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Homological Characterization of Convection Cycles for Multiplex Network Flows

Keywords: coupling strength, persistent homology, multilayer networks, homological indicator, multiplex Markov Chains

Extended Abstract

There are a bunch of approaches to construct or analyze a multilayer network or multiplex Markov chains (MMCs), ranging from using supra-Laplacian [1], comparing two multilayer nets by using graphlets multilayer technique [2], basing on the impact of high-order time delayed information [3] to computing Pareto Distance as in [4]. In the recent decade, utilizing Topological Data Analysis becomes an intensive tool for not just characterizing the intricate properties of such high-order networks but capturing heterogeneous properties simultaneously in these entities [5].

Topological Data Analysis (TDA) plays a crucial role in studying topological structures of point cloud data via an efficient tool called persistent homology (PH). Indeed, with the abundant applications, we can observe many key insights in various fields ranging from time series data [6, 7], image processing [8], machine learning [9], artificial intelligence [10, 11], the coloring patterns of fish [12] to RNA sequence data analysis [13, 14], brain analysis [15], to name a few. Complementing the study of point-cloud data, another line of research involves utilizing the TDA toolset to study complex systems, for which the applications include the analysis of spreading processes over social networks [16], network neuroscience [17, 18], mechanical-force networks [19], jamming in granular material [20], molecular structure [21, 22], material science [23], knot data analysis [24] and DNA folding [25].

In recent work [26], we developed an approach that leverages PH to study the topological behavior of flows over directed networks. Specifically, we utilized PH to automate the detection (and summarize the multiscale properties) of convection cycles that arise for the stationary distributions of irreversible Markov chains (MCs). MCs are known to have numerous applications across science and engineering including queuing theory [27], population dynamics [28], and machine learning algorithms that rely on Markov chain Monte Carlo [29], hidden Markov models [30], and Markov decision process [31]. Despite the prevalence of MCs, the emergence of convection cycles (i.e., cyclic flows) in Markov chains are insufficiently studied, especially from the perspective of homology. In fact, the study of convection cycles has been mostly limited to fluid dynamics, although in MCs such cycles have been used to model the "chiral edge flows" [26, 32] that are associated with the quantum Hall effect, polymer dynamics, and multiscale biological rhythms.

In our approach, we study convection via using a toolset of algebraic topology called *homology*, which formally studies the absence/presence of k-dimensional "holes" (and their connectivity) within a topological space such as a simplicial complex [33]. Because our consideration is the existence of cycles that are 1-dimensional (1D) holes, persistent homology is a natural fit to analyze convection cycles. To this end, we construct filtrations of graphs by removing edges according to the stationary flows across them, and we summarize the persistent homology of the filtered graphs' associated clique complexes. Numerically, we implement these techniques by building on a popular TDA framework called Gudhi [34], which we adapt to implement *edge-value clique (EVC) filtrations* of functions defined over the edges of graphs (Figure 1).

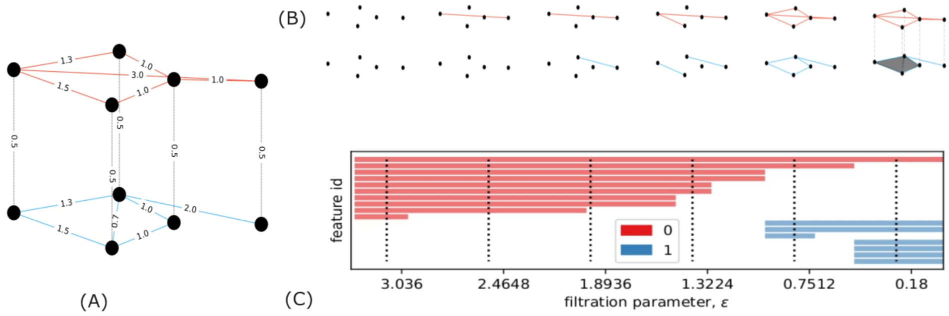

Figure 1: **Persistent homology according to an *edge-valued clique (EVC) filtration* for a weighted, multiplex network.** (A) Visualization of a multiplex network $\mathcal{G}$ with $L = 2$ layers, each consisting of $N = 5$ nodes and several weighted "intralayer" edges (which are colored red and blue in the respective layers). The network layers are coupled with "interlayer" edges having weight $\omega = 0.5$ (called the *coupling strength*). (B) Visualization of example simplicial complexes $\mathcal{S}_\varepsilon$ that arise during the EVC filtration for different $\varepsilon > 0$, which monotonically decreases from an initial value $\varepsilon_0 = 4$. Each $\mathcal{S}_\varepsilon$ is the clique complex for a graph $\mathcal{G}_\varepsilon$—that is, the graph $\mathcal{G}$ shown in panel (A) after removing edges having weight less than ε. (C) A *barcodes* summarize the persistence of 0-dimensional (red) and 1-dimensional (blue) *homological generators* for $\mathcal{S}_\varepsilon$, although we focus on 1-dimensional generators herein. Letting ε_b and ε_d denote the value of ε at which a given 1-cycle is born and dies, respectively, we define the cycle's "lifetime" $|\varepsilon_d - \varepsilon_b|$. Observe that there exists one short-lifespan cycle that appears (i.e., is born) at $\varepsilon \approx 1.1$ and disappears (i.e., dies) at $\varepsilon \approx 0.7$. This cycle can be observed in the lower, blue-colored network layer in panel (B).

In this present work, we extend this approach to the setting of multiplex Markov chains (MMCs) [35]. MMCs are a generalization of MCs in which a set of MCs are interconnected using another set of MCs. Intuitively, consider a random walk over a graph, but the walker can also stochastically jump onto to a different graph. Thus, there are stochastic transitions within a network (or graph) layer as well as stochastic transitions between layers. To control whether transitions occur mostly within a layer or between layers, a *coupling strength* ω is introduced to scale these. Prior work [35] found that ω plays a critical role in determining whether or not convection cycles arise, and in fact, some cycles can arise as an emergent property—that is, the coupling of reversible MCs lacking cycles can give give to MMCs that exhibit cycles.

Notably, that work did not utilize the techniques of topological data analysis. Herein, we utilize PH to provide new homological insights for this phenomenon (Figure 2). From the perspective of topology, the coupling strength ω can be understood as a "homological regularizer" of the multiplex diffusion process. Our methods provide mathematically principled (and automated) tools to gain a deeper understanding of convection cycles arising for network flows, and they are expected to be useful to myriad applications across the physical, social, biological and computational sciences.

Motivated by neuroscience and AI applications, we apply this modeling framework to investigate two applications. First, we study a leading mathematical framework for reinforcement learning called Markov decision processes (MDPs) and extend them using MMCs. We find PH to be an invaluable tool for tracking and quantifying optimal policies—that is, developing a homological understanding of decision making (or rather, indecision quiescence). Second, we build MMC models for fMRI-recorded brain activity for persons with and without Alzheimers, revealing homological differences between these two groups. Our work extends prior work

[35] that explored convective flows for these two groups but did not utilize TDA techniques. We find persistence barcodes to be useful features for disease classification.

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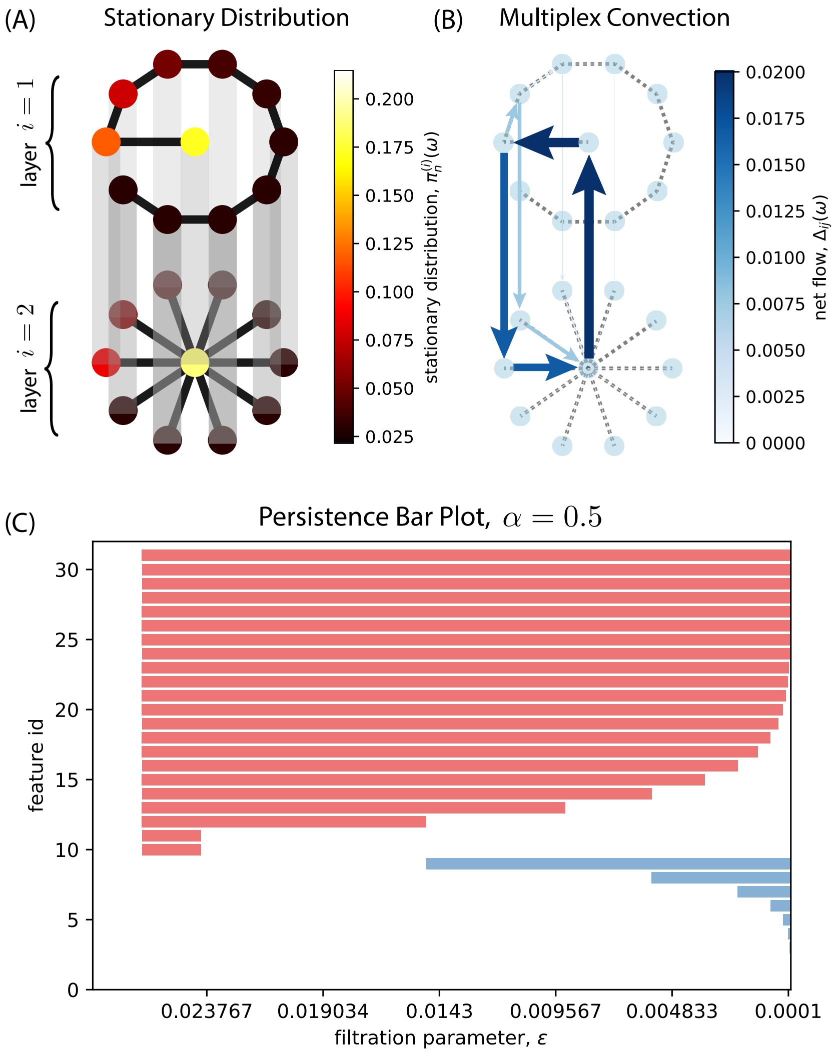

Figure 2: **Emergent convection over a multiplex Markov chain (MMC) [35]**. (A): Stationary distribution $\pi_n^{(i)}(\omega)$ for discrete-time MMC with interlayer coupling strength $\omega = 0.5$. The black and grey lines indicate edges in the intra- and interlayer Markov chains, respectively. (B): The stationary flow imbalance $\Delta_{pq}^{\omega} = \pi_{n_p}^{(i_p)}(\omega)[P(\omega)]_{pq} - \pi_{n_q}^{(i_q)}(\omega)[P(\omega)]_{qp}$ reveals for each edge (p,q) the extent to which diffusion moves in a biased direction after the system converges to its steady state. Observe the emergent multiplex convection cycle, which is a cyclical flow at stationarity that involves more than one layer. It arises due to multiplex imbalance, whereby the multiplexing of reversible Markov chains yields an irreversible MMC. (C): Persistent barcodes for 1-cycles track the appearance of these convective cycles.