Simplicial Neural Networks for Path Complexes

Heitor Baldo[*]
University of São Paulo, Brazil
Institute for Globally and Open Education (IGDORE)

Abstract

Simplicial neural networks (SNNs) generalise graph neural networks by performing message passing along simplices arranged in a simplicial complex. Here, we present a straightforward extension of SNNs to path complexes.

1 Introduction

Topological deep learning [7] extends the graph neural networks (GNNs) paradigm to higher-order relational structures, including simplicial complexes, cellular complexes, and hypergraphs. In particular, simplicial neural networks (SNNs) [3, 2, 1] associate a feature vector with each k-simplex and perform message passing through the simplicial Hodge Laplacian, enabling information exchange across different simplex dimensions. However, simplicial complexes are still limited strucutres since every face of a simplex must be present in the complex. This assumption is often unsuitable for directed relational data, such as causal networks, where only selected directed paths are meaningful. To model such data, a more general higher-order structure is required. Path complexes [4, 5] provide such a framework by replacing simplices with directed paths as the fundamental building blocks of the complex.

2 Path Complexes and Path Homologies

Throughtout this text, $G = (V, E)$ denotes a finite digraph with vertex set $V = \{0, \ldots, n-1\}$ and arc set $E \subseteq V \times V$ (no self-loops), and $\mathbb{K}$ denotes a field. The primary bibliography for this part is [4, 5].

Definition 2.1. *An* elementary p-path *on G is a sequence $e_{i_0 \ldots i_p} = (i_0, i_1, \ldots, i_p)$ of vertices such that each consecutive pair $(v_i, v_{i+1}) \in E$. Its* length *is p and it has $p+1$ vertices.*

Unlike a simplex, vertices in an elementary path may repeat (if cycles exist in G), and the ordering is essential.

Definition 2.2. *A p-*path *over a field $\mathbb{K}$ is any formal $\mathbb{K}$-linear combinations of elementary p-paths, that is, any p-path has a form*

$$u = \sum u^{i_0 \cdots i_p} e_{i_0 \ldots i_p},$$

where $u^{i_0 \cdots i_p} \in \mathbb{K}$. We denote by Λ_p the $\mathbb{K}$-linear space of all p-paths.

[*]Email address: heitor.baldo@igdore.org

Example 2.3. $\Lambda_0 = \mathit{Span}\{e_i : i \in V\}$, $\Lambda_1 = \mathit{Span}\{e_{ij} : i, j \in V\}$, $\Lambda_2 = \mathit{Span}\{e_{ijk} : i, j, k \in V\}$.

Morover, we say that an elementary path $e_{i_0 \ldots i_p}$ is *regular* if $i_k \neq i_{k+1}$ for all k, and *irregular* otherwise (some *consecutive* repeat).

Definition 2.4. *For any $p \geq 1$, we define the* p-th boundary operator $\partial_p : \Lambda_p \to \Lambda_{p-1}$ *by*

$$\partial_p e_{i_0 \ldots i_p} = \sum_{q=0}^{p} (-1)^q e_{i_0 \ldots \hat{i_q} \ldots i_p}.$$

For instance, $\partial_1 e_{01} = e_1 - e_0$ and $\partial_2 e_{012} = e_{12} - e_{02} + e_{01}$.

Definition 2.5. *An elementary p-path $i_0 \ldots i_p$ on V is called* allowed *if $i_k \to i_{k+1}$ for any $k = 0, .., p-1$ and* non-allowed *otherwise.*

Definition 2.6. *Let $\mathcal{A}_p$ the $\mathbb{K}$-linear space spanned by allowed elementary p-paths:*

$$\mathcal{A}_p = \mathit{Span}\{e_{i_0 \ldots i_p} : i_0 \ldots i_p \text{ is allowed}\},$$

and consider the following subspace of $\mathcal{A}_p$:

$$\Omega_p = \Omega_p(G) := \{u \in \mathcal{A}_p : \partial u \in \mathcal{A}_{p-1}\}.$$

The elements of Ω_p are called ∂-invariant p-paths.

Hence, we obtain a chain complex of ∂-invariant paths, $\Omega_\bullet = \Omega_\bullet(G)$:

$$0 \leftarrow \Omega_0 \xleftarrow{\partial} \Omega_1 \xleftarrow{\partial} \ldots \xleftarrow{\partial} \Omega_{p-1} \xleftarrow{\partial} \Omega_p \xleftarrow{\partial} \ldots$$

Example: A directed triangle is a sequence of three vertices a, b, c such that $a \to b \to c$, $a \to c$. A directed triangle determines a 2-path $e_{abc} \in \Omega_2$ because $e_{abc} \in \mathcal{A}_2$ and $\partial e_{abc} = e_{bc} - e_{ac} + e_{ab} \in \mathcal{A}_1$.

Definition 2.7. A path complex *over a set V is a non-empty collection $\mathcal{P}$ of (regular) elementary paths on V with the following property:*

- *for any $n \geq 0$, if $i_0 \ldots i_n \in \mathfrak{P}$ then also the truncated paths $i_0 \ldots i_{n-1}$ and $i_1 \ldots i_n$ belong to $\mathcal{P}$.*

Definition 2.8. *Given a* digraph $G = (V, E)$, $E \subseteq \{(i, j) : i \neq j\}$ *(no loops), its path complex $\mathcal{P}(G)$ consists of all regular paths $i_0 \cdots i_p$ that are* walks*: $(i_{k-1}, i_k) \in E$ for every k.*

Note that deleting the first or last vertex of a walk is still a walk, so $\mathcal{P}(G)$ is a path complex. Hence every digraph has a path homology.

Definition 2.9. *The* path homology *of $\mathcal{P}(G)$ is the homology of $(\Omega_\bullet, \bullet)$:*

$$H_p(G) = H_p(\mathcal{P}(G)) = \frac{\ker \partial\big|_{\Omega_p}}{\operatorname{Im} \partial\big|_{\Omega_{p+1}}}.$$

The p-th Betti number is defined as the dimension of the p-th path homology: $\beta_p(G) = \dim H_p(G)$.

3 Combinatorial Hodge Laplacians

We can build Hodge Laplacian operators for path complexes associated with digraphs as follows [6].

Consider an inner product in the spaces Λ_k, $k \geq 0$. Since Ω_k is a subspace of Λ_k, it inherits the inner product. Let $\partial_k : \Omega_k \to \Omega_{k-1}$ be the k-th boundary operator and $\partial_k^* : \Omega_{k-1} \to \Omega_k$ be its adjoint operator. The *Hodge p-Laplacian operator*, $\Delta_k : \Omega_k \to \Omega_k$, is defined by

$$\Delta_k = \partial_{k+1} \circ \partial_{k+1}^* + \partial_k^* \circ \partial_k.$$

The matrix representation of the Hodge k-Laplacian operator is given by

$$[\Delta_k] = B_{k+1}B_{k+1}^T + B_k^T B_k,$$

where $B_k = [\partial_k]$ is the matrix representation of the operator ∂_k. Let δ be the *coboundary* operator δ^* its adjoint operator. Since $[\partial_{k+1}]^T = [\delta_k]$ and $[\delta_k^*] = [\delta_k]^\dagger$, and if $[\delta_k] = A_k$, we can verify the following equalities: $[\delta_k^*\delta_k] = A_k^\dagger A_k$, $[\delta_{k-1}\delta_{k-1}^*] = A_{k-1}A_{k-1}^\dagger$, thus

$$[\Delta_k] = A_{k-1}A_{k-1}^\dagger + A_k^\dagger A_k. \tag{1}$$

4 Simplicial Neural Networks for Path Complexes

In this part, we propose a variant of the simplicial neural network (SNN) [3] for path complexes. This model is a higher-order extension of the graph neural networks (GNNs) paradigma.

Let's use the previously mentioned Hodge k-Laplacians (1) of a path complex $\mathcal{P}$ in terms of their matrices A_k, as they carry valuable topological information about the complex.

If $*$ denotes a convolution, a convolutional layer can be expressed by $\psi \circ (f * \phi_W)$, where ϕ_W is a function with small support parameterized by learnable weights W, and ψ is some nonlinearity and bias. Following Ebli et al. [3], we define the Fourier transform of real p-cochains on a path complex,

$$\mathcal{F}_k(c) = \big(\langle c, e_1\rangle_k, \langle c, e_2\rangle_k, ..., \langle c, e_{|\mathcal{P}_k|}\rangle_k\big), \tag{2}$$

where e_i are the eigencochains of the k-Laplacian $[\Delta_k]$, ordered by eigenvalues $\lambda_1 \leq ... \leq \lambda_{|\mathcal{P}_k|}$.

The function $\mathcal{F}_k$ is inversible since $[\Delta_k]$ is diagonalizable. Thus, for cochains $c, c' \in C^k(\mathcal{P})$ we define their convolution as the cochain $c *_k c' = \mathcal{F}_k^{-1}(\mathcal{F}_k(c)\mathcal{F}_k(c'))$ (pointwise product); we define a simplicial convolutional layer with input p-cochain c and weights W as being of the form $\psi \circ (\mathcal{F}_k^{-1}(\phi_W) *_k c)$. To ensure certain properties, we put, for a small N,

$$\phi_W = \sum_{i=0}^{N} W_i \Lambda^i = \sum_{i=0}^{N} W_i(\lambda_1^i, ..., \lambda_{|K_k|}^i). \tag{3}$$

Then we can write

$$\mathcal{F}_k^{-1}(\phi_W) *_k c = \sum_{i=0}^{N} W_i U \mathrm{diag}(\Lambda^i) U^T c = \sum_{i=0}^{N} W_i (U \mathrm{diag}(\Lambda) U^T)^i c = \sum_{i=0}^{N} W_i [\Delta_k]^i c. \tag{4}$$

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