the annealed case offering a probabilistic view over possible configurations.

In the quenched scenario, the observable is computed on a fixed structure, meaning that its evolution is determined solely by the dynamics of the system. For example, if the observable tracks the position of a random walker on the hypergraph, each time step reflects movement within the same structural constraints. On the other hand, in the annealed scenario, the observable is influenced by both the dynamics of the system and the varying structures at each time step. Here, the observable is recalculated each time a new structure from the ensemble is selected, offering a more generalized, averaged perspective across different realizations of the hypergraph. This duality in interpretation allows for a more flexible analysis of dynamic processes on hypergraphs.

These concepts are illustrated in Fig. 3.3, by means of a sketch portraying random walks on hypergraphs in the quenched and annealed cases, highlighting how we track the evolution of a chosen physical observable under each scenario.

3.4.3 Quenched fluctuations

In the quenched scenario, we consider averaged fluctuations in static hypergraph structures with η three-body interactions and investigate how higher-order network configurations impact the dynamics of random walks. To do so, we employ large deviations theory [101,102,160], making use of the leading scaling behavior of the probability distribution $\mathbb{P}_{\eta,n}(t) := \mathbb{P}_{\eta,n}(T_n = t)$ that is exponential in time, i.e.,

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Figure 3.3: Illustration of quenched and annealed scenarios in random walk on hypergraphs. In panel (a), the quenched case is shown where the hypergraph structure remains fixed. A random walker, represented by the red node, moves across the static structure. At each time step, we count a physical observable, such as whether the walker visits a specific node. In panel (b), the annealed case is depicted. Here, there is an ensemble of possible structures, with independent random walkers on each structure. At every time step, one structure from the ensemble is selected (highlighted by the small circles), and the observable is measured for that particular realization. The process is repeated with different structures selected at each time step, resulting in the observable being counted over varying structures.

$$\mathbb{P}_{n,n}(t) = e^{-nI_{\eta}(t) + o(n)} , \qquad (3.12)$$

where $I_{\eta}(t)$ is the non-negative large-deviation rate function containing the relevant information about rare events and o(n) denotes sub-linear corrections in n. Evaluating I_{η} directly is often non-trivial, thus we resort to a change of ensemble to get meaningful information on fluctuations. To this end, we introduce the Scaled Cumulant Generating Function (SCGF)

$$\Psi_{\eta}(s) = \lim_{n \to \infty} \frac{1}{n} \ln G_{\eta,n}(s) = \lim_{n \to \infty} \frac{1}{n} \ln \mathbb{E}\left[e^{nsT_n}\right]$$
(3.13)

which characterizes the leading exponential behavior of the moment generating function $G_{\eta,n}(s)$ associated with T_n . Here, s, the Laplace parameter that enters in the SCGF, plays the role of the conjugate parameter to T_n . Intuitively, as much as the inverse temperature in

equilibrium statistical mechanics is connected to the internal energy of a system through the derivative of the canonical free energy, s is connected to the observable T_n . When s > 0, T_n will more likely take values that are larger than the typical value and viceversa when s < 0. For finite and connected hypergraphs, $\Psi_{\eta}(s)$ is analytic, and one can calculate $I_{\eta}(t)$ via the Gartner–Ellis theorem [101, 102, 160, 161] that makes use of the Legendre–Fenchel (LF) transform

$$I_{\eta}(t) = \sup_{s \in \mathbb{R}} \left(st - \Psi_{\eta}(s) \right) , \qquad (3.14)$$

which links the Laplace parameter s with a fluctuation $T_n = t$ as

$$t = \Psi_n'(s) . \tag{3.15}$$

Because the random walk X is ergodic, the SCGF can be obtained as

$$\Psi_{\eta}(s) = \ln \zeta_s , \qquad (3.16)$$

where ζ_s , computed numerically, is the dominant eigenvalue of the so-called tilted matrix

$$\Pi_s = \{(\pi_s)_{ij}\} = \{\pi_{ij}e^{s\delta_{0,j}}\}$$
(3.17)

To account for average properties of the ensemble of hypergraphs considered, one can take a quenched average over the disorder—here characterized by the number η of higherorder interactions—of the function Ψ_{η} . Recalling that H is a binomially distributed random variable with parameter p and that the maximum number of higher-order interactions is N_{Δ} , the quenched average can explicitly be written as

$$\Psi_{\mathbf{q}}(s) = \sum_{\eta=0}^{N_{\Delta}} \mathbb{P}(\eta) \Psi_{\eta}(s) , \qquad (3.18)$$

where 'q' stands for quenched. Remarkably, the quenched average (3.18) takes such a simplified form because for a fixed number η of higher-order interactions, we have only one possible transition matrix. However, we note that more complicated models might lead to different disorder configurations and therefore different transition matrices. In the latter case, to disentangle disorder and dynamics one would need to carefully study combinatorially how many different configurations arise by fixing η . Given $\Psi_q(s)$ in (3.18), the quenched rate function $I_q(t)$ can be obtained via an LF transform of Ψ_q (rather than Ψ_{η}) in (3.14).

To understand the role of higher-order interactions, we first look at whether fluctuations of a given magnitude are more or less likely to appear on higher-order networks generated with different values of p. To understand this, we re-scale t in $I_q(t)$ with the typical fraction of time spent in 0 by the random walk at a fixed parameter p, namely T_{typ} , obtained by

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averaging (3.11) over $\mathbb{P}(\eta)$. In Fig. 3.4 we plot the rate functions $I_q(\tilde{t} = t/T_{typ})$ (\tilde{t} : time fraction on the core node relative to typical time) for different values of p and compare them with the rate function for a graph with no higher-order interactions (p = 0 case). Because of the re-scaling, all rate functions are 0 at the typical value $\tilde{t} = 1$. The likelihood is encoded in the shape of the rate function branches, the higher (lower) the branch the exponentially-less (more) likely is a fluctuation $\tilde{t} \neq 1$ to appear. We notice that with increasing p the average number of higher-order interactions pointing to node 0 grows generating a 'confinement' effect, which has two consequences on the dynamics.

On the one hand, at fixed p, fluctuations are more likely for times greater than the typical time, making it easier to visit the core node than peripheral nodes, as revealed by the asymmetric shape of the rate functions in Fig. 3.4. On the other hand, as p increases, more probability weight is concentrated in nodes connected to the core node via higher-order interactions. This means that, the greater the p, the harder it is for the random walk to leave earlier these nodes or stick to them for too long, as both behaviours become costly in terms of probability. In Fig. 3.5, the rate functions plotted against the non-rescaled time t show that typical time increases with p, but also that relative time changes are associated with bigger absolute fluctuations (the level lines of $I_q(p, t)$ are not parallel to T_{typ}). Thus, higher values of p result in wilder relative fluctuations and make it harder for the random walk to visit a core/localized or periphery/delocalized phase in the fluctuations.

More in detail, in Fig. 3.5 we show how I_q depends both on t and p. Comparing with the case of a fully pairwise graph (p = 0), on the one hand we show that the typical behavior at greater p is atypical for the case p = 0. On the other hand, rare values of T_n greater than the typical one for the case p = 0 can become typical just by increasing the number of higher-order interactions. By contrast, rare values of T_n smaller than the typical one become even more atypical by introducing higher-order interactions. We show fluctuations of the occupation time on peripheral nodes (all nodes but the core). Noticeably, we observe the opposite behavior, with an enhancement of fluctuations far off the typical occupation time. In summary, by introducing higher-order interactions we make it easier for the random walk to spend more time on the core node and less time on peripheral nodes.

Differently from the core-periphery case, in subsection 3.6.1 we also discuss the case of homogeneous hypergraphs, where higher-order interactions are not created around a given core node but distributed at random. There, we observe that the probability of the occupation time on a random node varies non-monotonically as a function of p, showing that there is an optimal value of higher-order interactions that generates wider fluctuations of the dynamics.

3.4.4 Dynamical fluctuations on peripheral nodes

Here we investigate the dynamical fluctuations of the time a random walk spends on peripheral nodes of the model presented in the section 3.4. Specifically, in Fig. 3.6, we show the



Figure 3.4: Rate functions $I_q(\tilde{t})$ as a function of the rescaled time \tilde{t} for different densities of higher-order interactions in the hypergraph p. The higher the p, the narrower the rate functions for $|\tilde{t}| > 1$.



Figure 3.5: Heatmap representing how the rate function $I_q(t)$ behaves as a function of t and p (for visualisation purposes we plot $\sqrt{I_q}$). The light-blue line represents the typical value T_{typ} which linearly increases with p. Plots obtained for a hypergraph with N = 1000 nodes.

rate functions considering as observable the occupation time on peripheral nodes (all nodes but the core), i.e., $\bar{T}_n = \frac{1}{n} \sum_{l=1}^n \sum_{i=1}^{N-1} \delta_{X_l,i}$. We refer to $\bar{I}_q(\tilde{t})$ as the rescaled rate function associated with the new observable \bar{T}_n . Noticeably, we observe the opposite behavior, with an enhancement of fluctuations far off the typical occupation time. In summary, by introducing higher-order interactions on a fully-pairwise network we make it easier for the random walk to spend more (less) time on the core (peripheral) node(s).



Figure 3.6: Rate functions $\bar{I}_q(\tilde{t})$ as a function of \tilde{t} observing the occupation time on all peripheral nodes ({1,...N - 1}).

3.4.5 Annealed fluctuations

We now consider random walks defined on non-static hypergraphs. Such annealed [162] scenario is relevant to predict dynamical behaviors in time-varying systems where the structure evolves at a rate which is comparable to the time-scale of the process on top [163], or in large systems whose precise characterization is often limited by lack of data or noise [164]. In particular, we investigate the annealed fluctuations of the occupation time observable in (3.10) over non-fixed realizations of three-body interactions for the model introduced above. In such a scenario, large fluctuations of a dynamical observable, such as T_n , could be generated by an optimal, albeit rare, realization of the underlying structure.

We consider the joint probability of obtaining a realization of the higher order structure and the occupation time in (3.10), and compute the moment generating function $G_n(s)$ associated with the observable T_n with respect to this probability. We notice that $G_n(s)$ takes the form of an *annealed* average of the moment generating function $G_{\eta,n}$ over the disorder
$$G_n(s) = \sum_{\eta=0}^{N_{\triangle}} \mathbb{P}(\eta) G_{\eta,n}(s) , \qquad (3.19)$$

where we remind the reader that fixing s corresponds to fixing a fluctuation t (on average) according to (3.15).

We consider the regime of long times and large graphs, with the condition $n \gg N_{\triangle} \gg 1$, and introduce the fraction of total triangles $h = \eta/N_{\triangle}$. The moment generating function $G_n(s)$ can be expressed using a saddle point approximation in (h, t), i.e.,

$$G_n(s) \approx e^{n\left(\ell^{-1}\log\mathbb{P}(h^*) + \Psi_{\eta^*}(s)\right)},$$
 (3.20)

where we call $\ell = n/N_{\triangle}$ the *annealing parameter* and indicate the saddle-point solution with (h^*, t^*) , adopting the shorthand notation $\eta^* = h^* N_{\triangle}$. In the following, we focus on the non-trivial exponent of (3.20):

$$\hat{\Psi}_{\ell}(s) \coloneqq \ell^{-1} \log \mathbb{P}(h^*) + \Psi_{\eta^*}(s) .$$
(3.21)

We can obtain the annealed SCGF from (3.21) by taking the infinite ℓ limit, that is $\Psi_a(s) := \hat{\Psi}_{\ell \to \infty}(s)$. The function $\Psi_a(s)$, together with its LF transform $I_a(t)$, completely describes atypical fluctuations of occupation times in the annealed regime. For large values of ℓ , disorder and dynamics 'interact' at the saddle-point solution of (3.20) selecting the most likely structure that realises the occupation-time fluctuation associated with s. We remark that (3.20) is valid as long as ℓ is large. In particular, for ℓ finite and small, one has $N_{\Delta} > n$ and therefore the ergodicity assumption necessary to derive $\Psi_{\eta^*}(s)$ falls. Indeed, for finite ℓ spurious contributions of $O(\ell^{-1})$ appear in (3.21) and shift \hat{I}_{ℓ} , the LF transform of $\hat{\Psi}_{\ell}(s)$ in (3.21), upwards. However, since the disorder is self-averaging, in the limit $\ell \to 0$ all probability concentrates around the typical number of higher-order interactions, recovering the quenched average (3.18) for a fixed p.

In Fig. 3.7 we plot I_{ℓ} for several values of ℓ . As expected, for small ℓ we retrieve the quenched rate function I_q (for the parameter p = 0.5 used here) which is realised by the typical number of higher-order interactions $\eta^* = h^* N_{\Delta} \sim \text{ceil} [N_{\Delta}/2]$ throughout all fluctuations shown in Fig. 3.8. As we increase ℓ , the function \hat{I}_{ℓ} tends to flatten, and in the limit $\ell \to \infty$ the annealed rate function I_a develops a plateau of zeros. That an annealed rate function is a lower bound of a quenched one is known in the mathematics literature [103, 111, 165, 166]. Intuitively, this is a consequence of picking an optimal structure to generate fluctuations in the dynamics rather than having it fixed as in the quenched case. Although I_a exhibits a continuous range where it equals zero, not every occupation time twithin this range is a typical event. Only the times resulting from the most probable network configurations, which manifest at the boundaries of this zero plateau, truly represent the



Figure 3.7: Rate functions \hat{I}_{ℓ} functions for different ℓ , as a function of t. Monte-Carlo quenched simulations for the three cases with no (left-most), maximum (right-most), and half-maximum (center) number of higher-order interactions are plotted as cross-shaped scatter points. Annealed simulations' results are plotted as round scatter points for different values of ℓ , colored according to the legend. Results are obtained for a hypergraph with N = 21 nodes and p = 0.5.

typical behavior of the observable T_n . These specific configurations emerge from the saddle point calculation (3.20) and, therefore, are statistically favored and dominate the ensemble. To further validate our observations, in Fig. 3.7 we also plot Monte-Carlo (MC) simulations for both the quenched and annealed case. Quenched simulations appear as coloured crossshaped scatter points for three different scenarios of random walks exploring a graph with no (left-most gray), max (right-most gray), and half-max (orange) number of higher-order interactions. Annealed simulations appear as enlarged green and gray scatter points for two different values of ℓ . In particular, orange crosses well describe the shape of the quenched rate function I_q and gray circles well show the flattening of the function \hat{I}_ℓ at large values of ℓ . Noticeably, from the saddle-point calculation in Fig. 3.8 it is evident that for large values of ℓ as one slightly moves from the typical scenario s = 0 and looks into fluctuations for either s < 0 or s > 0, the structure η^* optimally realising such fluctuations abruptly changes from, respectively, a graph with no higher-order interactions, i.e., min (η^*) = 0, to a structure that maximizes their number, i.e., max (η^*) = 10 for N = 21.

For finite ℓ we observe a continuous crossover centered in s = 0 between these two regimes. For large ℓ , such crossover appears to be much steeper, hinting at the existence of a transition in the limit $\ell \to \infty$ between two regimes, one where the random walk spreads over the entire graph, and one where it spends more time on the core node due to higherorder interactions. As discussed in the subsection, this is due to the use of the saddle-point approximation, and the existence of a phase transition is not confirmed by an analysis of the distribution of T_n at large ℓ of simulations of random walks on evolving hypergraphs,



Figure 3.8: The optimal value η^* of the number of higher-order interactions plotted as a function of s (the fluctuation parameter). Results are obtained for a hypergraph with N = 21 nodes and p = 0.5.

which converge to an unimodal distribution with $\ell \to \infty$. This suggests that the observed flattening might be due to neglecting sub-leading o(n) terms in Eq. (3.20). This results in heavier tails in the T_n distribution, allowing rare events to occur more frequently. In summary, while the saddle-point solution is limited in describing fluctuations of the system close to the typical time, it allows to correctly capture the extreme values of the annealed rate function, as confirmed by the good matching between MC simulations and analytical predictions in the tails of the rate functions.

3.4.6 Monte Carlo simulations for the quenched and annealed scenarios

Given a hypergraph of size N = 21 with a configuration of higher-order interactions η sampled from the binomial distribution in Eq. (3.8), we run 10^4 simulations (the more the smoother the statistic) of length $n = 10^4$ (the number of time steps of the random walk). The result of this is a histogram of values for the observable T_n (fraction of time the random walk has spent on the core node) for a given hypergraph. We then calculate the rate function (see Eq. (3.14)) for the observable T_n as

$$I_{\eta}^{\rm sim}(t) = -\frac{1}{n} \ln \mathbb{P}_{\eta}^{\rm hist}(t) , \qquad (3.22)$$

where superscript 'sim' indicates that the function is obtained from 'simulations' and 'hist' refers to the fact that the distribution is approximated by the 'histogram' related to the simulations. We repeat the procedure for 10^4 configurations of the hypergraph randomly selected from the binomial distribution in Eq. (3.8) and calculate the rate functions by averaging as

follows

$$I_{q}^{\rm sim}(t) = \sum_{\eta=0}^{N_{\Delta}} \mathbb{P}^{\rm hist}(\eta) I_{\eta}^{\rm sim}(t) , \qquad (3.23)$$

where $\mathbb{P}^{\text{hist}}(\eta)$ is the probability distribution of configurations η at a fixed p obtained with the random generation of graphs (it converges to Eq. (3.8) for infinitely many simulations). Notice that the cumulative statistics over different hypergraphs come only after re-scaling with $1/n \ln$ each distribution of T_n .

These are the quenched simulations represented as gray (p = 0 and p = 1) and orange (p = 0.5) circular dots in Fig. 3.7. They are used as a sanity check both for the quenched limit of our annealed calculation for p = 0.5 in the middle and, in the case of the annealed rate function, to check that the extrema of the zeros plateau corresponds to the two opposite situations of a graph with no triangular interactions for p = 0 (on the left) and a graph with N_{Δ} (the maximum possible) triangular interactions for p = 1 (on the right).

In order to carefully calculate (from simulations) the Legendre transform of Eq. (3.21), which is the asymptotic leading behaviour of Eq. (3.19), and visualise the rate functions appearing in Fig. 3.7 we generate 10^5 trajectories (the more the smoother the statistics) of the random walk of length $n = 10^4$ (which in turn fixes the parameter $\ell = n/N_{\Delta}$ for a graph of N = 21 nodes) where each one is initialised over a hypergraph with a number of triangular interactions picked up at random from the binomial distribution in Eq. (3.8). The graph is resampled over the trajectory of the random walk at a fast rate. For the simulations shown the graph is resampled at every time step of the random walk. However, we have seen that changing the rate slightly does not qualitatively change the results.

Once all the trajectories are obtained we calculate the cumulative statistic (the histogram) of the observable T_n and, only after that, re-scale the properly normalised histogram by $1/n \ln$. It is important to stress here that in the annealed scenario the re-scaling comes after obtaining the full statistics over all hypergraphs for the observable T_n (notice that this procedure is inverted in the quenched scenario), which is the reason why at the saddle point of Eq. (3.20) dynamics and disorder 'interact'. This procedure already generates a distribution $\mathbb{P}_a^{\text{hist}}$ for the observable T_n and from it we directly calculate the rate function

$$I_{\mathrm{a}}^{\mathrm{sim}}(t) = -\frac{1}{n} \ln \mathbb{P}_{\mathrm{a}}^{\mathrm{hist}}(t)$$
 .

This is the procedure followed to obtain the annealed simulations plotted in Fig. 3 (a). These, as expected, show a flattening of their shape towards the asymptotic annealed behaviour at increasing ℓ confirming our annealed large deviations approach to study fluctuations of the observable T_n .



Figure 3.9: Histograms of observable T_n from annealed simulations at different values of n $(\ell = n)$. The simulations are performed considering N = 21, and 10^5 different trajectories.

3.4.7 Histograms of T_n in annealed simulations for different n

In this section, we present the histogram of the observable T_n obtained from annealed simulations for different values of n. For all simulations, we consider the annealing parameter $\ell = n$, where n represents the time length of the simulations, with each simulation performed as described in the previous section. The histograms reveal a significant finding: there is no observable flattening across the simulations. Instead, as n increases, the histograms converge, indicating no true phase transition in the system. This suggests that the flattening of the rate function observed in the annealed scenario is caused by solely examining the saddle point in the study of dynamics using large deviations, neglecting sub-leading contributions.

3.4.8 Flattening of the rate function in the annealed scenario

Now, we further investigate the flattening of the rate function derived from large-deviation theory tools in the annealed scenario and presented in section 3.4. In subsection 3.4.8, after having defined how to numerically calculate rate functions in the annealed scenario, we will give further insights on the nature of such a presumed phase transition, showing that what we observe is actually caused by solely examining the saddle point in the study of dynamics neglecting sub-leading contributions.

Given this, resorting to the saddle point approximation defined in Eq. (3.20), as presented in Fig. 3.8, we observe that when one considers the two regimes of optimal number



Figure 3.10: (a) Quenched Ψ_q and annealed Ψ_a SCGFs as a function of s. The latter shows a discontinuity in its first derivative at s = 0.



Figure 3.11: Scaling, in log-log scale, of the width Δ_s as a function of the annealing parameter ℓ .

of higher-order interactions η^* for which the system maximizes the fluctuations, (one for $\eta^* = 0$ for s < 0 and another one for $\eta^* = max(eta)$ for s > 0), for finite ℓ we observe a continuous crossover centred in s = 0 between these two regimes. For large ℓ , such crossover appears to be much steeper, suggesting the existence of a phase transition in the limit $\ell \to \infty$. However, as discussed in detail in Section 3.4, where the large deviations solution is compared with simulations of random walk on evolving hypergraphs, this is due to neglecting sub-leading terms in the saddle point approximation.

In addition, we show the scaling analysis in Fig. 3.11 where we observe a power-law decay of $\Delta_s = s_{\max(\eta^*)} - s_{\min(\eta^*)}$, i.e., the distance in terms of s between the two extreme three-body interaction regimes, as a function of ℓ . Lastly, in Fig. 3.10, we plot $\Psi_q(s)$ and $\Psi_a(s)$. For the latter, differently from the quenched case, we observe a discontinuity in the first derivative at s = 0.

3.5 Results on more general processes

To validate the solidity of our results on more general dynamics, we apply our approach to a broader class of stochastic processes. Our method is easily adaptable to any stochastic process described by a transition matrix. Among the various processes, we focus on the biased random walk, which, being more general than the unbiased random walk, can portray diverse dynamics such as spreading where more connected nodes are either more repulsive or more attractive than usual. For example, the biased random walk can describe scenarios in social networks where influential individuals (more connected nodes) either facilitate or hinder the spread of information, or in transportation networks where certain hubs attract or repel traffic flow.

3.5.1 Biased random walk on hypergraphs

Here we introduce a new class of random walks on hypergraphs, specifically a hyper-degreebiased random walk. In analogy with the biased random walk on simple graphs [167], such a dynamic extends the unbiased random walk introducing a bias that enhances or hampers the attractiveness of nodes with respect to their hyper-degree.

For the first-order case (pairwise interactions only), every node j has a bias equal to k_j^{γ} (k_j is the degree of j) and the transition matrix reads

$$\Pi_{ij}^B = \frac{A_{ij}k_j^{\gamma}}{\sum_j A_{ij}k_j^{\gamma}},\tag{3.24}$$

where γ is the bias exponent. For $\gamma > 0$, the transition towards large-degree nodes is favoured, while for $\gamma < 0$ nodes with small degrees attract the walker more. For $\gamma = 0$, the

transition matrix retrieves the unbiased case, being $k_i^{\gamma} = 1$.

Following a similar approach, for the higher-order case we can define a hyper-degreebiased random walk that depends on the order-weighted hyper-degree k_j^H . Resorting the definition of k_j^H from Eq. (3.4) and (3.5), we can write the transition matrix as

$$\Pi_{ij}^{HB} = \frac{k_{ij}^{H} (k_{j}^{H})^{\gamma}}{\sum_{l} k_{il}^{H} (k_{l}^{H})^{\gamma}}.$$
(3.25)

Again, this dynamic favours the transition towards nodes with large k^H when $\gamma > 0$, makes less attractive the same nodes when $\gamma < 0$ and returns the unbiased case shown in Eq. (3.6) for $\gamma = 0$.

Intuitively, by means of this generalization of the random walk on hypergraphs, we can portray a large class of processes where one might need to tune the effects of group interactions. For instance, the diffusion of trends or norm adoption can be accelerated in large groups because of conformism mechanisms and peer pressure ($\gamma > 0$), or exploratory behaviors in information-seeking processes, where individuals or algorithms prioritize novel or less popular sources over well-known ones ($\gamma < 0$).

3.5.2 Results on biased random walk

In this Subsection, we detail the results of the biased random walk, previously defined. As an observable, we focus on the fraction of time spent on the core node over the hypergraph model introduced in section 3.4. Fig. 3.12 shows our findings for the quenched calculations. In panel (a), we plot the rate function for diverse values of the bias parameter γ . We observe that the rate functions (as a function of the rescaled time \tilde{t}) are narrower at increasing $\gamma > 0$, indicating that an attractive bias towards higher-order interactions reduces fluctuations beyond the unbiased scenario. This aligns with our observations in section 3.4 where higher-order interactions were seen to suppress fluctuations, with increased attractiveness further intensifying the 'confinement' effect and thus, reducing fluctuations. In contrast, $\gamma < 0$ leads to a broader rate function, signifying that this kind of higher-order interactions allows for larger fluctuations.

Panel (b) of Fig. 1 provides a complementary analysis by displaying the rate function in relation to both γ and t.

In Fig. 3.13 we show two heatmaps for distinct γ values, displaying the rate function's dependency on t and p.

Turning our attention to the annealed case, Fig. 3.14 delineates the rate functions for varying annealed parameters across two distinct values of γ . Remarkably, in Fig. 3.14, we observe a flattening of the rate function equivalently to the unbiased case (see discussion on



Figure 3.12: (a) Rate functions $I_q(\tilde{t})$ as a function of the rescaled time \tilde{t} for different bias parameters γ . The larger the γ , the narrower the rate functions for $|\tilde{t}| > 1$. (b) Heatmap representing how the rate function $I_q(t)$ behaves as a function of t and γ . Plots obtained for a hypergraph with N = 100 nodes and density of higher-order interactions p = 0.5.



Figure 3.13: Heatmaps representing how the rate function I_q behaves as a function of t and p for two different values of γ : $\gamma = -0.5$ panel (a) and $\gamma = 0.5$ panel (b).

the limits of the validity of the saddle-point approach presented in subsection 3.4.8 to fully capture such a behavior).



Figure 3.14: Annealed rate function \hat{I}_{ℓ} for different ℓ as a function of t, and the characteristic times (vertical dashed lines) for $\eta = 0$ and $\eta = max(\eta)$. The results are obtained considering $\gamma = -2$ (a) and $\gamma = 2$ (b).



Figure 3.15: The optimal value η^* of the number of higher-order interactions as a function of the tilting parameter s for p = 0.5, and different $\gamma : [-2, -1, 0, 1, 2]$.

Lastly, we examine which configurations of higher-order interactions maximize the fluctuations in the annealed scenario considering different values of the bias parameter γ . In Fig. 3.15, we show that the biased random walks maximize fluctuations in two different regimes. For $\gamma > -1$, the dynamical system behaves accordingly to the unbiased case, $\gamma = 0$, having the optimal configuration with no higher-order interactions for fluctuations of the residence time on the core node smaller than the typical value ($\eta^* = 0$, for s < 0) and with the totality of such interactions for fluctuations of the residence time greater than the typical value ($\eta^* = N_{\Delta}$, for s > 0). On the contrary, for $\gamma < -1$ in Fig. 3.15 (a), the

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optimal configurations are inverted with respect to positive and negative fluctuations. Intuitively, in the original unbiased case, the higher-order interactions increase the transition probability proportionally to the generalized hyper-degree k_i^H . When one inserts a negative bias with respect to k_i^H , the attractivity of nodes with higher-order interactions is reduced, and at $\gamma = -1$ the topological bias on higher-order interactions is compensated dynamically, with this interplay between structure and dynamics making the random walk not feel the effect of higher-order interactions anymore.



Figure 3.16: Heatmaps representing how the SCGF Ψ behaves as a function of η and s for five different values of $\gamma : [-2, -1, 0, 1, 2]$.

To further validate this idea, we plot in Fig. 3.16 the SCGF Ψ with respect to the number of triangular interactions η and the tilting parameter s. We observe that, for $\gamma = -1$, Ψ does not depend on η (panel (b)) and therefore is independent with respect to the number of higher-order interactions. While for $\gamma < -1$ (panel (a)), Ψ has an inverted behaviour with respect to the case $\gamma > -1$ (panels (c), (d), (e)).

3.6 Results on more general structures

The results presented so far are based on the model we have proposed, chosen for its computational simplicity that allows for the calculation of the SCGF knowing the probabilities of every configuration. Here, we consider more general structures whose configuration probabilities cannot be found analytically and must instead be determined through extensive Monte Carlo simulations. The rest of the approach remains equivalent, and we show that the findings are consistent with the results obtained previously. Specifically, we analyze various star-like hypergraph models with different topologies, such as those with overlapping or non-overlapping triangles and underlying random regular graphs.

3.6.1 Dynamical fluctuations in a homogeneous higher-order network

In the following, we investigate a model with no preferential / core node, where the threebody interactions are randomly distributed among any triplet of nodes (i, j, k) with probability p on top of a fully-connected structure in the quenched scenario.



Figure 3.17: Rate function $\underline{I}_q(\tilde{t})$ as a function of the rescaled time \tilde{t} for several densities of three-body interactions p in a hypergraph of N = 20 nodes with homogeneously distributed triangles. In the insets we zoom on both tails to highlight the non-monotonicity with respect to p.

In particular, in Fig. 3.17, we plot the large deviations rate function $\underline{I}_q(\tilde{t})$ associated with the occupation-time observable $\underline{T}_n = \frac{1}{n} \sum_{l=1}^n \delta_{X_l,j}$ for a randomly chosen node j as a function of the rescaled time \tilde{t} for several values of p. The two insets zoom on the non-monotonic tails –with respect to p– of the rate functions for values of \tilde{t} far from T_{typ} . Additionally, in Fig. 3.18, we plot the rate function, $\underline{I}_q(\tilde{t})$ as a function of p, for two values of \tilde{t} , one larger and one smaller than the typical time T_{typ} .

In summary, the magnitude of fluctuations in homogeneous hypergraphs with no preferential core node display a non-monotonic dependence on the density p of higher-order interactions. Remarkably, this indicates the existence of an optimal value of p that minimizes $\underline{I}_{q}(\tilde{t})$, and therefore maximizes the appearance of atypical occupation times.



Figure 3.18: \underline{I}_q for two fluctuations \tilde{t} as a function of p for two values of \tilde{t} , in a hypergraph of N = 20 nodes with homogeneously distributed triangles.

3.6.2 Dynamical fluctuations in star-like hypergraph models with more complex topology

In this section we discuss the atypical behavior of random walks on three additional starlike hypergraph models. While these models preserve the main features behind the model considered in section 3.4, their analysis presents additional complications. The model has the advantage of being extremely simple from a combinatorial point of view, allowing us to compute both quenched and annealed averages without making use of a numerical sample of all possible realizations of the model. Specifically, Eq. (3.8) describes the probability of drawing a hypergraph with a certain number of three-body interactions, and inserted in Eqs. (3.18) and (3.19) allows us to obtain respectively the quenched and the annealed Scaled Cumulant Generating Function. By contrast, these additional models are more costly because the weights $\mathbb{P}(\eta)$ used in both the quenched and annealed average (Eqs. (3.18) and (3.19)) can only be found by an extensive numerical sample.

Model S1: Core-node, All-possible triangles, underlying complete pairwise graph Model S1 extends Model A by allowing the formation of all possible triangles that include the central node 0 and any two peripheral nodes i and j. These triangles are generated with a probability p. Similar to Model A, this model also features a complete pairwise graph that fully interconnects all nodes.

Model S2: Core-node, Non-overlapping triangles, underlying random regular pairwise graph Model S2 maintains the same central node and non-overlapping triangles as the original Model A. However, the underlying pairwise connectivity is described by a regular random graph with pairwise degree k = 3, rather than being a complete graph. This introduces additional randomness in the connectivity patterns of the nodes.

Model S3: Core-Node, All-possible triangles, underlying random regular pairwise graph Model S3 combines elements of Model S1 and S2. In particular, it includes a central node 0 and allows the formation of all possible triangles involving 0 and any pair of peripheral nodes i and j as in Model S1. These triangles are realized with a probability p. The underlying pairwise connectivity of this model is a regular random graph with pairwise degree k = 3.

Results In Fig. 3.19 we investigate dynamical fluctuations in both the quenched and annealing scenario by reproducing some of the plots presented in section 3.4 for Models S1 (top row), S2 (middle row) and S3 (bottom row). In particular, the left panels (a, d and g) refer to the quenched scenario discussed in Figure 3.4. By contrast, the middle (b, e and h) and right panels (c, f and i) characterize the annealed scenario and should be compared with Figure 3.7 and Figure 3.8 respectively.

In particular, in Fig. 3.19, panels (a, d and g) for the quenched scenario we plot the quenched rate functions $I_q(\tilde{t} = t/T_{typ})$ as a function of the rescaled time $\tilde{t} = t/T_{typ}$ for various values of p. The rate function reflects the likelihood of dynamical fluctuations, with a higher one indicating a lower probability for fluctuations with $\tilde{t} \neq 1$. We observe that, for p > 0, the presence of higher-order interactions consistently reduces the probability of deviations from the typical value, thereby restricting the random walk's ability to visit either a core-localized or periphery-delocalized phase during fluctuations. Increasing p the average number of higher-order interactions pointing to node 0 grows generating the same 'confinement' effect on the dynamics discussed in section 3.4. As a consequence, escaping from node 0 becomes harder and dynamical fluctuations are suppressed.

In Fig. 3.19, panels (b, e and h), we display the annealed rate functions \hat{I}_{ℓ} sa a function of the rescaled time \tilde{t} for various levels of the annealing parameter ℓ , for a density of higherorder interactions given by p = 0.5. For lower values of ℓ , we recover the quenched rate function I_q , which is realised by the typical number of higher-order interactions η^* across all fluctuations. For higher values of ℓ , the function \hat{I}_{ℓ} begins to exhibit a flattening trend, in analogy to what we observed in the simpler model discussed in section 3.4.

Lastly, in Fig. 3.19, panels (c,f and i), for the same three values of ℓ we plot the optimal number of three-body interactions η^* that corresponds to the minimum of the rate functions in panels (b, e and h), namely the specific configuration that maximizes the fluctuations over the annealed average. For the lowest value of ℓ , the behavior of η^* is practically undistinguishable from the quenched scenario. For an intermediate value of the annealing parameter, $\ell = 2 \times 10^2$, we observe that for negative values of s the optimal fluctuations are obtained for small η^* , while for positive values of s these are obtained for large η^* . The continuous crossover between these two regimes, centered in s = 0, becomes much steeper for the highest value of the annealing parameter, $\ell = 2 \times 10^9$, supporting the existence of a transition between such two regimes in the limit of $\ell \to \infty$.

In summary, the patterns of dynamical fluctuations observed in the more complex higherorder topologies considered in Models S1, S2 and S3, are consistent to the ones observed in the simpler model of section 3.4, for both the quenched and annealed scenario.



Figure 3.19: (a,d,g) Quenched rate functions $I_q(\tilde{t})$ for different densities of higher-order interactions p. (b,e,h) Functions $\hat{I}_\ell(t)$ for different values of the annealing parameter ℓ for p = 0.5. (c,f,i) The optimal value η^* for the number of higher-order interactions as a function of the tilting parameter s for p = 0.5. Results are obtained for hypergraphs generated for Models S1 (top row), S2 (middle) and S3 (bottom), with N = 20 nodes.

3.7 Conclusions

In this chapter we have shed light on the impact of higher-order interactions on the atypical behaviors of dynamical processes on networks. In particular, we have investigated random walks dynamics in a simplified higher-order model, which allowed us to gain insights on dynamical fluctuations of diffusive processes in hypergraphs. By applying large deviations tools we have derived the leading exponential scaling of fluctuations for a dynamical observable, here considered to be the mean fraction of time the random walk spends on the system nodes. In the quenched case, where the structure of the system is fixed, higher-order interactions inhibit random walk fluctuations of the occupation time at the core, but enhance it elsewhere. In the annealed case, averaging over dynamics on non-fixed structures, the random walk dynamics select the optimal structure that realises a particular fluctuation. In such a scenario, rare events of the occupation time are more likely to appear, and by means of a saddle-point approximation, it is possible to capture dynamical fluctuations far from the typical time. We have also considered the case of homogeneous hypergraphs, showing the existence of a non-trivial value of density of higher-order interactions boosting fluctuations in higher-order networks. Finally, results shown here for random walks extend to broader dynamics, such as for large values of the biasing parameter for biased random walks on hypergraphs, where the bias promotes or hampers the visit of nodes with many higher-order interactions. In the future, it might be interesting to broaden our understanding of the impact of specific higher-order structural features, such as hypergraphs displaying a scale-free distribution of higher-order interactions [168], community structure [169], or directed hyperedges [170].

Beyond random walks, our work lays the groundwork for a broader and more general theory of fluctuations in higher-order networks. The framework developed here can be extended to a wide range of dynamical processes on networks, especially those that can be modeled as Markov processes. In particular, this approach has significant potential for applications in epidemiology, where studying rare events in contagion processes could yield valuable insights into the controllability and mitigation of disease spread. Epidemic models based on Markov chain approaches have been extensively studied in the literature [98, 171-173], providing a natural context for applying large deviations theory. By capturing the likelihood of extreme fluctuations in infection patterns, large deviations theory could inform strategies to prevent outbreaks or reduce their impact. Furthermore, higher-order interactions are known to alter the typical behavior of processes like social contagion [49] and percolation [1], making this framework especially relevant for analyzing rare and catastrophic events in complex systems. Extending these ideas to networks with features such as scale-free distributions, community structures [169], or directed hyperedges [170], will deepen our understanding of how structural characteristics influence both typical and rare dynamical behaviors in realworld systems.

Not a dog. Not a wolf. All he knows is what he's not. If only he could see what he is.

- Boris the Goose, Balto

4 Application of higher-order networks metrics to epilepsy

The network description of complex systems such as the brain is a remarkable tool to unveil their underlying organization and emergent dynamics. Such a description has enriched our understanding of brain organization both at the macroscopic [32, 174–176] and microscopic [177] levels, and has found remarkable clinical applications [178, 179]. The study of brain networks is crucial for understanding the neural basis of cognitive functions and behaviors [178]. By analyzing brain networks, researchers gain valuable insights into how different regions of the brain interact to orchestrate various cognitive processes [31].

Outline In this chapter, we focus on the application of a higher-order network perspective in the study of epilepsy. To investigate the role of regional brain organization in epilepsy surgery, we propose a neighbourhood-based description of brain connectivity. Firstly, we consider the differential connectivity between pairs of node types by implementing a threegroup partition of the brain regions, namely into resection area (RA), its neighbourhood and the remaining network. By doing so, we were able to specifically address the question of the emergence of pathological hubs in the vicinity of the RA, and its relation to surgical outcome. Secondly, we introduce a novel analysis framework to quantify regional brain organization based on the notion of extended neighbourhoods, following a previous theoretical study that generalizes the notion of clustering coefficient [180]. The extended neighbourhood of a node describes its area of influence, providing a mesoscopic description of brain organization that can inform us of e.g. the existence of regions with strong recurrent connectivity. By characterizing the network neighbourhood of each brain region through topological data analysis, we propose the generalization of local node-based centrality metrics to regional descriptors encoding regional organization.

4.1 Brain networks

The human brain operates as a highly complex system, wherein interactions between distinct regions of the brain enable the execution of cognitive, sensory, and motor functions. These interactions can be studied through the lens of network theory, where brain regions are treated as nodes and the connections between them as edges. The study of these interactions has led to the identification of two primary types of brain networks: structural and functional. While structural networks map the physical connections between brain regions, functional networks capture the dynamic interactions that emerge from brain activity.

Structural and functional brain networks Structural brain networks, formed by physical connections (white matter tracts) between brain regions, provide the anatomical foun-

dation for these interactions [181, 182]. Functional brain networks, on the other hand, are defined by statistical dependencies between the activities of different brain regions, reflecting dynamic interactions that can change over time [183]. The first provide insight into the physical pathways that enable connectivity, while functional networks reveal how these pathways are utilized during different cognitive tasks and states [184–186]. The integration of these two perspectives allows researchers to study the brain's architecture and its dynamic use, providing a holistic understanding of neural processes [187].

Furthermore, advancements in neuroimaging techniques, such as diffusion tensor imaging (DTI), functional magnetic resonance imaging (fMRI), electroencephalography (EEG), and magnetoencephalography (MEG), have significantly enhanced our ability to study brain networks [188]. These technologies provide detailed maps of structural connections and high-resolution data on functional interactions, enabling a deeper exploration of the brain's complex network dynamics [189].

Higher-Order Brain Networks A critical aspect of brain networks is their ability to support complex higher-order interactions, where multiple brain regions interact simultaneously, adding layers of complexity beyond simple pairwise connections [43]. These higher-order interactions are essential for capturing the full extent of brain network dynamics and organization.

A prominent example of higher-order structure in brain networks is the homological scaffold, identified using topological data analysis (TDA) to reveal multi-scale structures within brain networks. This approach uncovers the underlying geometric and topological properties that govern brain function, providing insights that are not evident through traditional pairwise analysis [38].

Another significant study utilized clique topology to uncover intrinsic geometric structures in neural correlations, highlighting the importance of higher-order connectivity patterns. Such studies illustrate the significance of higher-order interactions and introduce new tools and frameworks for analyzing brain networks [41].

Furthermore, recent advancements in higher-order information theory have significantly enhanced the understanding of brain networks. Techniques have been developed to decompose information into unique, redundant, and synergistic components, offering a nuanced view of brain network interactions [190–193]. This framework emphasizes the importance of higher-order interactions in understanding complex cognitive functions and their break-down in neurological disorders. Redundancy in brain networks is linked to robust communication within specialized sensorimotor systems, ensuring reliable information transfer. In contrast, synergistic interactions, which emerge from the integration of information across different regions, are crucial for higher-order cognitive functions and complex behaviors.

By applying such higher-order methods, researchers can unravel the informational ar-

chitecture of the brain, providing a comprehensive understanding of how multiple regions coordinate to perform tasks and how disruptions in these interactions can lead to cognitive impairments.

4.2 Clinical Applications of Brain Network Analysis

Disruptions in brain networks are closely linked to various neurological and psychiatric disorders, underscoring their significance in maintaining neurological health [178]. Understanding how these networks function normally and how they are altered in disease states can lead to better diagnostic and therapeutic strategies [194].

The insights gained from studying brain networks have significant clinical applications, particularly in diagnosing and treating neurological disorders [178].

For instance, Alzheimer's disease is characterized by reduced clustering and increased path length in brain networks, indicative of a loss of small-world properties crucial for efficient information transfer [195]. Schizophrenia involves disruptions in network hierarchy and connectivity patterns, contributing to the cognitive deficits observed in patients [196–198].

4.2.1 Brain Networks for Epilepsy

A remarkable example, which is the focus of this chapter, is the case of epilepsy surgery. This is the treatment of choice for drug-resistant epilepsy patients, and it entails the removal or disconnection of a set of brain regions –the epileptogenic zone (EZ)– with the goal of stopping seizure generation and propagation [199, 200].

Epilepsy surgery is preceded by an extensive presurgical evaluation, involving different imaging modalities such as magnetic resonance imaging (MRI) or electro- and magnetoencephalography (E/MEG). However, positive outcome rates (i.e. seizure freedom after the surgery) are not optimal, and around 30% of the patients continue to present seizures one year after the resection, although this number can go up to 50% for cohorts with complicated etiology. With the goal of improving these outcome rates, network-based studies have investigated in detail the brain network organization of epilepsy patients in order to unveil pathological effects that may predict surgical outcome [201, 202]. In practice, there is no gold standard to identify the actual EZ, instead this may be approximated by the resection area (RA) in combination with surgical outcome: for patients with good outcome the EZ is included in the RA, whereas for patients with bad outcome the EZ was at least partially preserved by the surgery. Within this context, a big conceptual leap has taken place, from the notion of individual epileptogenic zones, to the consideration of epileptogenic networks that arise from the interplay between different brain regions in promoting and inhibiting ictal activity [187, 203–205]. According to this perspective, the effect of a given surgery cannot be determined alone by the characteristics of the RA, but needs to measured against the whole epileptogenic network [194]. Data-driven and modeling studies seem to support this hypothesis, and thus network mechanisms are recognized to participate in the generation and propagation of seizures [188, 189, 206–213].

Substantial evidence underscores changes in structural and functional brain networks in epilepsy [214, 215], particularly related to the epileptogenic zone [181]. Whether there is an increase or decrease in connectivity of the EZ compared to healthy individuals, however, remains an open question. fMRI-based studies initially pointed towards a disconnection of the EZ [216–218], but more recently MEG and invasive EEG studies have suggested hyperconnectivity of the EZ and neighbouring regions [181,183,187,219–224], which may indicate the tendency to generate and spread seizures [219]. At the same time, however, the suppression hypothesis of the EZ has been supported by other invasive EEG [225] and MEG studies [226].

Pathological changes in brain connectivity in epilepsy are disproportionally associated with the network hubs [227] -highly central or important regions in the network architecture of the brain- a finding echoed in other neurophysiological disorders such as Azheimer's Disease, multiple sclerosis, or stroke [195, 214]. In the case of epilepsy, pathological hubs that facilitate seizure generation and propagation may be present. The spatial and network properties of brain hubs, as well as their removal during surgery, are both associated with epilepsy surgery outcome [228–233]. Notably, however, hubs can also have an inhibitory effect to prevent the ictal state [225,232], and it should be noted that hub removal is associated with increased side-effects from the surgery. The RA and the EZ have been associated with brain hubs by several studies, both in the ictal [234–236] and interictal [221, 234, 236] states. Such studies found associations between hub removal and seizure-freedom with different MEG-based connectivity measures [221, 237], although in a recent study involving a large cohort (n = 91) of epilepsy surgery patients we could not confirm these findings [222]. In a recent MEG study with a smaller cohort of 31 epilepsy patients, [224] were able to classify epilepsy surgery patients according to surgical outcome (79% accuracy and 65%specificity) by comparing the degree centrality (a measure of *hubness* given by the number of neighbours of a node) of the RA to the remaining network nodes.

Overall, although hub removal has been associated with a favorable outcome of epilepsy surgery, this does not seem to be a necessary condition for a good outcome. Indeed, brain hubs do not always overlap with the RA, even for patients with a good outcome [207, 208, 210, 222]. These findings motivated the hypothesis that the *epileptogenic focus*, the region where seizures start (i.e., the seizure onset zone), need not coincide with the pathological hubs but may be strongly connected to them, in which case removal of either the epileptogenic focus, the pathological hub, or even the connection between them may be enough to prevent seizure propagation and achieve a good outcome [207, 222]. Thus,

regional brain organization around the epileptogenic focus, as opposed to only its centrality, becomes a promising target to understanding the effect of a given resection.

4.3 Dataset description

4.3.1 Patient group

The patient cohort derived from the one presented in [222]. Three cases were removed, two due to existence of a previous resection, and one due to withdrawal of patient consent. The final patient cohort thus consisted of 91 patients with refractory epilepsy, with heterogeneous seizure etiology. All included patients (i) received a clinical MEG recording as part of their presurgical evaluation between 2010 and 2015 at Amsterdam University Medical Center, location VUmc; (ii) subsequently underwent epilepsy surgery at the same center; (iii) surgery outcome information was available following the Engel classification [200] either 1 year (88 patients) or at least 6 months (3 patients) after the surgery. No rules or procedures were imposed other than routine clinical care, accordingly no approval for this study by the institutional review board (Medisch Ethische Toetsingscommissie VUmc) and informed consent were needed according to the Dutch health law of February 26, 1998 (amended March 1, 2006), i.e. Wet Medisch-Wetenschappelijk Onderzoek met mensen (WMO; Medical Research Involving Human Subjects Act), division 1, section 1.2.

The patient group was heterogeneous with temporal and extratemporal resection locations and different etiology. Surgical outcome was classified according to the Engel classification [200]. 64 patients were deemed seizure free (SF).

4.3.2 Individualized Brain Networks

Individualized brain networks were derived for each patient from 10 to 15 minute restingstate MEG (magnetoencephalography) recordings, using the Automated Anatomical Labeling (AAL) atlas [238] to define a brain parcellation of 90 Regions of Interest (ROIs), with 78 cortical and 12 subcortical ROIs, excluding the cereberallar ROIs [239]. The pre-processing steps, as well as the procedures to reconstruct the activity of each source are described in detail in [222]. We derived 7 brain networks for each patient: a broadband network (*B*, 0.5 - 48.0Hz) and six frequency-band specific networks: $\delta (0.5 - 4.0Hz)$, $\theta (4.0 - 8.0Hz)$, $\alpha_1 (8.0 - 10.0Hz)$, $\alpha_2 (10.0 - 12.0Hz)$, $\beta (12.0 - 15.0Hz)$ and $\gamma (15.0 - 30.0Hz)$, by filtering the source-reconstructed data in the corresponding frequency bands.

Each ROI defined one node in the network, and the coupling strength or link weight between each pair of nodes w_{ij} was estimated with the Phase Lag Index (PLI). The PLI is a functional connectivity metric that measures the asymmetry in the distribution of instantaneous phase differences between two times series [240]. The PLI is insensitive to zero-lag coupling and thus it is robust against volume conduction or field spread [240]. 174 epochs of 4096 samples (3.28s) where used for each patient to estimate functional coupling.

4.3.3 PLI matrices thresholding

Raw PLI matrices were thresholded and binarized with a disparity filter method [241]. The disparity filter extracts the connectivity backbone $(a_{ij} > 0)$ if there is a significant connection between *i* and *j* and 0 otherwise) of a network by removing connections that are not statistically significant. The disparity filter accounts for node heterogeneity in the edge weight distribution: weak edges are identified on a node-by-node basis, by comparing their strength to that of the remaining node's edges with a given significance threshold α which we set to 0.1. This resulted in sparse networks (with network densities of about 5%; range: 0.047 - 0.051, see Table 4.1) with giant components spanning the majority of the nodes (range: 84.49 - 89.1).

Band	В	δ	θ	α_1	α_2	β	γ
L	384.15	416.63	393.74	395.90	403.04	385.15	392.84
S	84.49	89.91	89.09	89.32	89.38	89.10	89.81

Table 4.1: Basic network statistics. We report the average number of edges L remaining in the network after the thresholding procedure, and the average size of the largest component S, for each frequency band.

In figure 4.1 we report the distribution of node-set sizes for each frequency band.

4.3.4 Resection area and node sets

We consider the differential connectivity between pairs of node types by implementing a three-group partition of the brain regions, namely into resection area (RA), its neighbourhood and the remaining network. The resection area is the region of the brain removed during surgery, conducted on subjects suffering from epilepsy and who have shown resistance to pharmacological treatments. It is typically associated with the presence of hubs identified as central in the brain network. The resection area was determined for each patient from the three-month post-operative MRI. This was co-registered to the pre-operative MRI (used for the MEG co-registration) using FSL FLIRT (version 4.1.6) 12 parameter affine transformation. The resection area was then visually identified and assigned to the corresponding AAL ROIs, namely those for which at least 50% or the centroid had been removed during surgery.



Figure 4.1: Distributions of the size of each node-set (as indicated by the general legend) over the patient population, for each frequency band as indicated by the panel title (*B* stands for the broadband).

Based on the resection area, we identified four sets of nodes: \mathcal{RA} , or resected nodes, are the nodes that belong to the resection area. $\overline{\mathcal{RA}}$, or non-resected nodes, are the nodes that do not belong to \mathcal{RA} . We further considered two subsets of $\overline{\mathcal{RA}}$ nodes. This partition was based on the connectivity of the resection area, and was thus different for each frequency band: \mathcal{N} , or neighbours, are the nodes that are connected to \mathcal{RA} nodes and that do not themselves belong to the resection area. \mathcal{O} , or other nodes, are the remaining nodes in the network, that is, nodes that do not belong to the resection area and are not connected to any \mathcal{RA} nodes.

4.4 Simplicial complex description of brain data

Simplicial complexes represent higher-order networks which allow for interaction between two but also more nodes, described by simplices. A *d*-simplex is formed by a set of d + 1nodes and all their possible connections. For instance, a 0-simplex is simply a node, a 1simplex a link and the two corresponding nodes, a 2-simplex is a triangle, a 3-simplex is a tetrahedron and so on. A simplicial complex \mathcal{K} is formed by a set of simplices such that i) if a simplex belongs to \mathcal{K} then any simplex formed by a subset of its nodes is also included in \mathcal{K} , and ii) given two simplicies of \mathcal{K} , their intersection either also belongs to \mathcal{K} , or it is a null set [180]. A simplicial complex representation of a network can be built deterministically by defining the *clique complex* of the network. A *k*-clique is a subgraph of the network formed by *k* all-to-all connected nodes. That is, 1-cliques correspond to nodes, 2-cliques to links, 3-cliques to triangles, and so on. Thus, in order to build a simplicial complex of dimension *d* from a network, we identify all d + 1-cliques [180, 242]. This choice for creating simplices from cliques has the advantage of using pairwise signal processing to create a simplicial complex from brain networks [243]. Other strategies to build simplicial complexes beyond pairwise signal processing have been proposed, such as approaches combining information theory and algebraic topology [190, 244–248].

The mesoscopic structure of a complex network can be described in terms of extended neighbourhoods or ego networks [180], as illustrated in figure 4.2 Starting from a given node *i*, we define its *d*-extended neighbourhood \mathcal{EN}_i^d as the subgraph induced by the set of nodes at hopping distance δ equal or smaller to $d, \delta \leq d$ (see figure 4.2b). \mathcal{EN}_i^d generalizes the concept of clustering coefficient, as it allows us to capture the connectivity not only between the first neighbours of a node, but of its general area of influence characterized by the hopping distance parameter d.

 \mathcal{EN}_i^d can be characterize by its size (number of nodes, $N_{\mathcal{EN}^d}$) and connectivity (number of links, $E_{\mathcal{EN}^d}$). $N_{\mathcal{EN}^d}$ generalizes the notion of node degree, and indeed the degree of a node equals to $N_{\mathcal{EN}^{d=1}}$. Similarly, the local clustering coefficient reduces to $CC_i = 2 \frac{E_{\mathcal{EN}^{d=1}}}{N_{\mathcal{EN}^{d=1}}(N_{\mathcal{EN}^{d=1}}-1)}$.

Finally, we also characterized the topological organization of the extended neighbourhoods by the notion of *Betti numbers*. The first Betti number β_0 measures the number of connected components on a network. Subsequent Betti numbers β_i describe the topology of the simplicial complex associated with the network. Generally, the Betti numbers β_i , $i \ge 1$ are topological invariants derived from the simplifical complex that measure the number of linearly independent *i*-dimensional holes in the simplicial complex. Thus, β_1 provides the number of 1-dimensional cycles that are not boundaries of 2-dimensional simplices of the associated simplicial complex, and similarly β_2 indicates the number of 2-dimensional cycles (i.e. over triangles) that are not boundaries of 3-dimensional simplices of the simplicial complex. β_0 indicates the number of connected components of the local neighbourhood. Thus, large values indicate a hub that connects otherwise disconnected regions of the network [180]. β_1 indicates the number of cycles forming 1-dimensional holes. Therefore, a large value of the ratio β_1/β_0 indicates a sparse neighbourhood. Similarly, larger values of β_2 indicate the tendency to form planar (i.e. triangular) structures. The Betti numbers are non-linearly influenced by the size and density of the neighbourhood, and integrate information of the mesoscopic structure of the network in a non-trivial manner.

4.5 **Topological metrics**

To quantify the connectivity and network properties of brain nodes, we utilized a variety of metrics. These metrics can be categorized into node-level metrics and neighbourhood-level metrics. Below is a detailed description of each metric:

4.5.1 Node-level Metrics

We characterized the local structure of the network by three nodal properties. In particular, for each node i we considered its centrality (as given by the betweenness centrality BC_i), clustering coefficient CC_i , and curvature C_i .

- The **Betweenness Centrality** BC measures the influence of a node over the flow of information within the network. It is calculated by determining the fraction of all shortest paths in the network that pass through a given node. Nodes with high betweenness centrality are considered critical for information transfer and can be identified as hubs within the network [18].
- The Local Clustering Coefficient c quantifies the extent to which nodes in a graph tend to form clusters or groups. For a given node i, the clustering coefficient is defined as the ratio of the number of closed triplets (or triangles) to the total number of triplets (both open and closed) centered on that node. Mathematically, it is given by:

$$c_i = \frac{2 \times \text{Number of closed triangles including node } i}{k_i(k_i - 1)}$$
(4.1)

where k_i is the degree of node *i*. A higher clustering coefficient indicates a greater tendency for node *i* to form tightly-knit groups with its neighbors [18].

• The Local Curvature C captures how paths bend around a node in its vicinity, offering insights into the local geometric structure More specifically:

$$C_i = \sum_{k=1}^{k_{max}} (-1)^{k+1} \frac{Cl_{ik}}{k},$$
(4.2)

where Cl_{ik} is the number of k-cliques to which i belongs, and k_{max} represents the size (i.e. number of nodes) of the largest clique in the network ($k_{max} = 3$ considering interactions up to three-node ones.). It generalizes the concept of curvature from differential geometry to network theory. Nodes with high curvature tend to have a significant influence on the robustness and stability of the network [249].

4.5.2 Neighbourhood-level Metrics

The extended neighbourhood \mathcal{EN} of a node encompasses all nodes within a certain distance (or hops) from the given node, excluding the node itself [180].

• The Number of Nodes in the Extended Neighbourhood N measures the size of the \mathcal{EN} and it generalizes the concept of node degree.

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Figure 4.2: Schematic description of extended neighbourhoods. (A) Illustrative representation of the extraction of a node's neighbourhood for d = 2. The nodes are color-coded to show the central node (red), its first (orange) and second (yellow) neighbours and the remaining network nodes (green). (B) Extended neighbourhood of the node. The central node is not included in its neighbourhood, therefore it is shown here with low opacity (light pink node) and its edges are removed (dashed lines). The topological organization of the neighbourhood can be observed. In this case, e.g. two different connected components emerge, as well as two closed triangles.

- The Number of Edges in the Extended Neighbourhood E quantifies the total number of pairwise edges within the \mathcal{EN} , reflecting the local connectivity density.
- The **Betti Numbers** $(\beta_0, \beta_1, \beta_2)$ are topological invariants that describe the connectivity of simplicial complexes (contructed in this case from the node neighbourhoods) at different dimensions, generalizing the notion of clustering coefficient:
 - β_0 represents the number of connected components in the \mathcal{EN} , indicating the degree of fragmentation. A higher β_0 indicates a node that acts as a broker between different communities.
 - β_1 quantifies the number of one-dimensional holes or open loops representing independent cycles within the \mathcal{EN} . It provides information on the presence of circular structures that are not filled in by higher-dimensional simplices.
 - β_2 measures the number of two-dimensional voids, reflecting higher-order connectivity patterns such as cavities within the \mathcal{EN} .



Figure 4.3: Illustration of the properties of simplicial complexes and extended neighbourhoods. (a) Schematic network where we highlight two nodes: a regional hub (node H) with high degree (7 neighbours) and high BC since it brokers two communities, and a local hub (node W) with high degree (5 neighbours) but low BC. Panels (b) and (c) illustrate extended neighbourhoods of W and H, respectively. The different topology of \mathcal{EN}_W and \mathcal{EN}_H is encoded by the regional and local metrics, as shown in panel (d). Whenever there is a closed clique in the original network, simplices are built in the extended neighbourhood. For instance, in panel (b), the grey triangle represents a 2-dimensional simplex built according to this rule.

4.6 Neighbourhood topology to characterize epilepsy seizures

To characterize regional brain organization, we have considered the notion of the extended neighbourhood \mathcal{EN} of a node [180]. Extended neighbourhoods, also called ego-centered networks, define the area of influence of a node. Mathematically, the extended neighbourhood of node *i*, \mathcal{EN}_i^d , is defined as the subgraph conformed by nodes at distance δ , $0 < \delta < d$, of node *i* (which, crucially, excludes node *i*), as depicted in figure 4.2. By changing the radius d of the extended neighbourhood we can access different scales of network organization, going from the local to the global perspective. To quantify the structure of \mathcal{EN}_i^d , and thus regional network organization, we have considered five topological measures: the size or number of nodes N_i^d , the number of edges E_i^d , and the first three Betti numbers quantifying the number of connected components $\beta_{0,i}^d$, the number of loops $\beta_{1,i}^d$ (not accounting for triads which are always considered to be filled), and the number of cavities or 2-dimensional loops, $\beta_{2,i}^d$. These metrics quantify the topology of the extended neighbourhood of each node. The number of nodes and edges indicate the regional connectivity of the node, and can be interpreted as centrality metrics. Similarly, a high value of the first Betti number indicates that node i acts as a broker between different otherwise disconnected components of its neighbourhood [180]. In figure 4.3 we provide an illustration of these different metrics.

In order to quantify the structure of \mathcal{EN}_i^d , and thus regional network organization, we consider the following two classes of metrics: neighbourhood-level and node level metrics. The first class refers to those metrics that describe the structure around a node i.e depending

on the connectivity of its first and second neighbours, while the second class gather metrics that directy depend on local node properties such as node's edges.

Concerning neighbourhood-level metrics, we have considered five topological measures: the size or number of nodes of N_i^d , the number of edges E_i^d , and the first three Betti numbers quantifying the number of connected components $\beta_{0,i}^d$, the number of loops $\beta_{1,i}^d$ (not accounting for triads which are always considered to be filled), and the number of cavities or 2-dimensional loops, $\beta_{2,i}^d$. These metrics are node-dependent as they quantify the topology of the extended neighbourhood of each node. The number of nodes and edges indicate the regional connectivity of the node, and can be interpreted as centrality metrics. Similarly, a high value of the first Betti number indicates that node *i* acts as a broker between different otherwise disconnected components of its neighbourhood [180]. In figure 4.3 we provide an illustration of these different metrics.

As a benchmark, we have considered also three node-based metrics, namely the betweenness centrality BC_i , the local clustering coefficient c_i , and the local curvature C_i . The betweenness centrality is a standard measure to quantify node-centrality and define *hubbness* [207, 214, 221]. It quantifies the extent to which a node lies on the shortest paths between other nodes, thus capturing its role in controlling information flow in the network [18]. Node curvature measures how paths in the simplicial complex diverge or converge around a node, capturing the local geometric properties of the space. Specifically, in a simplicial complex, curvature reflects how higher-dimensional simplices (such as triangles or tetrahedra) connect around a node, influencing the shape and flow of the network structure. It is associated with network robustness, and also identifies brain hubs, with large negative values being indicative of hub status [250]. The clustering coefficient captures the connectedness of a node's neighbours, and has previously been associated with epilepsy surgery outcomes [206].

4.7 Analysis

4.7.1 Statistical analysis

We first performed an individualized node-based analysis by which we tested whether the hub-status of the different node-sets differed significantly for each patient and metric \mathcal{X} . We considered two types of comparisons: a) two-node-set setting, where we tested whether $\mathcal{X}(\mathcal{RA}) > \mathcal{X}(\overline{\mathcal{RA}})$, and b) three-node-set setting, where we tested whether $\mathcal{X}(\mathcal{RA}) > \mathcal{X}(\overline{\mathcal{RA}}) > \mathcal{X}(\overline{\mathcal{RA}}) > \mathcal{X}(\overline{\mathcal{O}}), \mathcal{X}(\mathcal{N}) > \mathcal{X}(\overline{\mathcal{O}})$. We quantified whether the hubness distributions were significantly different via bootstrapping analyses with 10⁴ replicas to determine the *z*-score and *p*-value of the difference. The sign of the difference indicated whether it was in the direction of the hypothesis or against it. The *z*-score was computed as the mean of the differences of the bootstrapped samples divided by the standard deviation of

these differences. The 2-tailed *p*-value associated with the *z*-score was determined using the cumulative distribution function of a standard normal distribution. Considering the large number of comparisons performed, we applied the Bonferroni correction to account for multiple testing and control the false discovery rate. Specifically, the Bonferroni correction was applied by dividing the original significance level ($\alpha = 0.05$) by the number of comparisons made. For each pairwise comparison of node-sets, we conducted 56 statistical comparisons (7 bands times 8 metrics). Thus, for every pair of nodes, we used the Bonferroni correction by adjusting the significance level to $\alpha' = 0.05/56 \approx 8.9^{-4}$.

To determine whether the results held at the group level, for each patient we estimated the average of each hubness metric for each of the node sets. We then performed a paired bootstrapping analysis to test whether the distribution of average metrics was significantly different, for each of the four pairs of node-comparisons as defined above.

We subsequently utilized the results of the node-based analyses to perform a receiver operating characteristic (ROC) curve classification of the patients (SF or NSF). The result of each node-based test was quantified in the variable $r_{n_1,n_2}^i(\mathcal{X})$ for each patient *i*, hubness metric \mathcal{X} , and node-set sets n_1 and n_2 . $r_{n_1,n_2}^i(\mathcal{X}) = 1$, -1 or 0 indicating whether the node-sets were significantly different in the direction of the hypothesis, contrary to it, or not significantly different, respectively. We then summed over hubness metrics to define a *distinguishability* score D_{n_1,n_2}^i for each patient and node-based comparison [224]. To sum up the results of the three-node-set analysis, we defined a combined distinguishability score, D_{comb}^i , by summing over the corresponding three pairwise comparisons. The distinguishabbility score according to each test was then used to classify the patients with a ROC curve analysis, and the goodness of the classification was measured with the area under the curve (AUC).

Finally, to enable a more direct comparison with the previous study by [224], we also estimated the distinguishability score as originally proposed by calculating the AUC of the node ROC-classification (instead of using $r_{n_1,n_2}^i(\mathcal{X})$), for each metric \mathcal{X} and pair of nodesets. Patient-classification based on this score was then performed similarly to the previous analysis. For this test we also considered the node strength (the sum of its non-zero weights after thresholding) as a metric to allow for a more direct comparison with [224].

4.7.2 Topological characterization of the epileptogenic zone

Following the hypothesis that the EZ is either a hub or connected to a hub, we hypothesized that RA nodes and their neighbourhoods will be more central than other nodes in the network. To test this hypothesis, we considered an existing database comprising 91 patients who underwent epilepsy surgery at Amsterdam UMC, location VUmc. This database had been studied with a combination of network metrics and machine learning previously [222].

The brain organization for each patient was encoded in a functional brain network comprised of 90 regions of interest (ROIs) (according to the AAL atlas [251]), derived from resting-state MEG, and thresholded to keep only the strongest links. MEG networks were derived in different frequency bands, which account for different aspects of brain function. For simplicity we have considered here first the broadband (0.5 - 48.0Hz), but refer back to a multi-frequency analysis in later sections. The resection area of each patient was derived from post-operative MRI and was encoded in terms of AAL nodes.

Each node in the network was described by means of the 8 metrics defined in the previous section, with high values of these metrics associated with higher generalized centrality, except for the curvature where the direction is the opposite as discussed above. Initially, two sets of nodes were defined for each patient and network: resected nodes \mathcal{RA} and nonresected nodes $\overline{\mathcal{RA}}$. We analysed whether these nodes differed at the individual level in any of the 8 metrics considered (bootstrapping and a Bonferroni correction were used to establish statistical significance). Details of this analysis for an exemplary case are shown in Figure 4.5. We found that, at the individual level, \mathcal{RA} nodes were significantly more central according to all neighbourhood metrics, except β_0 , for 15% to 30% of patients (respectively for 23, 27, 20 and 14 cases for N, E, β_1 and β_2). Traditional node-based metrics were less efficient at detecting differences between the node groups: according to these metrics \mathcal{RA} nodes were significantly more central than \mathcal{RA} nodes only for a handful of patients (respectively 6, 3 and 6 for c, C and BC). We note that, for a few patients, the opposite result was found and \mathcal{RA} nodes were significantly less central than \mathcal{RA} nodes, both with the node- and neighbourhood-based metrics (respectively 5, 5, 7 and 3 cases for N, E, β_1 and β_2 ; and 3 and 1 cases for c and C; whereas no case was found for BC). These results are summarized in figure 4.4 (a), whereas numerical results can be found in the Appendix in Tables A.1 and A.2.

Our results agree with previous studies according to which the RA is not always a network hub, but it is often strongly connected to a pathological hub [207, 214, 222]. Consequently, the $\overline{\mathcal{RA}}$ node set may include both nodes that are less and more central than \mathcal{RA} nodes. To account this effect, we split the $\overline{\mathcal{RA}}$ set into two: nodes that were neighbours of the \mathcal{RA} (*neighbours*, \mathcal{N} set) and nodes that were not (*other*, \mathcal{O} set). According to our initial hypothesis, within this division of the node sets we expected that both \mathcal{RA} and \mathcal{N} nodes were more central than \mathcal{O} nodes, and that \mathcal{RA} and \mathcal{N} nodes were similarly highly central. As expected, we found that the node sets \mathcal{RA} and \mathcal{N} were in most cases significantly more central that the \mathcal{O} set (see figure 4.4 panels b and d). As before, neighbourhood-based metrics were able to capture this difference more consistently across patients than node-based metrics. Regarding the relative hub-status of the RA and its neighbourhood, we only found significant differences between \mathcal{RA} and \mathcal{N} nodes for a small fraction of the patients (figure 4.4 panel c). These went in both directions, with a tendency towards a higher centrality of \mathcal{N} nodes at the group level, as we discuss below. For instance, for the metric that picked up



Figure 4.4: Patient-specific comparison of different node groups for the two-group (a) and the three-group (b, c, d) set-ups. For each panel, the hypothesis of the relation in centrality between the two metrics is shown in the panel title. The fraction of patients for whom there was a significant difference in the direction (opposite direction) of the hypothesis is shown by the blue (red) triangles in the upper-right (bottom-left) corner of each cell, respectively for each frequency band (rows) and metric (columns), color-coded as indicated by the colorbar. The corresponding numerical values are shown in Tables A.1 and A.2. The vertical black line separates node-based (left) from neighbourhood-based (right) metrics. $\mathcal{X}(S)$ stands for the generalized centrality metric \mathcal{X} measured on the nodes in set S.



Figure 4.5: Distribution of generalized centrality metrics for an exemplary case (SF patient, broadband network) for each node-set. Each panel corresponds to a generalized centrality metric as indicated by the labels. For each panel we show the results for the two analysis that were performed: the two-node-set partition (left) accounting for the \mathcal{RA} and $\overline{\mathcal{RA}}$ node sets, and the three-node-set partition (right) accounting for the \mathcal{RA} , \mathcal{N} and \mathcal{O} node sets. In all panels we show the distribution of values for each node-set as a violin plot, and indicate the mean and median values with solid lines. The box-plots indicate the median, the 25% and 75% percentiles and the extreme values. Significant differences between two groups are indicated by black lines connecting the corresponding violins.

the most differences in the broadband, β_1 , \mathcal{RA} nodes were more central than \mathcal{N} nodes for 10 cases, but the opposite was true for 12 cases. These findings indicate heterogeneity in the patient population regarding the relative hub-status of the resection area and its neighbours. For most cases, these two sets could not be distinguished based on centrality metrics (either node- or neighbourhood-based), indicating a similar highly-central status (note that the remaining nodes were found to be less central).

4.7.3 Group level analyses

To gain a population-level perspective of the relative hub-status of the RA, we repeated the previous analyses at the group level. To do so, we measured the average centrality of the nodes in each node-set, for each patient and frequency band. We found that, when all patients were pooled together, the differences between node-sets became more subtle, likely



Figure 4.6: Group-level comparison between nodes sets, for each considered frequencyband (y-axis) and network metric (x-axis). From left to right, the panels indicate the difference between the node sets: i) \mathcal{RA} vs $\overline{\mathcal{RA}}$, ii) \mathcal{RA} vs \mathcal{N} , iii) \mathcal{RA} vs \mathcal{O} , iv) \mathcal{N} vs \mathcal{O} . $\mathcal{X}(S)$ stands for the generalized centrality metric \mathcal{X} measured on the nodes in set S. The color code indicates the z-score of the difference between the average values of each node set, computed by bootstrapping the data (sampling size of 10⁴). Single asterisks indicate significant differences (p < 0.05) that did not survive the Bonferroni correction (n = 56), and double asterisks the ones that did ($p < 8.9^{-4}$). The corresponding numerical values are shown in the Appendix in Tables A.3 and A.4

due to patient-specific variability, as shown in figure 4.6. Overall, we found in the two nodegroup analysis that the \mathcal{RA} and $\overline{\mathcal{RA}}$ node-sets could not be significantly distinguished at the group level, for most metrics and frequency bands, with the most notable exception of the broadband. The three node-group analysis recovered for the most part the findings of the individual-level analyses, i.e. \mathcal{O} nodes were the least central, and \mathcal{N} were somewhat more central than \mathcal{RA} . At the group level the betweeness centrality became the most robust metric across frequency bands, and the broadband network was the network for which differences between node-groups were more prevalent across metrics. Notably, three of the metrics, the local clustering c, β_0 and β_2 , performed poorly for the remaining frequency bands.

4.7.4 Topological signatures of the RA and surgical outcome

In order to investigate whether the hub-status of the \mathcal{RA} was associated with surgical outcome in this dataset, we assigned each patient a *distinguishability* score $D_{\mathcal{RA},\overline{\mathcal{RA}}}$ to quantify the distinguishability between the \mathcal{RA} and $\overline{\mathcal{RA}}$ node-sets [224]. For each patient, $D_{\mathcal{RA},\overline{\mathcal{RA}}}$ measures the number of tests (over the 8 network metrics considered) for which the hypothesis of the hub-status of the RA is significantly fulfilled. Following our previous findings that a three-node-group division is more informative at the node level, we also assigned distinguishability scores to the pairwise comparisons between the three node-sets $\mathcal{RA}, \mathcal{N}$ and \mathcal{O} , namely $D_{\mathcal{RA},\mathcal{N}}, D_{\mathcal{RA},\mathcal{O}}$ and $D_{\mathcal{N},\mathcal{O}}$.

Next, to summarize the results of the three-node-group analysis into one score, we de-



Figure 4.7: Classification of SF and NSF patients based on the two-node-group (a) and threenode-group (b) distinguishability scores. $\mathcal{X}(S)$ stands for the generalized centrality metric \mathcal{X} measured on the nodes in set S. Panels (a) and (b) show the ROC curves corresponding to the broadband, the remaining bands are shown in Figure 4.8. The resulting AUC is indicated by the figure legends. Panel (c) shows the resulting AUC for all frequency bands, for this same analysis. In this representation, the SF group is assigned to be the positive class. The color-scale is centered around AUC = 0.5, which indicates a lack of association. Bluecolors stand for an association in the direction of the hypothesis (AUC > 0.5, i.e. the SF group presents a higher distinguishability score) whereas red-colors stand for the opposite (AUC < 0.5, the NSF group presents a higher distinguishability score).
fined a combined score of the three-node-group analysis D_{comb} by summing over the corresponding three pairwise comparisons. The derivation of these metrics is illustrated in Figure 4.11. We used each distinguishability score to classify the patients between the *seizure-free* (SF) and *non-seizure-free* (NSF) groups, as shown in figure 4.7 (a statistical comparison between the two groups was also performed, see Figure 4.12, but no statistical differences between the two groups survived after Bonferroni correction). We found that patient classification was fair at best for any of the frequency bands or node-group montages (panel c). The best results were found for the broadband when considering the combined information of the three-node-group analyses, which resulted in an area under the curve AUC = 0.68.

Finally, to better contextualize and validate our findings, we considered an alternative definition of the node distinguishability, D', as introduced by [224]. In this case D' is simply the area under the curve resulting from the classification of \mathcal{RA} and $\overline{\mathcal{RA}}$ nodes (see Figure 4.9). In their original study, [224] found that they could classify the patients according surgical outcome with an AUC of 0.76 using D' based on the degree-centrality as metric. For our dataset, however, we found an AUC of only 0.65 when using D' based on the degree-centrality (see Table 4.2). When applying D' to the 8 metrics considered, we found AUC values ranging from 0.68 (for the neighbourhood metric N in the α_1 -band) and 0.36 (neighbourhood metric β_1 , α -band) for the two-node-sets analysis, with similar results also for the three-node-set partition (see Figure 4.9).

	$\mathcal{X}(\mathcal{R}\mathcal{A}) > \mathcal{X}(\overline{\mathcal{R}\mathcal{A}})$	$\mathcal{X}(\mathcal{RA}) > \mathcal{X}(\mathcal{N})$	$\mathcal{X}(\mathcal{RA}) > \mathcal{X}(\mathcal{O})$	$\mathcal{X}(\mathcal{N}) > \mathcal{X}(\mathcal{O})$
B	0.56	0.51	0.57	0.49
δ	0.57	0.56	0.59	0.57
θ	0.42	0.46	0.43	0.44
α_1	0.39	0.41	0.40	0.51
α_2	0.60	0.55	0.61	0.60
β	0.48	0.47	0.45	0.50
γ	0.64	0.58	0.65	0.57

Table 4.2: Results of the patient classification following the methodology in [224]. We report the area under the curve (AUC) of the patient classification (SF versus NSF) based on the distinguishability D' between \mathcal{RA} and $\overline{\mathcal{RA}}$ nodes (first column), when using the weighted degree as nodal centrality metric. $\mathcal{X}(S)$ stands for the generalized centrality metric \mathcal{X} measured on the nodes in set S. The latter three columns extend this analysis to the three-node-set framework by considering the distinguishability between the i) \mathcal{RA} and \mathcal{N} nodes; ii) \mathcal{RA} and \mathcal{O} nodes; and \mathcal{N} and \mathcal{O} node sets, respectively. Each row corresponds to a different frequency band. We highlight in bold the results for with |AUC - 0.5| > 0.1.

4.7.5 Alternative distinguishability score

In order to compare our findings with a recent study by Ramaraju and colleagues [224], we repeated the patient-classification analysis using their original definition of the distinguishability score, D'_i . We also consider the same centrality metric used by [224], the weighted degree or strength of a node (the sum of its link weights after thresholding the PLI matrix with the disparity filter). The distinguishability score for each patient D'_i was defined by [224] as the AUC of the ROC-classification analysis of the \mathcal{RA} and $\overline{\mathcal{RA}}$ node sets. A D' value close to 0.5 indicates that the two node sets cannot be classified according to the corresponding metric, whereas values close to 0 or 1 indicate that the node sets are easily classifiable. In particular, AUC > 0.5 indicates that the \mathcal{RA} set is more central than the $\overline{\mathcal{RA}}$ set, and vice versa for AUC < 0.5. The results of this analysis are shown in Table 4.2 (first column).

We did not find a good patient classification for any frequency band. The best classification results were obtained for the γ band with AUC = 0.64, followed by the α_1 (AUC = 0.39) and α_2 (AUC = 0.60) bands. Interestingly, the direction of the classification changed across frequency bands: for α_2 and γ SF patients presented higher distinguishability scores D'_i than NSF patients, whereas for α_1 the opposite was true.

To exploit the three-node-set partition framework defined in subsection 4.3.4, we extended this analysis to account for three more two-class node-based classifications, namely i) \mathcal{RA} and \mathcal{N} nodes; ii) \mathcal{RA} and \mathcal{O} nodes; and \mathcal{N} and \mathcal{O} nodes (Table 4.2). Swarm plots depicting distinguishability scores are presented in figure 4.10 for the case of broad band for a visual representation of the classification. We found that the results for the latter two cases were very similar to the original \mathcal{RA} and $\overline{\mathcal{RA}}$ distinguishability. As expected from the results in Figure 4.4, the \mathcal{RA} and \mathcal{N} cannot be easily classified, resulting in low node-distinguishability scores and in a poor patient classification.

We repeated this analysis on our proposed framework of 8 generalized centrality metrics, the results are shown in Figure 4.9. The results were similar to those using the weighted degree, with only fair patient classification results. The best findings were obtained when considering the two-node-set partition (i.e. \mathcal{RA} versus $\overline{\mathcal{RA}}$) in the broadband (AUC = 0.68 for the metric E), and overall showed large variability also in the direction of the AUC (that is, whether SF or NSF patients presented larger distinguishability scores). Thus this extended analysis was not able to improve upon our initial results.



Figure 4.8: Additional results to Figure 4.7. ROC analysis of the SF and NSF groups based on the patient scores, for each band (rows) and node-groups analysis (columns). The final column corresponds to the compounded score of the three-node-group analysis. We indicate the area under the curve (AUC) of each curve as the legend.



Figure 4.9: Patient classification results using the methodology by [224] combined with our proposed generalized centrality metrics. Each panel corresponds to a node-based comparison as indicated by the panel titles, with the vertical line separating the two-node-set case from the three-node-set cases. $\mathcal{X}(S)$ stands for the generalized centrality metric \mathcal{X} measured on the nodes in set S. Rows correspond to frequency bands and columns to generalized centrality metrics. We show the resulting AUC both with the color-code and by numerical values.



Figure 4.10: Swarm plot depicting distinguishability values (D'_{RS}) for SF and NSF surgical outcomes for different node-based comparisons, based on the node strength. $\mathcal{X}(S)$ stands for the generalized centrality metric \mathcal{X} (node strength here) measured on the nodes in set S. Values close to 0 (1) indicate that high strength nodes are resected (spared). Each scatter point represents an individual patient. The results for every band are reported in Table 4.2.

4.7.6 Multi-frequency analysis: Individual patient results

In this subsection we detail the definition of the distinguishability score \mathcal{D} and provide details on the statistical analyses involving this metric. In Supp. Figure 4.11 we show the results of the node-based analyses. Each panel corresponds to a frequency band and a comparison between node-sets, as indicated by the panel title. For each panel, we show the result $x_i^{\mathcal{X}}$ of the statistical comparison between the two node-sets, using each of the centrality metrics \mathcal{X} and for each patient *i* with a color code. The color code indicates whether there is a significant difference in the direction of the hypothesis (blue, $x_i^{\mathcal{X}} = 1$), against it (red, $x_i^{\mathcal{X}} = -1$), or there is no significant difference (grey, $x_i^{\mathcal{X}} = 0$). The patient distinguishability score D_i is simply defined as the sum of the results of this statistical comparison over generalized centrality metrics: $D_i = \sum_{\mathcal{X}} x_i^{\mathcal{X}}$. Given that central nodes have large negative curvature, this term is multiplied by -1 in the sum. The resulting patient

distinguishability score D_i is thus a number between -8 and 8, where $D_i = 8$ (-8) indicates that the two node-sets were highly different in the direction of the hypothesis (against the hypothesis), and $D_i = 0$ indicates no significant or inconsistent differences (across metrics) for the patient.

In Figure 4.12 we show the results of the statistical comparison between the SF and NSF groups based on the distinguishability scores D_i , for each of the node-based tests. We observed a tendency towards higher scores for SF patients for the broadband, θ and α_1 bands, and in the opposite direction for δ and γ , however none of the differences are significant after Bonferroni correcting for multiple comparisons.

Additionally, we also performed a ROC

patient-classification analysis based on the distinguishability scores, the results of which were reported in Figure 4.7. Here we show in Figure 4.8 the ROC curves corresponding to each of the node-based tests, for the broadband.



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Figure 4.11: Disthinguishability score D_i . Each panel corresponds to the comparison between two node-sets as indicated by the panel titles, and a frequency band (from top to bottom: broadband, δ , θ , α_1 , α_2 , β , γ). We show the result for each metric x_i^H in the top rows of each panel and D_i in the bottom row. Both metrics are color-coded as indicated by the colorbar. The vertical white line on each panel separate SF (left) and NSF (right) cases.



Figure 4.12: Statistical comparison between the SF and NSF patient groups based on the patient distinguishability score D_i , for each node-group-comparison (columns) and frequency band (rows), as indicated by the axis labels. The final column combines the results of the three-node-groups tests by adding up the patient scores. The color-code indicates the difference between the average scores of the SF and NSF groups, as given by the color-bar. The cross markers indicate differences with p-value < 0.05 before Bonferroni-correcting for multiple comparisons. None of the differences were significant after the correction.

4.8 Discussion of results

In our study involving 91 patients who underwent epilepsy surgery, we investigated the hubstatus of the resection area and its region of influence to shed new light onto the presence of pathological hubs in the brains of epilepsy-surgery patients and their role in the outcome of epilepsy surgery. We proposed a novel methodology based on node-neighbourhoods and topological data analysis to quantify node centrality at a mesoscopic level. As a validation of our novel approach, we compared our findings against established node-based metrics such as the betweenness centrality and clustering coefficient. Moreover, by leveraging the same database previously analyzed by [222] with traditional methodologies, we enabled a direct comparison between the two studies.

In our study, we found that (a) the neighbours of the resection area play an important role in brain-network organization in epilepsy and are significantly different from the remaining nodes in the networks (thus a three-group partition of the brain regions, where RA neighbours are separated from the remaining brain network, is more representative than a two-group partition); (b) the RA and its neighbours are more central than the remaining brain regions, which holds true at the group level and also individually for most patients; (c) the RA and its neighbours are similarly highly-central, with only some differences at the individual level (for 10 to 20% of patients) that go in both directions, whereas at the group level the neighbours are weakly but significantly more central; and (d) the difference in hub-status between either the RA or its neighbours and the remaining network nodes, but not between them, is weakly associated with surgical outcome (AUC = 0.62, 0.64 and 0.46, respectively). A main consequence of our findings is that a three-node-group partition of the brain regions as we have introduced here, such that the RA-neighbouring regions are separated from the remaining brain regions and considered specifically, is more representative than a two-node-group partition, in particular yielding better node-classification results. These findings support the hypothesis of the emergence of pathological hubs in refractory epilepsy that do not necessarily overlap with the RA, a finding that was valid for patients with good and bad outcome. These results further highlight the need for individualized studies that take into account patient-specific brain connectivity.

4.8.1 Hub status of the RA

In this study we considered the emergence of pathological hubs in epilepsy and their overlap with the resection area [214, 221]. The RA has been associated with brain hubs both in functional and structural studies ([187,208,219–224,234–236,252,253]; see also [214,254] for recent reviews), and their overlap has been related to surgical outcome, with several MEG studies finding that hub removal was associated with good postsurgical outcomes [221, 223, 224, 253]. In particular, [221] found that the brain network hubs (defined via the betweenness centrality on a minimum-spanning-tree, MST, description) were localized within the resection cavity in 8 out of 14 SF patients and none (out of 8) NSF patients (73% accuracy). Similarly, [253] found that removal of the most central hubs (defined via the eigenvector centrality on weighted PLI networks) had predictive value in a study with 31 patients (17 SF). Considering a simple correlation metric as the basis for connectivity, [224] found, in a study with 31 patients (12 SF), that SF patients had significantly more hubs surgically removed. Finally, [223] also found higher functional connectivity (defined via both the amplitude-envelope coupling and phase-locking-value on the MST description) inside than outside the RA for SF patients, and few differences between the two for NSF patients in a study with 37 (22 SF) patients involving both children and young adults with refractory epilepsy. The functional connectivity measures predicted weakly the EZ location and surgical outcome (sensitivity and specificity above 0.55 with leave-one-out cross-validation).

However, the relationship between hub-removal and surgical outcome could not be validated in our previous study [222] (94 patients, 64 SF) which used the same patient cohort as we have considered here. Nissen and colleagues defined the hub-status on the basis of the MST betweenness centrality, and only a weak association with the RA was found (60.34%accuracy with a random forest classifier) and none with surgical outcome (49.03% accuracy). In line with the suggestion that the relationship between the RA and the brain hubs is not straightforward, several studies have pointed towards the functional isolation of the EZ, both in invasive EEG [225] and MEG [226]. In particular, [221, 226] found that SF patients presented a more isolated resection area (relative to the contralateral hemisphere) than NSF patients in a study with 12 patients (7 SF) based on amplitude-envelope-correlation networks. [225] found that the seizure onset zone (SOZ) and the early propagation zone presented increased inwards and decreased outwards functional connectivity in an invasive EEG study involving 81 drug-resistant epilepsy patients undergoing presurgical evaluation. Interestingly, they found that the largest difference between SF and NSF patients appeared in the propagation zone: the connectivity profile of the propagation zone was intermediate to that of the SOZ and the remaining networks for SF patients, whereas for NSF patients it consistently and closely resembled that of the remaining network. It is worth noting that this result may just reflect a difference in invasive EEG sampling between SF and NSF patients, such that e.g., the true propagation zone of NSF patients may have been undersampled [225].

The existence of pathological hubs can reconcile these findings: a pathological hub that may or may not coincide with the SOZ may be present facilitating seizure propagation. Then, removal of either the SOZ, the pathological hub, or even the connection between them, could lead to seizure freedom [210, 221]. In a previous modeling study, for instance, we found that the link-based resections that led to the best postsurgical outcome in the model were those linking the RA to the network hubs [207]. Our findings in the current study support this hypothesis, as we have found that the relative hub-status of the RA varies largely within the patient cohort, and that whether it is more or less central than its neighbours does

not determine outcome. Therefore, removal of a hub region was not necessary in this study to achieve seizure freedom. Of note, in this study we have considered the RA as a proxy for the epileptogenic zone, as it commonly done in epilepsy-surgery studies [209, 222, 224]. However, this adds a level of inaccuracy: for NSF cases it is known to be inaccurate, but even for SF cases it might have been larger that needed [207, 208]. This can lead to inaccuracies in the definition of the RA, and as a consequence of the neighbourhood regions. In contrast, the differences between either the RA or its neighbours with the remaining brain regions proved to be a stronger indicator of surgical outcome (albeit still weak, with AUC = 0.62and 0.64, respectively). The proposed three-node-set partition may thus provide new insight into the effect of a particular resection, which may be missed with the standard two-nodeset partition approach. This is in agreement with the methodology and findings in [225], but here we propose a methodology based only on resting-state MEG brain connectivity, without the need for invasive or ictal recordings, as the notion of the propagation zone is substituted by that of the neighbours of the RA.

4.8.2 Centrality metrics and node neighbourhoods

We proposed the use of regional centrality metrics to better account for the effect of a given resection, following previous theoretical works [180, 255, 256]. Most previous clinical studies have considered traditional centrality metrics that do not take the local networkneighbourhood into account, of which the degree [221-224], betweenness centrality [221,222], and eigenvector centrality [207, 257, 258] are predominant. Here we found that neighbourhood-based metrics, with the exception of β_0 (which equaled 1 in most cases for the considered parameters, as a consequence of the high level of recurrent connectivity in the networks), were able to more consistently pick up differences between \mathcal{RA} and \mathcal{RA} nodes at the individual level across all frequency bands, and in particular for the broadband, than nodal measures such as the betweenness centrality or the clustering coefficient (figure 4.4). These findings indicate that the neighbourhood of the RA is significantly different from the neighbourhood of other nodes in the brain network, in particular denoting a higher (generalized) centrality. In contrast, at the group level (figure 4.6) the metric that revealed the strongest difference between \mathcal{RA} and \mathcal{RA} nodes was the betweenness centrality, which is also the metric most often considered in the literature. We note this as an interesting venue for future research: at the theoretical level to understand whether different centrality metrics might be more or less sensitive to individual variations, and at the clinical level to validate the generalizability of these findings. Notably, whereas the betweenness centrality requires of global information, extended neighbourhood metrics can be computed with only regional information, and are thus more efficient to compute for large systems.

In the case of the three-node-set partition, at the group-level the differences between local and regional centrality metrics were larger (figure 4.6). This may be caused by the

neighbourhood-based partition of the node sets, such that the RA neighbourhood is considered explicitly, even for the node-based metrics. At the individual level the neighbourhoodbased metrics were also slightly more sensitive to differences between both the RA (\mathcal{RA} set) and its neighbours (\mathcal{N} set) with the remaining network nodes (\mathcal{O} set). Differences between the \mathcal{RA} and \mathcal{N} node-sets were sparse as discussed above, and generally all metrics performed similarly except for the clustering coefficient c, and the first and third Betti numbers, β_0 and β_2 , with very low sensitivity. In particular β_0 and β_2 , showed little variation across nodes for the parameters considered. At the group level, however, the betweenness centrality and curvature found the strongest and more consistent differences between nodesets. Further studies, considering e.g., larger networks or different connectivity thresholds, could validate the generalizability of these findings.

In order to better contextualize our study, we also considered the node strength (or weighted degree) as a centrality metric, following [224]. In their original study the authors found that this metric could classify \mathcal{RA} and \mathcal{RA} nodes for 8 out of 12 SF patients, and that, using the area under the curve of this classification (distinguishability D') as a patient score, they could classify SF and NSF patients with an AUC of 0.76. In our study, however, we have only found an AUC of 0.65 when implementing their methodology, and an optimal value of AUC = 0.68 for the α_1 band with the combined distinguishability score. These results are in agreement with those found in subsection 4.7, and with our previous findings with this same dataset [222]. Further studies are needed to elucidate the origin of the lower performance found here compared to Ramaraju et al. We identify methodological considerations, such as the choice of connectivity metric –we considered here a phase metric, the PLI, that is insensitive to volume conduction, whereas Ramaraju et al. used uncorrected amplitude correlations [224] – or the thresholding procedure used (simple thresholding vs the disparity filter considered here). Moreover, the small dataset considered by Ramaraju et al. could have driven the higher performance of the classification analysis. The findings may also reflect intrinsic differences between the patient populations: the cohort in this study is highly heterogeneous, including patients with different etiologies.

4.8.3 Multi-frequency analysis

We adopted a multi-band description, in analogy with some previous studies [226, 228, 253, 259–262]. These studies found for the most part comparable results across frequency bands, with significant differences in brain network organization between epilepsy patients and controls, or between SF and NSF epilepsy-surgery patients, arising predominantly in the θ and α bands [226, 228, 260–262], although differences have also been observed in the δ and γ bands [259] and in the ripple and fast ripple bands [259, 260].

In our study we also found comparable results across frequency bands for the node-based analyses, both at the individual and group level. Some metrics such as the local clustering *c*,

 β_0 and β_2 however only picked up differences between node sets in the broadband network. Notably, only in this band were the sizes of the \mathcal{N} and \mathcal{O} node-groups markedly different (when considering all ROIs and patients, see Figure 4.1 for more details). The bands for which we found the best patient classification were the broadband and α_1 , in agreement with the literature [226,228,260,262]. Remarkably, we found the strongest variations across frequency bands in the patient classification analysis (figure 4.7). Whereas in the broadband and the lower frequency bands (in particular δ and α_1) we found a somewhat better outcome for patients with high distinguishability score, this was not the case for higher frequency bands (in particular β and γ , see figure 4.7).

4.8.4 Methodological considerations

In this study we considered the same patient database as in our previous study [222]. In this previous study, a machine learning analysis was used to classify network nodes as belonging or not to the resection area, and to classify patients as having good (SF) or bad (NSF) outcomes. The performance of the node classifier was fair (60.37% accuracy), but the patient classification failed (49.03% accuracy). We have introduced several methodological changes relative to this original study, from the consideration of multiple frequency bands, the three-node-group partition, and the inclusion of node-neighbourhoods and topological data analysis. The methodologies of the two studies can be compared via the betweenness centrality, a benchmark centrality measure considered in both studies: [222] found that hub nodes overlapped more than expected by chance with the \mathcal{RA} . This is in qualitative agreement with our finding that \mathcal{RA} nodes are, at the group level, significantly more central than $\overline{\mathcal{RA}}$ nodes.

Regarding the patient classification, [222] performed a classification based on a combination of individual and average metrics, namely the averages over (a) \mathcal{RA} nodes, (b) the resection lobe, (c) nodes contralateral to the \mathcal{RA} , (d) $\overline{\mathcal{RA}}$ nodes, and two metrics measuring the difference between the average over \mathcal{RA} and the contralateral nodes, and over \mathcal{RA} and $\overline{\mathcal{RA}}$ nodes. No significant differences between SF and NSF patients were identified at group level, and a machine learning analysis was also unable to classify the patients according to surgical outcome. In our study, instead of using the centrality values directly, we exploited the results of the node-based analyses to perform a patient classification analysis, similarly to [224]. In particular, we defined a distinguishability score based on the difference between each of the node sets, and we found an AUC of 0.68 for the broadband network (the same used in [222]). In this manner we were able to exploit a patient-specific analysis, accounting for heterogeneity in the patient population, which can be lost if comparisons of absolute values among patients are performed. The differences in findings between the two studies, and our finding that a population-based analysis is less sensitive than the patient-specific analysis, highlight the need to consider methodologies that allow for individualized patient characterization [209, 210].

Whereas some of the studies mentioned above [224], as well as other recent studies [209], have found better classification results than the ones found in this study, the strength of this study lies in the much larger patient cohort considered here, which is two to three times larger than typical cohort sizes in similar studies. Moreover, we further validated the robustness of our findings with respect to several methodological choices, including the frequency band of the MEG-based brain networks and specific analysis details, benchmarking our findings and analysis pipelines against previous studies [222, 224].

4.9 Conclusions

In this chapter, we explored the application of higher-order network representations in understanding the functional organization of brain networks, with a particular focus on epilepsy. Our findings highlight the critical role of topological features in identifying pathological hubs within the epileptogenic zone (EZ). Through the integration of topological data analysis (TDA) with network neuroscience, we demonstrated that the resection area and its surrounding regions exhibit increased centrality in the network, shedding light on the structural and functional abnormalities associated with seizure dynamics. This higher-order perspective not only enhances our understanding of epilepsy's network structure but also provides predictive power in classifying resected versus non-resected areas.

One of the significant takeaways from this analysis is the variability observed across patients. The differences in the centrality metrics suggest that personalized approaches to epilepsy surgery are essential, given the unique network topologies associated with each patient's condition. While our findings offer a framework for improved prediction of surgical outcomes, the variability among patients also points to the necessity of further research in developing more individualized models.

Looking forward, there are several promising avenues for future research. Expanding the application of TDA and higher-order networks to other neurological disorders, such as Alzheimer's and schizophrenia, could uncover new insights into the underlying dynamics of these diseases. Additionally, the integration of these methods with other dynamical processes, such as social contagion or disease spreading models, presents an exciting opportunity for cross-disciplinary research. By continuing to explore the rich complexities of higher-order networks, we can further refine our models and improve their applicability to a broader range of clinical and theoretical contexts.

5 Conclusions and outlook

This thesis set out to advance our understanding of complex networks by moving beyond the limitations of traditional pairwise interaction models. Across various domains, from social to biological systems, interactions within networks often involve groups of entities rather than just pairs. Recognizing this complexity, our work focused on the role of higherorder interactions and their significant impact on both the structure and dynamics of these systems.

We began by examining the structural properties of networks that incorporate higherorder interactions, aiming to understand how these interactions influence network topology, including the distribution of connections, the formation of degree correlations, and overall connectivity. To achieve this, we introduced the Hidden Variables (HV) formalism, a mathematical framework designed to capture the complexity of higher-order interactions within temporal networks—where interactions evolve over time, adding layers of dynamism to the network structure. Our study revealed that higher-order interactions could drastically alter key network properties, such as percolation thresholds—the critical points at which a network transitions from a disconnected to a connected state—and the network's robustness against failures or targeted attacks. These findings underscore the importance of considering higher-order interactions in analyzing network structure, particularly in systems where the timing and sequence of interactions are pivotal to network functionality.

In the context of dynamical processes, we explored how group interactions shape system behavior, particularly in scenarios where the system is driven out-of-equilibrium. By developing models such as random walks and diffusion processes on hypergraphs, we investigated how higher-order interactions influence system dynamics, focusing on the emergence of rare events—extreme or unexpected outcomes with significant impacts. We demonstrated that higher-order interactions are not merely secondary features but critical factors that can profoundly affect system dynamics, leading to atypical behaviors often invisible in models restricted to pairwise interactions. The presence of higher-order interactions could either suppress or amplify fluctuations depending on the network configuration, affecting the likelihood and nature of rare events. This provided new insights into the dynamics of complex systems, especially in understanding how out-of-equilibrium processes and fluctuations are shaped by the network's underlying interaction structure.

Bridging the gap between theory and practice, we applied these concepts and models to the study of brain networks in epilepsy patients. We focused on identifying and analyzing pathological hubs—regions of the brain that, while not the primary epileptogenic focus, are crucially connected to it and may influence the spread of epileptic seizures. By integrating higher-order network metrics with empirical patient data, we gained a deeper understanding of the organization of these brain networks. This analysis provided novel insights into how these networks function, suggesting that considering group interactions could lead to more effective surgical strategies. Specifically, surgical planning should not only target the epileptogenic zone but also account for the broader network interactions involving pathological hubs, potentially improving patient outcomes by minimizing seizure recurrence and preserving critical brain functions.

The work presented in this thesis opens several avenues for future research, both in expanding the theoretical frameworks introduced and in applying these concepts to new domains and challenges. For example, the HV formalism, successfully applied to model higher-order interactions in activity-driven networks, can be extended to other established network models. Spatial network models, where connections are influenced by physical proximity, can be enhanced to consider group interactions based on geographic clustering, with the HV formalism providing a framework for analyzing the resulting network properties. Similarly, gravity models, which consider the "mass" of nodes and distance in determining connection probabilities, can be generalized to higher-order scenarios where groups of nodes interact based on collective attributes like combined mass or distance. Geometric and hyperbolic models, which embed networks in abstract spaces, can also be extended to consider higher-order geometrical relationships, with HV offering a method to solve and analyze these complex structures. Furthermore, fitness models, where connections are formed based on a node's intrinsic ability to attract links, can be expanded to higher-order fitness landscapes, allowing for the study of networks where group dynamics are driven by collective fitness. Integrating the HV formalism into these higher-order versions of classical models will enable a better understanding of how complex global behaviors emerge from localized, group-based interactions, offering more accurate representations of real-world networks such as transportation systems, social dynamics, and biological interactions.

In addition to these structural extensions, future research should explore how specific higher-order structural features influence dynamical fluctuations and rare events. Investigating hypergraphs that exhibit a scale-free distribution of higher-order interactions could reveal how these heterogeneous structures affect the likelihood of rare events, such as extreme fluctuations in diffusion processes. Similarly, examining the role of community structures or directed hyperedges in hypergraphs may provide new insights into the emergence of atypical dynamics, especially in systems where group interactions follow a non-random or preferential pattern. Beyond random walks, the methodologies developed in this thesis can be applied to other dynamical processes sensitive to higher-order interactions. For instance, in models of social contagion, where the spread of information or behavior is influenced by group dynamics, understanding the role of higher-order interactions could lead to better predictions of how ideas or innovations propagate through social networks. Extending this work to percolation processes could also improve our understanding of how connectivity thresholds and critical phenomena are affected by higher-order interactions, particularly in networks with complex, multi-body connections.

Another important area for future research is developing a more general theory of fluc-

tuations in higher-order networks. While this thesis laid the groundwork by examining specific cases, a comprehensive framework that captures the impact of higher-order interactions across various network types and dynamical processes would be invaluable. Such a theory could provide the tools needed to analyze the stability and robustness of networks under various conditions, offering insights into how higher-order interactions influence the emergence of catastrophic events, such as systemic failures in infrastructure networks or the rapid spread of diseases in populations.

Finally, the insights gained from applying higher-order network analysis to the study of brain networks in epilepsy patients open up several promising avenues for future research, particularly in improving the understanding and treatment of neurological disorders. A significant direction for future research is the further exploration of how higher-order interactions within brain networks contribute to the onset and propagation of epileptic seizures. While this thesis focused on pathological hubs and their connections within the network, future studies could investigate the broader network environment, including how different brain regions contribute to or inhibit seizure activity when interacting in complex, multinode configurations. Mapping the higher-order topological features of brain networks in more detail, such as identifying subgraphs or motifs prone to pathological synchronization, could provide new targets for therapeutic interventions.

Another promising area is the development of personalized models of brain networks that incorporate higher-order interactions. Given the heterogeneity observed in patient populations, as highlighted by this work, creating individualized network models that consider a patient's unique higher-order interactions could lead to more precise and effective treatment strategies. These models could simulate different surgical approaches or other interventions, allowing clinicians to tailor treatments to each patient's specific network structure, potentially improving surgical success rates and reducing the risk of post-operative complications.

Additionally, future research could extend higher-order network analysis beyond epilepsy to other neurological conditions characterized by abnormal network activity, such as Alzheimer's disease, Parkinson's disease, or schizophrenia. Understanding how higher-order interactions differ between healthy and diseased brains could lead to the development of biomarkers for early diagnosis or new therapeutic targets aimed at restoring normal network function.

Moreover, there is potential for integrating higher-order network analysis with real-time brain activity monitoring, such as EEG or fMRI data. Dynamically tracking changes in the brain's higher-order network structure could improve seizure onset prediction or even develop closed-loop systems that can intervene to prevent seizures before they fully develop. This approach could lead to advanced neuromodulation techniques that adapt in real-time to the evolving state of the brain, offering a new frontier in treating epilepsy and other neurological disorders.

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Appendix

A 1 Code availability

The data used for the material presented in Chapter 4 are not publicly available because the patients did not consent for the sharing of their clinically obtained data. Access to the data-sets can be provided through AUMC, access requests should be directed to the corresponding author. All user-developed codes are available in github: https://github.com/LeonardoDiGaetano/TDA-Epilepsy.

A 2 Supplementary information to patient-specific comparison

Here we report the number of patients for whom there was a significant difference in the direction of the hypothesis (Table A.1) and in opposite direction (Table A.2) relative to the results presented in Figure 4.4.

	(a) $\mathcal{X}(\mathcal{R}\mathcal{A}) > \mathcal{X}(\overline{\mathcal{R}\mathcal{A}})$										(b) $\mathcal{X}(\mathcal{RA}) > \mathcal{X}(\mathcal{O})$									
	BC	c	\mathcal{C}	N	E	β_0	β_1	β_2			BC	c	\mathcal{C}	N	E	β_0	β_1	β_2		
B	6	6	1	23	27	0	20	14		В	16	17	1	49	50	2	46	37		
δ	3	0	1	4	6	1	6	2		δ	5	4	0	15	18	1	15	5		
θ	3	4	1	11	14	0	8	9		θ	10	8	1	23	25	0	24	15		
α_1	0	4	4	6	6	0	5	1		α_1	6	6	3	22	26	0	25	10		
α_2	0	1	1	2	5	0	3	4		α_2	5	3	0	14	16	0	17	7		
β	0	5	4	4	5	0	4	3		β	4	9	4	17	21	0	17	9		
γ	1	0	2	5	4	0	4	1		γ	5	1	1	11	12	0	9	2		
		(c) .	$\mathcal{X}(\mathcal{R})$	(\mathcal{A}) :	$> \mathcal{X}$	(\mathcal{N})						(d)	$\mathcal{X}(J)$	V) >	> X($\mathcal{O})$				
	BC	c	\mathcal{C}	N	E	β_0	β_1	β_2			BC	c	\mathcal{C}	N	E	β_0	β_1	β		
B	5	3	7	9	5	0	10	4		B	61	29	1	71	68	24	73	54		
δ	2	0	2	2	2	1	2	1		δ	45	6	0	57	54	0	56	1		
θ	2	3	2	1	1	1	2	0		θ	41	15	0	57	55	2	55	2		
α_1	0	2	11	1	1	0	1	1		α_1	48	10	1	61	59	2	60	1		
010	0	1	3	0	0	0	0	1		00	11	1	0	45	46	1	18	6		

Table A.1: Number of patients for whom there was a significant difference in the direction of the hypothesis of Figure 4.4.

53

37

β

13 0 56 56

4 | 0

56

44

2

44 46

20

4

β

0

5 6

0

1

0

0

0

1

0

(a) $\mathcal{X}(\mathcal{RA}) > \mathcal{X}(\overline{\mathcal{RA}})$

	BC	c	\mathcal{C}	N	E	β_0	β_1	β_2
B	0	2	3	5	5	0	7	3
δ	0	1	0	3	2	0	3	0
θ	0	1	7	3	2	0	2	1
α_1	0	0	1	6	5	1	4	0
α_2	1	2	2	3	5	1	6	2
β	3	1	1	5	6	1	5	0
γ	0	1	2	2	1	0	3	0

(c) $\mathcal{X}(\mathcal{RA}) > \mathcal{X}(\mathcal{N})$

	BC	c	\mathcal{C}	N	E	β_0	β_1	β_2
B	15	4	2	14	9	3	12	7
δ	4	2	0	5	6	0	6	2
θ	7	1	4	5	4	0	4	3
α_1	10	3	0	10	10	1	8	2
α_2	5	1	3	5	5	0	9	1
β	10	4	1	10	8	0	11	4
γ	10	2	0	4	4	0	5	0

(b) $\mathcal{X}(\mathcal{RA}) > \mathcal{X}(\mathcal{O})$

	BC	c	\mathcal{C}	N	E	β_0	β_1	β_2
B	0	2	11	5	5	0	7	4
δ	0	1	4	3	3	0	3	0
θ	0	2	9	1	1	0	1	0
α_1	0	1	6	6	5	1	4	1
α_2	1	3	6	2	3	1	4	3
β	2	1	4	5	6	1	4	0
γ	0	1	4	1	1	0	2	0

(d) $\mathcal{X}(\mathcal{N}) > \mathcal{X}(\mathcal{O})$

	BC	c	\mathcal{C}	N	E	β_0	β_1	β_2
B	0	6	30	0	0	0	0	0
δ	0	3	25	0	0	0	0	0
θ	0	3	20	1	1	1	0	0
α_1	0	3	24	1	0	2	0	0
α_2	0	0	33	1	1	1	0	0
β	0	1	32	0	0	0	0	0
γ	0	4	27	0	0	0	0	0

Table A.2: Number of patients for whom there was a significant difference in opposite direction of the hypothesis of Figure 4.4.

Supplementary information to group-level comparison A 3

Here we report the numerical values presented in Figure 4.6. Table A.3 presents z-scores presented through colors in Figure 4.6 and Table A.4 the corresponding p-values.

	(a) $\mathcal{X}(\mathcal{R}\mathcal{A}) > \mathcal{X}(\overline{\mathcal{R}\mathcal{A}})$										(b) $\mathcal{X}(\mathcal{RA}) > \mathcal{X}(\mathcal{O})$									
	BC	С	С	N	E	β_0	β_1	β_2]		BC	с	C	N	E	β_0	β_1	β_2		
B	2.2	1.5	-1.7	4.2	3.8	2.7	2	1.4		B	-4.2	0.1	1.6	-1.9	-1.4	-3.3	-1.2	-0.39		
δ	0.49	0.27	0.62	0.57	0.47	0.5	0.39	0.17		δ	-3.2	0.3	3.5	-3.6	-3	0.25	-2.9	-0.38		
θ	0.87	1.8	-0.48	3.1	3.2	-0.097	1.2	0.9		θ	-3.6	1	1.2	-2.5	-1.7	-0.68	-1.5	0.16		
α_1	-2.1	0.52	0.83	0.25	0.67	-2.2	0.56	0.46		α_1	-6.5	0.92	2.7	-2.9	-2.3	-1.9	-1.9	-0.21		
α_2	-0.92	-0.99	-1.2	0.5	0.47	-0.75	-0.4	-0.12		α_2	-5.6	0.5	0.5	-1.1	-2.3	-2.3	-0.044	0		
β	-1.2	1	0.36	0.39	0.41	-1.1	0.53	0.58		β	-7.5	0.5	2.8	-4.1	-3.5	-1.5	-4.1	-0.42		
γ	-2.1	-1.8	-0.42	-0.74	-0.64	-1.4	0.34	0.38		γ	-6.8	-0.97	-3.7	-4.2	-4.1	-1.8	-0.2	0.052		

(c)	$\mathcal{X}($	R.	A)	>	\mathcal{X}	(Л	ſ
(-)	,		- /	-			· .

		-		-				
	BC	С	C	N		β_0	β_1	β_2
B	5.7	3.4	-3.7	8.1	7.7	5.4	4.4	2.9
δ	3.4	0.7	-1.6	4	3.6	0.64	0.82	0.86
θ	3.9	2.6	-2.1	6.1	6.5	0.46	3.2	2.2
α_1	2.1	0.78	-0.51	4.8	3.5	0.72	0.41	1
α_2	-0.6	-0.93	-0.5	4.7	3.1	-0.51	2	0.094
β	3.1	-1.5	-1.5	3.5	3.5	-0.72	1.2	1.4
γ	1.6	-2.1	-2.1	3.5	3.1	-0.1	1.3	0.61

(d) $\mathcal{X}(\mathcal{N}) > \mathcal{X}(\mathcal{N})$	$\mathcal{X}(\mathcal{O})$
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			```	/	```	/		
	BC	c	С	N	E	$\beta_0$	$\beta_1$	$\beta_2$
B	15	4.1	-5.7	13	12	8	6.2	1.2
δ	17	0.65	-7	11	8.1	7.9	7.1	1.2
θ	7.5	2.1	-3.6	11	11	1.5	5.2	2.2
$\alpha_1$	10	-0.25	-4.8	11	8.3	5.6	1.2	1
$\alpha_2$	15	-0.29	-4.7	7	7	-0.46	5.5	0.057
β	18	1.3	-5.7	13	10	1.8	7.3	1.8
$\gamma$	13	-1.5	-6.5	8.5	7.9	1.4	8	0.63

-0.38 0.16 -0.21 0 -0.42

Table A.3: Numerical values corresponding to results of Figure 4.6. Group-level comparison between nodes sets, for each considered frequency-band (y-axis) and network metric (xaxis).  $\mathcal{X}(S)$  stands for the generalized centrality metric  $\mathcal{X}$  measured on the nodes in set S. The numbers indicate the z-score of the difference between the average values of each node set, computed by bootstrapping the data (sampling size of  $10^4$ ).

(a)  $\mathcal{X}(\mathcal{RA}) > \mathcal{X}(\overline{\mathcal{RA}})$ 

#### (b) $\mathcal{X}(\mathcal{RA}) > \mathcal{X}(\mathcal{O})$

	BC	с	C	N	E	$\beta_0$	$\beta_1$	$\beta_2$		BC	с	C	N	E	$\beta_0$	$\beta_1$	$\beta_2$
B	0.03	0.145	0.083	0.0	0.0	0.007	0.05	0.176	B	0.0	0.919	0.121	0.062	0.17	0.001	0.249	0.693
δ	0.622	0.79	0.533	0.57	0.64	0.619	0.699	0.868	δ	0.001	0.763	0.001	0.0	0.003	0.801	0.003	0.706
θ	0.386	0.07	0.632	0.002	0.002	0.923	0.212	0.218	θ	0.0	0.306	0.215	0.013	0.087	0.495	0.122	0.872
$\alpha_1$	0.039	0.603	0.405	0.805	0.503	0.025	0.574	0.645	$\alpha_1$	0.0	0.359	0.008	0.003	0.01	0.053	0.056	0.8
$\alpha_2$	0.359	0.323	0.241	0.618	0.637	0.453	0.662	0.901	$\alpha_2$	0.0	0.546	0.262	0.024	0.023	0.965	0.05	0.92
β	0.214	0.295	0.722	0.7	0.684	0.268	0.599	0.562	β	0.0	0.517	0.005	0.0	0.0	0.121	0.0	0.671
$\gamma$	0.038	0.069	0.676	0.457	0.523	0.807	0.462	0.701	$\gamma$	0.0	0.331	0.0	0.0	0.0	0.525	0.0	0.958

(c)  $\mathcal{X}(\mathcal{RA}) > \mathcal{X}(\mathcal{N})$ 

(d)  $\mathcal{X}(\mathcal{N}) > \mathcal{X}(\mathcal{O})$ BC BC F  $\frac{\beta_2}{0.004}$  $\beta_0$  $\frac{\beta_2}{0.0}$  $\beta_0$  $\beta$ 0.001 0.0 0.0 0.0 BB0.0 0.0  $\delta \\ \theta \\ \alpha_1$  $\delta \\ \theta \\ \alpha_1$ 0.001 0.485 0.11 0.0 0.0 0.522 0.002 0.387 0.0 0.516 0.0 0.0 0.272 0.0 0.0 0.224 0.0 0.0 0.645 0.043  $\begin{array}{c} 0.0 \\ 0.0 \end{array}$  $\begin{array}{c} 0.0\\ 0.0 \end{array}$  $\begin{array}{c} 0.0 \\ 0.0 \end{array}$ 0.0 0.0 0.0 0.01 0.079 0.0 0.001 0.03 0.039 0.0 0.14 0.025 0.034 0.433 0.611 0.003 0.006 0.315 0.806 0.0 0.408 0.248  $\alpha_2 \\ \beta$  $0.001 \\ 0.002$ 0.352 0.139 0.002 0.0 0.067 0.002 0.0 0.064 0.61 0.472 0.01 0.003 0.925 0.163  $\alpha_2 \\ \beta$ 0.0 0.0 0.775 0.191 0.0 0.0 0.0 0.0 0.0 0.0 0.646 0.069 0.0 0.0 0.0 0.0 0.0 0.955 0.071 0.531 0.003 0.122 0.108 0.038 0.042 0.891 0.185 0.539 0.0 0.127 0.519 0.0

Table A.4: p-values corresponding to results of Figure 4.6. Group-level comparison between nodes sets, for each considered frequency-band (y-axis) and network metric (x-axis).  $\mathcal{X}(S)$  stands for the generalized centrality metric  $\mathcal{X}$  measured on the nodes in set S. The numbers indicate the p-values of the comparison between the average values of each node set presented in Table A.3 and Figure 4.6.