Time Dimension Dances with Simplicial Complexes: Zigzag Filtration Curve based Supra-Hodge Convolution Networks for Time-series Forecasting

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Abstract

Graph neural networks (GNN) offer a new powerful alternative for multivariate time series forecasting, demonstrating remarkable success in a variety of spatio-temporal applications, from urban flow monitoring systems to health care informatics to financial analytics. Yet, such GNN models pre-dominantly capture only lower order interactions, that is, pairwise relations among nodes, and also largely ignore intrinsic time-conditioned information on the underlying topology of multivariate time series. To address these limitations, we propose a new time-aware GNN architecture which amplifies the power of the recently emerged simplicial neural networks with a time-conditioned topological knowledge representation in a form of zigzag persistence. That is, our new approach, Zigzag Filtration Curve based Supra-Hodge Convolution Networks (ZFC-SHCN) is built upon the two main components: (i) a new highly computationally efficient zigzag persistence curve which allows us to systematically encode time-conditioned topological information, and (ii) a new temporal multiplex graph representation module for learning higher-order network interactions. We discuss theoretical properties of the proposed time-conditioned topological knowledge representation and extensively validate the new time-aware ZFC-SHCN model in conjunction with time series forecasting on a broad range of synthetic and real world datasets: traffic flows, COVID-19 biosurveillance, Ethereum blockchain, surface air temperature, and vector autoregressions. Our experiments demonstrate that ZFC-SHCN achieves the state-of-the-art performance with lower requirements on computational costs.

1 Introduction

Over the last few years, graph neural networks have emerged as a new powerful alternative to traditional statistical and machine learning models in conjunction with multivariate time series forecasting tasks. Such successful applications of GNNs range from urban traffic analytics to forecasting COVID-19 hospitalizations to electrocardiogram monitoring. However, most GNNs remain inherently static and do not explicitly incorporate the inherent time characteristics of the encoded knowledge. In turn, limitations in capturing the time dimension in the knowledge representation and learning mechanisms for time-evolving data results in GNNs becoming less relevant over time and requiring frequent and often costly model updates.

Furthermore, GNNs tend to pre-dominantly focus only on information propagation among nodes and be limited in their ability to describe polyadic relationships among multiple substructures of multivariate time series or multi-node interactions in dynamics graphs. However, as recently shown by [6], such higher-order interactions might be the key toward better understanding of the underlying mechanisms of many real world graph-structured phenomena. One of the recent approaches to

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systematically address such polyadic graph interactions is to model higher order substructures as simplices and then, by borrowing the concepts of the Hodge Theory, to generalize the ideas of the combinatorial graph Laplacian which describes diffusion from node to node via edges to diffusion over simplices. This Hodge Laplacian construction allows for extending the notion of convolution operation to simplicial convolution, and the resulting simplicial neural networks (SNNs) are arguably one of the frontlines in graph learning today, though these ideas have never been yet applied in conjunction with knowledge representation and learning of time-evolving objects.

Our goal here is to bridge the emerging concept of time-aware learning with the recent notions of simplicial convolution, with a particular focus on explicitly integrating the core time-conditioned topological characteristics. In particular, we amplify the power of SNNs with a time-conditioned topological knowledge representation in a form of zigzag persistence for time-indexed data and, more specifically, its new highly computationally efficient summary, Zigzag Filtration Curve. As a result, our new approach, Zigzag Filtration Curve based Supra-Hodge Convolution Networks (ZFC-SHCN) enables us to systematically learn the most intrinsic time-conditioned information both on the underlying topology of the time-evolving data and higher-order interactions among various substructures.

Significance of our contributions can be summarized as follows:

- ZFC-SHCN is the first approach bringing the concepts simplicial convolution and SNNs to time-aware learning.
- We propose a new highly computationally efficient summary of persistence for time-indexed data, Zigzag Filtration Curve, and derive its theoretical stability guarantees.
- We validate utility of ZFC-SHCN in conjunction with forecasting multivariate time series from diverse application domains such as traffic networks, COVID-19 biosurveillance, surface air temperature, token prices on Ethereum blockchain, and vector autoregressions. Our findings indicate that ZFC-SHCN delivers the state-of-the-art forecasting performance, with a significant margin and demonstrates higher computational efficiency.

2 Related Work

Time-series Forecasting with Graph Convolutional Networks The field of applying graph convolutional networks (GCN)-based models for the spatio-temporal network data forecasting have received a large amount of attention in recent years. DCRNN [27] introduces the spectral graph convolution into spatio-temporal network data prediction, which can capture spatio-temporal dependencies. STGCN [41] uses convolutional neural networks (CNN) to model temporal correlations. Moreover, to infer the hidden inter-dependencies between different traffic variables, some efforts [40, 3, 8] conduct convolution operation in spatial dimension through the adaptive adjacency matrices. Recent Z-GCNETs [14] develops a zigzag topological layer equipped with zigzag persistence image into GCN framework to model temporal correlations. However, all of above methods only focus on the node-level representations, in this paper, we focus on both higher-order structures representation and topological information learning.

Zigzag Persistent Homology Persistent homology [18, 43] is a suite of tools within topological data analysis (TDA) that provides a way for measuring topological features of shapes and of functions. However, the regular persistent homology does not explicitly model the geometric and topological information from a sequence of topological spaces. To address this limitation, a generalization of ordinary persistence, i.e., zigzag persistent homology, based on the theory of quiver representation, has been proposed by [10]. Zigzag persistence allows us to systematically describe how the homology changes over a sequences of spaces. Despite its high potential, especially in conjunctions with analysis of time-evolving data, zigzag persistence still remains largely a theoretical concept, and its applications are yet scarce. The recent results for time-dependent data studies include, for example, zigzag-based clustering [24], bifurcation analysis of dynamic systems [39], and time series forecasting [14]. The memory and computational efficiency of zigzag persistence is one of the daunting challenges. Inspired by [29], in this paper we propose a novel highly computationally efficient representation of zigzag persistence for learning time-evolving data, that is, zigzag filtration curve.

Simplicial Neural Networks Modeling higher-order interactions on graphs is an emerging direction in graph representation learning. While the role of higher-order structures for graph learning has been documented for a number of years [1, 22] and involves such diverse applications as graph signal processing in image recognition [16], dynamics of disease transmission and biological network, integration of higher-order graph substructures into deep learning on graphs has emerged only in 2020. As shown by [6, 35], higher-order network structures can be leveraged to boost graph learning performance. Indeed, several most recent approaches [17, 34, 7, 12] propose to leverage simplicial information to perform neural networks on graphs. However, neither of these Simplicial Neural Networks (SNNs) are integrated with a topology-based graph convolution layer allowing us to learn both time-aware persistent topological features and simplicial geometry of graphs. In this paper, we propose ZFC-SHCN to address this limitation.

3 Time-Aware Topological Learning with Zigzag Curves

Spatio-temporal Graph Construction A spatio-temporal graph is a collection of snapshots at different time steps, denoted by $\boldsymbol{\mathcal{G}} = \{\mathcal{G}_1, \mathcal{G}_2, \cdots, \mathcal{G}_{\mathcal{T}}\}$, where $\mathcal{T}$ is the maximum timestamp. Here $\mathcal{G}_t = (\mathcal{V}_t, \mathcal{E}_t, \boldsymbol{\mathcal{A}}_t, \boldsymbol{X}_t)$ is the graph observed at time step $t \in [1, \mathcal{T}]$, where $\mathcal{V}_t$ is a finite set of $|\mathcal{V}| = N$ nodes, $\mathcal{E}_t$ is a set of edges, $\boldsymbol{\mathcal{A}}_t \in \mathbb{R}^{N \times N}$ is the adjacency matrix, and $\boldsymbol{X}_t \in \mathbb{R}^{N \times d}$ is the node feature matrix. Specifically, each row of $\boldsymbol{X}_t$ is a d-dimensional feature vector of the corresponding node. For simplicity, wherever applicable below, we omit the subscript t and denote graph $\mathcal{G}_t$ at time t as $\mathcal{G}$.

Background on Ordinary Persistence Tools of ordinary persistence, or persistent homology (PH), allow us to study salient data shape patterns along various dimensions. By shape here we broadly understand data properties which are invariant under continuous transformations, that is, transformations which do not alter "holes" in the data, for examples, bending, twisting, and stretching. The key idea is to choose some suitable scale parameter ν and then to study graph $\mathcal{G}$ not as a single object but as a nested sequence of graphs, or *graph filtration* $\mathcal{G}_1 \subseteq \ldots \subseteq \mathcal{G}_n = \mathcal{G}$ which is induced by monotonic changes of scale ν. For example, if $\mathcal{G}$ is an edge-weighted graph $(\mathcal{V}, \mathcal{E}, w)$ with weight function $w : \mathcal{E} \mapsto \mathbb{R}$, then for each ν_j, $j = 1, \ldots, n$, we set $\mathcal{G}_{\leq \nu_j} = (\mathcal{V}, \mathcal{E}, w^{-1}(-\infty, \nu_j])$, yielding the induced edge-weighted filtration. We can also consider only induced subgraphs of $\mathcal{G}$ with maximal degree of ν_j for each $j = 1, \ldots, n$, resulting in the degree sublevel set filtration. (For more discussion on graph filtrations see [21].) Armed with this construction, we can track which shape patterns, for example, independent components, loops, and voids, emerge as scale ν varies. To make the process of pattern counting more systematic and efficient, we build an abstract simplicial complex $\mathscr{K}(\mathcal{G}_j)$ on each $\mathcal{G}_j$. We also record complex indices j_b (birth) and j_d (death) at which we first or last observe each shape feature. Topological features with longer lifespan are said to persist and likelier to yield important information on the structural organization of $\mathcal{G}$.

Learning Shapes of Time-Conditioned Data with Zigzag Persistence This construction enables us to extract the key topological descriptors from a single graph $\mathcal{G}$. However, in our case we observe not a single graph but a sequence of time-evolving graphs $\{\mathcal{G}^1, \ldots, \mathcal{G}^{\mathcal{T}}\}$. How can we track shape signatures which are not just individualistic for each time stamp but characterize intrinsic properties of the observed object over time? One approach how we can bring PH tools to analysis of time-conditioned objects is zigzag persistence. Based on the theory of quiver representations, zigzag persistence generalizes ordinary persistence to tracking characteristics of graphs (or other topological spaces) with inclusions going in different directions [10, 9]. In particular, given a time-indexed sequence of graphs $\{\mathcal{G}^1, \ldots, \mathcal{G}^{\mathcal{T}}\}$, we first form a set of graph inclusions over time

$$\begin{tikzcd}
 & \mathcal{G}_1 \cup \mathcal{G}_2 & & \mathcal{G}_2 \cup \mathcal{G}_3 & & \mathcal{G}_3 \cup \mathcal{G}_4 & & \ldots \\
\mathcal{G}_1 \arrow[ur] & & \mathcal{G}_2 \arrow[ul] \arrow[ur] & & \mathcal{G}_3 \arrow[ul] \arrow[ur] & & \mathcal{G}_4 \arrow[ul] \arrow[ur] &
\end{tikzcd}$$

and then assess compatibility of persistent topological features across unions of graphs. That is, we record indices at which topological features (dis)appear, for some given scale ν_*. If for a given ν_* topological feature ρ (i.e., p-dimensional hole, $0 \leq p \leq \mathcal{K}$, where $\mathcal{K}$ is the dimension of the simplicial complex $\mathbb{K}(\mathcal{G})$) is first recorded in $\mathbb{K}(\mathcal{G}^j)$, we say that the feature's birth is j, and if ρ first appears in $\mathbb{K}(\mathcal{G}^j \cup \mathcal{G}^{j+1})$, we record its birth as $j + 1/2$. In turn, if ρ is last seen in $\mathbb{K}(\mathcal{G}^j)$, we record its death as j, while if it is last seen in $\mathbb{K}(\mathcal{G}^j \cup \mathcal{G}^{j+1})$, we say that its death is at $j + 1/2$. Let $\mathfrak{J}$ be the set of all observed topological features for a given ν_*. Collecting then births and deaths over $\mathfrak{J}$, we

summarize all extracted information as a multiset $\mathcal{D}_{\nu_*} = \{(b_\rho, d_\rho) \in \mathbb{R}^2 | b_\rho < d_\rho, \rho \in \mathfrak{J}\}$, called a zigzag persistent diagram (ZPD) (where b_ρ and d_ρ are the birth and death of the topological feature ρ respectively).

This makes zigzag persistence particularly attractive for analysis of dynamic objects which are naturally indexed by time. However, the idea of zigzag persistence is an applicable way beyond learning time-evolving objects. Nevertheless, zigzag persistence still remains largely a theoretical concept, with yet only a handful of applications, and one of the roadblocks hindering a broader proliferation of zigzag-based methods in practice is their computational costs. Here we make a step toward bringing more computationally efficient summary of zigzag persistence to real world applications.

Time-Aware Zigzag Filtration Curves Consider a sequence of time intervals associated with a zigzag filtration over time period $[t_1, t_\mathcal{N}]$

$$\left(t_1, t_1 + \frac{1}{2}\right), \left(t_1 + \frac{1}{2}, t_2\right), \left(t_2, t_2 + \frac{1}{2}\right), \ldots, \left(t_{\mathcal{N}-1} + \frac{1}{2}, t_\mathcal{N}\right).$$

Let DgmZZ_{ν_*} be the resulting ZPD for a given ν_* and $\mathcal{M}$ be the number of off-diagonal topological features in ZPD, i.e., DgmZZ_{ν_*}. Inspired by the recent results on stabilized Betti sequences by [23] and filtration curves by [29] for ordinary persistence, we propose a new simple and computationally efficient summary of zigzag persistence, called *Zigzag Filtration Curve*.

Definition 3.1 (Zigzag Filtration Curve (ZFC))**.** The zigzag filtration curve evaluated at $\Delta t_i^- = (t_{i-1} + \frac{1}{2}, t_i)$, $i = \{1, 2, \ldots, \mathcal{N}\}$, for a given ν_*, is defined as

$$\text{ZFC}^p_{\nu_*}(\Delta t_i^-) = \sum_{j=1}^{\mathcal{M}} \xi_i(t_{b_j}, t_{d_j})\omega_i,$$

where $(t_{b_j}, t_{d_j}) \in \mathbb{R}^2$ is a vector containing birth and death of the j-th off-diagonal p-dimensional topological feature in DgmZZ_{ν_*} (as such, $t_{b_j} < t_{d_j}$), $j = \{1, 2, \ldots, \mathcal{M}\}$, $0 \leq p \leq \mathcal{K}$; $\xi_i : \mathbb{R}^2 \mapsto \mathbb{R}$ is some suitable Lipschitz continuous function with Lipschitz constant L_i, for example, Gaussian density; and $\omega_i > 0$, $i = \{1, 2, \ldots, \mathcal{N}\}$ are weights such that $\sum_i \omega_i = 1$. Zigzag filtration curve at $\Delta t_i^+ = (t_i, t_i + \frac{1}{2})$ is defined analogously. (For sake of notation, wherever applicable in the further exposition we suppress index p in ZFC.)

Motivated by [23], here as Lipschitz continuous function ξ_i for intervals Δt_i^-, we use a Gaussian density f with mean $(t_{i-1} + 1/2, t_i)$, while for intervals Δt_i^+, we set mean of f to $(t_i, t_i + 1/2)$, $i = 1, 2, \ldots \mathcal{N}$. For both Δt_i^- and Δt_i^+, we set a 2×2-variance-covariance matrix Σ as identity matrix. (See Appendix C.5 for more discussion on sensitivity analysis.) Other suitable choice of ξ include arctan function.

As we show below, the proposed ZPC also enjoys the important theoretical stability guarantees in terms of Wasserstein-1 distance.

Proposition 3.2 (Stability of Zigzag Filtration Curve)**.** *Let DgmZZ_{ν_*} be a zigzag persistence diagram and DgmZZ'_{c_*} be its perturbed copy such that $\mathcal{W}_1\big(\text{DgmZZ}_{\nu_*}, \text{DgmZZ}'_{\nu_*}\big) < \epsilon$, where $\mathcal{W}_1$ is Wasserstein-1 distance. Then, ZFC is stable with respect to Wasserstein-1 distance.*

In practice topological features of various dimensions p, $p = 0, 1, \ldots, \mathcal{K}$, may play different roles in the learning task performance, and these roles are not known a-priori. Hence, to harness time-conditioned information encoded in ZFC corresponding to different dimensions p, we propose Multi-Zigzag Filtration Curves (M-ZFCs) $\text{M-ZFCs}_{\nu_*} \in \mathbb{R}^{K \times \frac{\mathcal{N}-1}{2}}$ by stacking $\text{ZFC}^0, \text{ZFC}^1, \ldots, \text{ZFC}^\mathcal{K}$. Figure 1 in Appendix B shows the both 0- and 1-dimensional ZFCs obtained from the proposed ZFC.

4 Zigzag Filtration Curve based Supra-Hodge Convolution Networks

Given a graph $\mathcal{G}$ and its historical ω step graph signals $\boldsymbol{X}^\omega = \{\boldsymbol{X}_{t-\omega+1}, \ldots, \boldsymbol{X}_t\} \in \mathbb{R}^{\omega \times N \times F}$ (F is the node feature dimensionality), the time-series forecasting problem is to learn a mapping function f which maps the historical data $\{\boldsymbol{X}_{t-\omega+1}, \ldots, \boldsymbol{X}_t\}$ into the next h step data $\{\boldsymbol{X}_{t+1}, \ldots, \boldsymbol{X}_{t+h}\}$. The mapping relation is represented as follows $\{\boldsymbol{X}_{t-\omega+1}, \ldots, \boldsymbol{X}_t\} \xrightarrow{f} \{\boldsymbol{X}_{t+1}, \ldots, \boldsymbol{X}_{t+h}\}$.

4.1 Graph convolution in spatial dimension

Given the node embedding dictionary $\boldsymbol{W}^{\phi} = (w_1^{\phi}, w_2^{\phi}, \ldots, w_N^{\phi}) \in \mathbb{R}^{N \times d_c}$ (where $x_u^{\phi} \in \mathbb{R}^{d_c}$ and d_c is the dimension of node embedding), we aim to seek a non-negative function $\boldsymbol{S}_{u,v} = \mathscr{G}(w_u^{\phi}, w_v^{\phi})$ which represents the pairwise similarity between any two nodes u and v. Concretely, the multiplication between $\boldsymbol{W}^{\phi}$ and $(\boldsymbol{W}^{\phi})^{\top}$ can (i) give a sum pooling of second-order features from the outer product of all the embedding vector pairs (w_u^{ϕ}, w_v^{ϕ}) and (ii) infer the hidden spatial dependencies of nodes

$$\boldsymbol{S}_{uv} = \mathscr{G}(w_u^{\phi}, w_v^{\phi}) = \frac{\exp\left(\text{ReLU}(w_u^{\phi}(w_v^{\phi})^{\top}\right)}{\sum_{u=1}^{N} \exp\left(\text{ReLU}(w_u^{\phi}(w_v^{\phi})^{\top}\right)},$$

where $\text{ReLU}(\cdot) = \max(0, \cdot)$ is a nonlinear activation function, which is used to eliminate weak connections proactively, and the role of the softmax function is applied to normalized the learned graph $\boldsymbol{S}$. Inspired by the recent advancements in random walk-based graph embedding learning [32, 19], we make a graph convolution in spatial dimension, feeding a power series of learned graph $\boldsymbol{S}$ with varying random walk steps $\{1, 2, \cdots, r\}$ ($r \in \mathbb{Z}_+$), as follows

$$\boldsymbol{H}_{t,\text{GC}}^{(\ell+1)} = \sigma(\text{Stack}(\boldsymbol{I}, \boldsymbol{S}, \cdots, \boldsymbol{S}^r)\boldsymbol{H}_{t,\text{GC}}^{(\ell)}\boldsymbol{\Theta}_{\text{GC}}^{(\ell)}), \tag{1}$$

where $\sigma(\cdot)$ stands for a nonlinear activation function, $\text{Stack}(\cdot)$ is the function which stacks r powered learned graphs, $\boldsymbol{H}_{t,\text{GC}}^{(\ell)}$ and $\boldsymbol{H}_{t,\text{GC}}^{(\ell+1)}$ are the input and output activations for layer ℓ (where $\boldsymbol{H}_{t,\text{GC}}^{(0)} = \boldsymbol{X}_t \in \mathbb{R}^{N \times F}$), and $\boldsymbol{\Theta}_{\text{GC}}^{(\ell)} \in \mathbb{R}^{d_{\ell}^{\text{GC}} \times d_{\ell+1}^{\text{GC}}}$ is the ℓ-th layer's trainable weights.

4.2 ZFC convolution: a bridge between spatial and time dimensions

To preserve and propagate both spatial and time-aware topological information simultaneously, the ZFC convolution is proposed. The intuition behind ZFC convolution is that learn a strong connection between two dimensions via two 1D convolution layers, i.e., time-wise and node-wise. ZFC convolution consists of three key components: (i) a linear embedding on M-ZFCs, which can learn the importance of time-aware topological features for each node to form a time-dimension-specific node embedding; (ii) a 1D convolution layer along time-wise, where it gathers time-aware topological features from the entire space into a compact set; (iii) a 1D convolution layer along node-wise, where can capture relations between different nodes. The resulted ZFC convolution operation over a M-ZFCs$^{\omega}$ is defined as

$$\boldsymbol{H}_{t,\text{ZFC}} = \mathscr{F}_{\theta}(\mathscr{F}_{\psi}(\boldsymbol{\Theta}_{\text{ZFC}}\text{M-ZFCs}^{\omega})^{\top})^{\top}, \tag{2}$$

where ω is the size of the window for sequence learning, M-ZFCs$^{\omega}$ denotes the M-ZFCs feature extracted from the time window with size ω, $\boldsymbol{\Theta}_{\text{ZFC}} \in \mathbb{R}^{N \times d_q}$ is a weight matrix to be learned, $\mathscr{F}_{\theta}$ and $\mathscr{F}_{\psi}$ are 1D convolutional layers, and $\boldsymbol{H}_{t,\text{ZFC}} \in \mathbb{R}^{N \times d_{\text{out}}^{\text{ZFC}}}$ is the $d_{\text{out}}^{\text{ZFC}}$-dimensional output.

4.3 Supra-Hodge convolution in temporal dimension

Time-evolving data such as multivariate time series, spatio-temporal processes, and dynamic networks, often exhibit a highly complex dependency among its substructures which is way beyond what can be described by dyadic interactions or pairwise relations among nodes. Instead, such higher-order polyadic interactions can be systematically addressed using the Hodge Theory. In particular, the discrete Hodge theory allows us to generalize the notion of a standard combinatorial graph Laplacian which describes diffusion on graph $\mathcal{G}$ from node to node via edges to diffusion over higher-order substructures of $\mathcal{G}$ [28, 6]. In turn, higher-order substructures can be modeled as k-simplices of $\mathcal{G}$. (See Appendix B for the background information on the Hodge Laplacians.) In the last year, convolutional architectures on simplicial complexes based on the associated concepts of the Hodge theory have emerged as the most recent direction in graph neural networks but have never been yet applied to learning time-evolving data. Our goal here is to introduce the notion of simplicial convolution and the ideas of Hodge-Laplacians to time-aware learning.

In particular, to capture time-conditioned higher-order interactions on $\mathcal{G}$ and to describe diffusion of information over simplices along the temporal dimension, we build a supra-Hodge convolution operation, based on the multiplex network representation learning. (In the following for simplicity, we assume the notations without sub/superscript k stands for node-level and in our experiments we always consider $k \in \mathbb{Z}_+$).

First, given the historical spatio-temporal network series $\boldsymbol{\mathcal{G}}_{t-\omega+1:t} = \{\mathcal{G}_{t-\omega+1}, \mathcal{G}_{t-\omega+2}, \ldots, \mathcal{G}_t\}$, we consider a directed connected node-aligned multiplex network, which is made up of ω layers with N nodes on each layer. That is, adjacency matrix $\boldsymbol{\mathcal{A}}^{\alpha} = \{a^{\alpha}_{uv}\}_{N\times N}$ (where $\alpha \in \{t-\omega+1, \ldots, t\}$) defines the intra-connection between nodes u and v in layer α and a distance matrix $\boldsymbol{\mathcal{D}}^{\alpha\beta} = \{d^{\alpha\beta}_{uu}\}_{N\times N}$ quantifies the transition probability of moving from node u of layer α to node u of layer β. (Here $\beta > \alpha$, since we consider information diffusion procedures only along the temporal dimension). Next, based on the discrete Hodge theory, we propose a new Hodge k-Laplacian for multiplex graphs, called *supra-Hodge k-Laplacian* $\boldsymbol{\mathcal{L}}^{Sup}_k \in \mathbb{R}^{\phi_k\omega\times\phi_k\omega}$

$$\boldsymbol{\mathcal{L}}^{\text{Sup}}_k = \begin{pmatrix} (\boldsymbol{\mathcal{L}}^{11}_k)^r & \boldsymbol{D}^{12}_{k+1} & \cdots & \boldsymbol{D}^{1\omega}_{k+1} \\ \boldsymbol{0} & (\boldsymbol{\mathcal{L}}^{22}_k)^r & \cdots & \boldsymbol{D}^{2\omega}_{k+1} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & (\boldsymbol{\mathcal{L}}^{\omega\omega}_k)^r \end{pmatrix}, \tag{3}$$

where $\boldsymbol{\mathcal{L}}^{\alpha\alpha}_k$ is the Hodge k-Laplacian in layer α, $\boldsymbol{D}_{k+1}$ is the diagonal matrix of degrees of each k-simplex, i.e., $\boldsymbol{D}_{k+1} = \max\left(\text{diag}(|\boldsymbol{B}_{k+1}|\boldsymbol{1}, \boldsymbol{I})\right)$ and $\boldsymbol{B}_{k+1}$ is the k-simplex-to-$(k+1)$-simplex incidence matrix, and r-th of $\boldsymbol{\mathcal{L}}^{\alpha\alpha}_k$ represents r-step random walk on Hodge k-Laplacian of layer α which will allow every k-simplex to accumulate information from its neighbors. Hence, when $k = 1$, we can infer the spatial dependencies between each pair of edges and capture meaningful edge information in both spatial and temporal dimensions – through the lens of supra-Hodge 1-Laplacian. For instance, in molecule networks, each node represents an atom and each edge is a bond connecting two atoms; the bond (i.e., edge) features include bond type, ring status, molecular charge which are closely related to atom (i.e., node) features (such as atomic total and partial charges).

Since the goal of forecasting task is to predict node (i.e., 0-simplex) attribute(s) in the next few time steps, we propose a novel diffusion supra-Hodge convolution on the sliding window $\boldsymbol{\mathcal{G}}_{t-\omega+1:t}$. We then update nodes' representations by transforming the multiplex k-simplex embedding to nodes via incidence matrices

$$\boldsymbol{H}^{(\ell+1)}_{t,k,\text{SH}} = \sigma(\boldsymbol{\mathcal{L}}^{\text{Sup}}_k \boldsymbol{H}^{(\ell)}_{t,k,\text{SH}} \boldsymbol{\Theta}^{(\ell)}_{k,\text{SH}}), \tag{4}$$

$$\boldsymbol{H}^{(\ell+1)}_{t,\text{SH}} = (\boldsymbol{B}^{\top}_1 \cdots \boldsymbol{B}^{\top}_k)\boldsymbol{H}^{(\ell+1)}_{t,k,\text{SH}}, \tag{5}$$

where (i) in Equation 4: $\boldsymbol{\Theta}^{(\ell)}_{k,\text{SH}} \in \mathbb{R}^{d^{\text{SH}}_{k;\ell}\times d^{\text{SH}}_{k;\ell+1}}$ is a learnable filter matrix for layer ℓ (here $d^{\text{SH}}_{k;\ell}$ and $d^{\text{SH}}_{k;\ell+1}$ are the intermediate and output dimensions to the ℓ-th layer), $\boldsymbol{H}^{(\ell)}_{t,k,\text{SH}}$ and $\boldsymbol{H}^{(\ell+1)}_{t,k,\text{SH}}$ are the input and output activations for layer ℓ (where $\boldsymbol{H}^{(0)}_{t,k,\text{SH}} = \bar{\boldsymbol{X}}_{k;t-\omega+1:t} \in \mathbb{R}^{\phi_k\omega\times d^{\text{in}}_k}$ and the historical k-simplex features of the spatio-temporal networks $\boldsymbol{X}_{k;t-\omega+1:t} = \{\boldsymbol{X}_{k;t-\omega+1}, \boldsymbol{X}_{k;t-\omega+2}, \ldots, \boldsymbol{X}_{k;t}\} \in \mathbb{R}^{\phi_k\times\omega\times d^{\text{in}}_k}$ is reshaped as a matrix $\bar{\boldsymbol{X}}_{k;t-\omega+1:t}$ with shape $\phi_k\omega \times d^{\text{in}}_k$) and (ii) in Equation 5: we transform the k-simplex embedding $\boldsymbol{H}^{(\ell+1)}_{t,k,\text{SH}}$ to node embedding $\boldsymbol{H}^{(\ell+1)}_{t,\text{SH}} \in \mathbb{R}^{N\times d^{\text{SH}}_{k;\ell+1}}$ through incidence matrices. We then combine the embeddings from graph convolution, M-ZFCs convolution, and Supra-Hodge convolution to get the final embedding $\boldsymbol{H}^{(\ell+1)}_{t,\text{out}}$

$$\boldsymbol{H}^{(\ell+1)}_{t,\text{out}} = [\boldsymbol{H}^{(\ell+1)}_{t,\text{GC}}, \boldsymbol{H}_{t,\text{M-ZFCs}}, \boldsymbol{H}^{(\ell+1)}_{t,\text{SH}}], \tag{6}$$

where $[\cdot,\cdot,\cdot]$ denotes the concatenation of the outputs from three convolution operations, and $\boldsymbol{H}^{(\ell+1)}_{t,\text{out}} \in \mathbb{R}^{N\times d_{\text{out}}}$ (where $d_{\text{out}} = d^{\text{GC}}_{\ell+1} + d^{\text{ZFC}}_{\text{out}} + d^{\text{SH}}_{\ell+1}$).

4.4 Gate Recurrent Unit with ZFC-SHCN

To describe the complex spatio-temporal dependencies among time series and assess a hidden state of nodes at a future timestamp, we feed the final embedding $\boldsymbol{H}^{(\ell+1)}_{t,\text{out}}$ into Gated Recurrent Units (GRU). Formally, we set the forward propagation equations of GRU as

$$\begin{aligned} \boldsymbol{\Re}_t &= \eta\left(\boldsymbol{W}_{\Re}\left[\boldsymbol{\Psi}_{t-1}, \boldsymbol{H}^{(\ell+1)}_{t,\text{out}}\right] + \boldsymbol{b}_{\Re}\right), \qquad \boldsymbol{\Im}_t = \eta\left(\boldsymbol{W}_{\Im}\left[\boldsymbol{\Psi}_{t-1}, \boldsymbol{H}^{(\ell+1)}_{t,\text{out}}\right] + \boldsymbol{b}_{\Im}\right), \\ \boldsymbol{\Psi}_t &= \tanh\left(\boldsymbol{W}_{\Psi}\left[\boldsymbol{\Im}_t \odot \boldsymbol{\Psi}_{t-1}, \quad \boldsymbol{H}^{(\ell+1)}_{t,\text{out}}\right] + \boldsymbol{b}_{\Psi}\right), \quad \tilde{\boldsymbol{\Psi}}_t = \boldsymbol{\Re}_i \odot \boldsymbol{\Psi}_{t-1} + (1-\boldsymbol{\Re}_t)\odot\boldsymbol{\Psi}_t, \end{aligned}$$

where $\eta(\cdot)$ is an activation function (e.g., ReLU, LeakyReLU), $\odot$ is the elementwise product, $\boldsymbol{\Re}_t$ is the update gate and $\boldsymbol{\Im}_i$ is the reset gate. Here $\boldsymbol{b}_{\Re}$, $\boldsymbol{b}_{\Im}$, $\boldsymbol{b}_{\Psi}$, $\boldsymbol{W}_{\Re}$, $\boldsymbol{W}_{\Im}$, and $\boldsymbol{W}_{\Psi}$ are learnable

parameters, while $\left[\boldsymbol{\Psi}_{t-1}, \boldsymbol{H}_{t,\text{out}}^{(\ell+1)}\right]$ and $\boldsymbol{\Psi}_t$ are the input and output of GRU model, respectively. We then obtain $\tilde{\boldsymbol{\Psi}}_t$ which contains both the spatio-temporal and time-aware information.

5 Experiments

5.1 Datasets

We validate our ZFC-SHCN model on five diverse data types: (i) COVID-19 datasets [36]: CA, PA, and TX represent the number of COVID-19 hospitalizations in California (CA), Pennsylvania (PA), and Texas (TX) respectively; (ii) traffic datasets [11]: PeMSD4 and PeMSD8 are two real time traffic datasets in California; (iii) synthetic multivariate time-series (MTS) datasets based on vector autoregression (VAR) [20, 30] (where the VAR model is a generalization of the univariate AR process with more than one time-evolving component); (iv) daily surface air temperature in CA, PA, and TX over 02/01/2020–12/31/2020, and (v) Bytom token prices of Ethereum blockchain over 07/27/2017–05/07/2018. The results on (i)–(iii) are presented in the main body, and the analysis on (iv) and (v) are in Appendix C.2 and C.4. The detailed description of each dataset is in Appendix C.1.

5.2 Baselines

We compare our proposed ZFC-SHCN with 14 types of state-of-the-art baselines (SOAs), including FC-LSTM [38], SFM [42], N-BEATS [31], DCRNN [27], LSTNet [25], STGCN [41], TCN [4], DeepState [33], GraphWaveNet [40], DeepGLO [37], LRGCN [26] AGCRN [3], StemGNN [8], and Z-GCNETs [14].

5.3 Experimental settings

We implement ZFC-SHCN with Pytorch framework on NVIDIA GeForce RTX 3090 GPU. We optimize all the models by Adam optimizer for maximum of 200 epochs. The learning rate is searched in $\{0.001, 0.003, 0.005, 0.01, 0.05\}$ and the embedding dimension is searched in $\{1, 2, 3, 5, 10\}$. Our ZFC-SHCN is trained with batch sizes of 64 and 8 on PeMSD4 and PeMSD8, respectively. On both COVID-19 and surface air temperature datasets (i.e., CA, PA, and TX), we set the batch size to be 8. We train two 1D convolutional layers for ZFC representation learning with the same hidden layer dimension $nhid$ where $nhid \in \{8, 16, 32, 64, 128\}$. For PeMSD4 and PeMSD8, we consider the window size $\omega = 12$ and the horizon $h = 3$; for both COVID-19 and surface air temperature datasets, we consider window size $\omega = 5$ and horizon $h = 15$; for two simulated VAR datasets VAR_{T_1} and VAR_{T_2}, we set the window size as $\omega = 10$ and horizon as $h = 5$, and set the batch size as 8; for Bytom, we consider the window size $\omega = 7$ and horizon $h = 7$, and set the batch size as 8. All models are evaluated in terms of Mean Absolute Error (MAE), Root Mean Square Error (RMSE), and Mean Absolute Percentage Error (MAPE). The best results are in **bold** font and the results with *dotted underline* are the best performance achieved by the runner-ups. We also perform a one-sided two-sample t-test between the best result and the best performance achieved by the runner-up, where *, **, *** denote p-value < 0.1, 0.05, 0.01 (i.e., denote significant, statistically significant, highly statistically significant results, respectively. The source code is available at `https://www.dropbox.com/sh/9wmwhkgabqqry0r/AAACZdPI_ja5UpoWXJ-zi0eva?dl=0`.

5.4 Experimental results

Real datasets The experimental results on PeMSD4 and PeMSD8 traffic data are reported in Table 2. As Table 2 shows, ZFC-SHCN achieves the best MAE, RMSE, and MAPE compared with SOAs on both PeMSD4 and PeMSD8. Compared to the RNN-based methods such as FC-LSTM, SFM, N-BEATS, LSTNet, and TCN, ZFC-SHCN achieves relative gains in RMSE over the runner-ups, ranging from 17.68% to 65.41% for both PeMSD4 and PeMSD8. In turn, DCRNN, STGCN, GraphWaveNet, AGCRN, and StemGNN only focus on learning node-level representations. Compared to them, ZFC-SHCN captures interactions and encodes higher-order structures correlations beyond pairwise relations among nodes and yields a relative gain from 2.06% to 5.63% in RMSE on the traffic datasets. In addition, we compare ZFC-SHCN with the method based on zigzag persistence image, i.e., Z-GCNETs, and find that ZFC-SHCN outperforms Z-GCNETs

by 1.75% on PeMSD4 and 5.36% on PeMSD8 in terms of RMSE. Table 3 presents COVID-19 hospitalization prediction results (RMSE) in CA, PA, and TX, and we observe the following findings. First, our proposed ZFC-SHCN achieves state-of-the-art performance on all three datasets. For instance, ZFC-SHCN yields 3.61%, 1.47%, 65.55% relative gains in RMSE over the runner-ups (including both GCN-based and zigzag persistence image-based methods) on three biosurveillance datasets. These results indicate that the ZFC mechanism and higher-order representation learning module play significant roles in capturing both topological information and higher-order structures. Second, as shown in Figure 2 in Appendix C, we find that, compared to the runner-up (i.e., Z-GCNETs), the predicted value of COVID-19 hospitalizations is more consistent with the ground-truth. Finally, Tables 3 and 4 in Appendix C present the overall prediction performances of ZFC-SHCN and representative baselines on surface air temperature and Ethereum blockchain datasets. We find that our proposed ZFC-SHCN consistently outperforms all baselines with either a significant or (highly) statistically significant margin across all data, except surface air temperature in TX, where ZFC-SHCN still yields the best performance across all models.

Table 1: Forecasting performance (RMSE) of ZFC-SHCN and top three baselines on synthetic time series following vector autoregressions (VAR).

Model	**VAR**$_{T_1}$	**VAR**$_{T_2}$
AGCRN [3]	0.50±0.03	0.44±0.02
StemGNN [8]	0.51±0.02	0.42±0.02
Z-GCNETs [14]	0.49±0.02	0.44±0.01
ZFC-SHCN (ours)	*****0.45±0.01**	*****0.38±0.01**

Table 2: Performance on PEMSD4 and PEMSD8 traffic data. Standard deviations are reported in Table 1 in Appendix C, for sake of space.

Model	**PeMSD4**			**PeMSD8**		
	MAE	RMSE	MAPE (%)	MAE	RMSE	MAPE (%)
FC-LSTM [38]	27.14	41.59	18.20	22.20	34.06	14.20
SFM [42]	24.36	37.10	17.20	16.01	27.41	10.40
N-BEATS [31]	25.56	39.90	17.18	19.48	28.32	13.50
DCRNN [27]	24.70	38.12	17.12	17.86	27.83	11.45
LSTNet [25]	24.04	37.38	17.01	20.26	31.96	11.30
STGCN [41]	22.70	35.50	14.59	18.02	27.83	11.40
TCN [4]	26.31	36.11	15.62	15.93	25.69	16.50
DeepState [33]	26.50	33.00	15.40	19.34	27.18	16.00
GraphWaveNet [40]	26.85	39.70	17.29	19.13	28.16	12.68
DeepGLO [37]	25.45	35.90	12.20	15.12	25.22	13.20
AGCRN [3]	17.78	29.17	11.79	14.59	23.06	9.29
StemGNN [8]	20.20	31.83	12.00	15.83	24.93	9.26
Z-GCNETs [14]	18.05	29.08	11.79	14.52	23.00	9.28
ZFC-SHCN (ours)	*****17.58**	*****28.58**	*****11.68**	*****13.86**	*****21.83**	*****8.92**

Table 3: Performance on COVID-19 hospitalizations in CA, PA and TX.

Model	**CA**			**PA**			**TX**		
	MAE	RMSE	MAPE (%)	MAE	RMSE	MAPE (%)	MAE	RMSE	MAPE (%)
FC-LSTM [38]	167.86±3.25	502.29±4.16	90.71±7.17	47.60±2.36	108.74±2.28	69.37±2.38	20.75±0.50	71.66±2.15	89.16±8.96
SFM [42]	103.98±1.46	475.66±3.23	66.91±5.70	45.91±2.42	106.12±1.87	70.15±5.60	17.49±0.58	70.18±1.91	85.85±8.25
N-BEATS [31]	105.99±1.51	476.10±2.89	67.55±5.16	46.91±2.82	105.86±1.95	15.82±4.39	21.25±0.56	69.26±1.61	85.11±8.77
DCRNN [27]	107.20±1.00	492.10±2.96	69.83±5.57	47.49±2.13	107.21±1.63	67.15±3.94	17.15±0.55	70.47±2.28	88.95±8.01
LSTNet [25]	105.63±1.82	480.61±3.91	67.72±2.17	46.01±2.70	105.67±1.76	72.33±4.21	13.06±0.53	72.93±2.20	84.23±9.01
STGCN [41]	102.88±1.11	470.52±3.06	69.73±5.69	52.69±2.40	106.78±1.87	69.36±4.59	12.69±0.49	63.26±2.25	60.47±8.37
TCN [4]	110.82±1.35	492.82±3.54	70.00±6.92	49.80±2.36	105.07±1.90	69.86±4.91	13.70±0.40	67.08±1.89	65.23±8.61
DeepState [33]	100.57±1.58	469.15±3.71	68.24±5.79	48.46±2.70	107.61±2.31	67.69±4.21	13.24±0.46	59.47±1.93	62.38±8.60
GraphWaveNet [40]	89.64±1.80	394.83±3.35	67.61±5.36	48.08±2.18	109.41±1.91	69.39±4.27	12.66±0.56	58.98±1.22	60.33±8.87
DeepGLO [37]	95.58±1.94	455.80±3.18	67.35±5.99	47.66±2.57	103.74±2.07	68.71±4.09	12.02±0.60	53.09±1.97	62.88±8.83
AGCRN [3]	87.24±1.77	448.27±2.78	66.30±5.17	44.69±2.49	103.79±3.08	63.45±4.00	10.93±0.49	52.96±3.92	59.92±8.99
StemGNN [8]	82.36±2.23	377.25±3.91	67.90±5.94	42.98±2.80	103.15±1.87	63.47±4.11	9.57±0.80	51.00±2.60	59.60±8.81
Z-GCNETs [14]	81.22±2.15	356.35±3.20	62.81±5.75	43.52±2.20	106.22±1.27	65.89±4.66	9.37±0.50	46.04±1.78	59.21±8.73
ZFC-SHCN (ours)	**79.33±1.70**	****343.92±3.66**	**61.25±5.80**	**42.74±2.24**	**101.65±1.53**	**61.90±4.07**	****9.20±0.39**	*****27.81±1.72**	**55.34±8.60**

Synthetic datasets The evaluation results on two VAR datasets are summarized in Table 1. Compared to the three strongest baselines (i.e., AGCRN, StemGNN, and Z-GCNETs), we observe that our pro-

posed ZFC-SHCN consistently yields the best performance for all synthetic datasets. More precisely, ZFC-SHCN outperforms the runner-ups from 8.89% to 10.52% for VAR_{T_1} and VAR_{T_2}. Furthermore, to assess the time-wise and high network interactions, we use the global clustering coefficient (GCC) and Euler-Poincaré characteristic (EPC) as measures of higher order substructures [5]. We find that for GCC for VAR_{T_1} and VAR_{T_2} are 4.96 and 5.87, respectively; while the average EPC for VAR_{T_1} and VAR_{T_2} are 7.47 and 6.91, respectively. Interestingly (though intuitively it can be expected), higher GCC and lower EPC tend to be associated with higher relative gains delivered by ZFC-SHCN. Finally, in Appendix C.5 we present the sensitivity analysis for ZFC as a function of covariance matrix in VAR models.

5.5 Ablation studies

To evaluate the performance of different components in our ZFC-SHCN model, we perform an expansive ablation study. The ablation study is made with three setups: (i) ZFC-SHCN without graph convolution in spatial dimension (W/o Graph convolution in spatial dimension), (ii) ZFC-SHCN without ZFC convolution (W/o ZFC convolution), and (iii) ZFC-SHCN without supra-Hodge convolution (W/o Supra-Hodge convolution). The experimental results are shown in Table 4 and prove the validity of each component. As Table 4 indicates, compared to ZFC-SHCN w/o ZFC convolution, the zigzag homological feature is vital for capturing the topological structure of spatio-temporal graph and our proposed graph convolution operation on ZFC significantly improves forecasting performance. By comparing to ZFC-SHCN w/o supra-Hodge convolution, we illustrate the significance of higher-order structures representation learning for guiding the model how to capture information on higher-order interactions. Also, ZFC-SHCN w/o graph convolution in spatial dimension demonstrates that the learned graph obtained from trainable weights can learn hidden information and enhance (multivariate) time-series representation learning.

Table 4: Ablation study on PeMSD4 and COVID-19 hospitalizations in TX.

	Architecture	RMSE
PeMSD4	**ZFC-SHCN**	*****28.58±0.15**
	W/o Graph convolution in spatial dimension	28.82±0.28
	W/o ZFC convolution	28.66±0.20
	W/o Supra-Hodge convolution	28.69±0.19
COVID-19	**ZFC-SHCN**	****27.81±1.72**
	W/o Graph convolution in spatial dimension	29.17±1.73
	W/o ZFC convolution	29.75±1.96
	W/o Supra-Hodge convolution	30.11±1.77

5.6 Computational Complexity

For higher-order simplices, incidence matrices $\boldsymbol{B}_1$ and $\boldsymbol{B}_2$ can be calculated efficiently with the computational complexity $\mathcal{O}(N + M)$ and $\mathcal{O}(M + Q)$ respectively, where N is the number of 0-simplices (i.e., nodes), M is the number of 1-simplices (i.e., edges), and Q is the number of 2-simplices (i.e., filled triangles). The computational complexity of ZFC is $\mathcal{O}(\Upsilon^{\delta})$ [2, 15], where Υ represents the number of points in time interval and $\delta \in [2, 2.373)$. We also compare our ZFC-SHCN with the most recent approach based on multipersistence-GNN [13] (i.e., TAMP-S2GCNets). We find that ZFC-SHCN yields either on-par or more competitive performance than TAMP-S2GCNets, while our proposed ZFC-SHCN significantly improves the computational efficiency (see Appendix C.3 for more details). More details about running time comparison can be found in Appendix C.4.

6 Conclusion

We have proposed a novel framework for time aware deep learning of time-evolving objects which takes the advantages of both the higher-order interactions among the data substructures, described as simplices, and the most intrinsic time-conditioned topological information exhibited by the object, characterized via zigzag persistent homology. By leveraging the power of simplicial convolution operation and zigzag persistence for time-indexed data, ZFC-SHCN is capable to to yield the most competitive forecasting performance, while requiring less computational resources than its closest competitors. Still, computational complexity and limited theoretical results on statistical inference for zigzag persistence remain one of the major existing limitations of ZFC and, more generally, all topological methods for time dependent processes. In the future, we will investigate these theoretical and methodological challenges and will extend the ZFC-SHCN idea to anomaly detection in streaming time-dependent processes.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] See the Conclusion Section 6.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See the Broader Impact Section in Appendix D.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] See Section 3 and Appendix A.
   (b) Did you include complete proofs of all theoretical results? [Yes]
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] See Section 5.3.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Section 5.3.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes]
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See Section 5.3.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
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5. If you used crowdsourcing or conducted research with human subjects...

(a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]

(b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]

(c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]