Simplicial Neural Networks

Author
Affiliation
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Author
Affiliation
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Author
Affiliation
Address
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Abstract

In this paper we present simplicial neural networks (SNNs), a generalization of graph convolutional neural networks to data that live on a class of topological spaces called simplicial complexes. These are natural multi-dimensional extensions of graphs which encode more than just pairwise relationships, namely higher-order relationships between nodes (represented geometrically as filled triangles, tetrahedra, and so forth). We define an appropriate notion of convolutions for such data, which we leverage to construct the desired convolutional neural networks. This allows us to consider richer data than traditional methods, including n-fold collaboration networks and vector field data.

1 Introduction

Graph-based convolutional neural networks (GNNs) have recently become popular techniques in machine learning [[**Stefania says:** cite]]. Compared to classical deep neural networks dealing with regular grid-structured data, graph neural networks take into account irregular graphs to better learn complex interactions in the data. Although graphs can describe complex systems of relations ranging from biology to social science, they are intrinsically limited to modeling pairwise interactions. [[**Stefania says:** rewrite this paragraph, taken from G and mine article]] The success of topological methods in studying data, and the parallel establishment of *topological data analysis (TDA)* as a field [1, 2] (see also [3, 4, 5, 6] for modern introductions and surveys), have confirmed the usefulness of viewing data through a higher-dimensional analog of graphs [7, 8]. Such a higher-dimensional analog is called a *simplicial complex*, a mathematical object whose structure can describe n-fold interactions between points. Their ability to capture hidden patterns in the data has led to various applications from neurobiology [9, 10] to material science [11]. [[**Stefania says:** end paragraph]] In this paper we present *simplicial neural networks (SNNs)*, a novel neural network framework designing local operations that do message passing on simplicial complexes. Our method, like GNNs, offers an efficient architecture thanks to our formulation of strictly localized filters only involving operations with a sparse matrix. Differently from hypergraph neural networks, in SNNs the message passing operator on *simplices* (of a fixed degree) is sensitive to the topological structure of the complex, a highly relevant feature in TDA.

2 Proposed Technique

In this section we introduce the simplicial neural networks (SNNs). The first step to generalize GNNs to simplicial complexes [12] is to design localized convolutional filters on simplicial complexes or equivalently to define a localized message passing operator on simplices. This role will be played by the simplicial laplacians, a well-known operator encoding topological information on the simplcial complex [13], [14].

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2.1 Simplicial Complexes

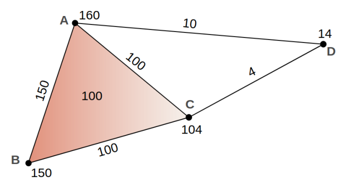
A *simplicial complex* is a collection of finite sets closed under taking subsets. We refer to a set in a simplicial complex as a *simplex* of *dimension* p if it has cardinality $p+1$. Such a p-simplex has $p+1$ *faces* of dimension $p-1$, namely the sets omitting one element, which we will denote as $[v_0, \ldots, \hat{v}_i, \ldots, v_p]$ when omitting the i'th element. While this definition is entirely combinatorial, we will soon see that there is a geometric interpretation, and it will make sense to refer to and think of 0-simplices as *vertices*, 1-simplices as *edges*, 2-simplices as *triangles*, 3-simplices as *tetrahedra*, and so forth (see Figure 1, (b)). Let $C_p(K)$ be the free real vector space with basis K_p, the set of p-simplices in a simplicial complex K. The elements of $C_p(K)$ are called *p-chains*. The p-cochain (vector) space $C^p(K)$ is defined as the dual of $C_p(K)$, i.e. $C^p(K) = \{\hom(K, \mathbb{R})\}$. The basis of C^p is given by the dual basis K_p^*. These vector spaces come equipped with *coboundary maps*, namely linear maps $\delta^p : C_p \to C^{p+1}$ defined by

$$\delta_p(f([v_0, \ldots, v_{p+1}])) = \sum_{i=0}^{p+1} (-1)^i f([v_0, \ldots, \hat{v}_i, \ldots, v_{p+1}])$$

where $\hat{v}_i$ denotes that the i-th vertex has been omitted.

Papers	Authors	Citations
Paper I	A, B, C	100
Paper II	A, B	50
Paper III	A, D	10
Paper IV	C, D	4

(a) Data



(b) Co-authorship complex

$$\begin{array}{cc} \begin{array}{ccccc} \text{AB} & \text{AC} & \text{AD} & \text{BC} & \text{CD} \end{array} & \\ \begin{pmatrix} 3 & 0 & 1 & 0 & 0 \\ 0 & 3 & 1 & 0 & -1 \\ 1 & 1 & 2 & 0 & 1 \\ 0 & 0 & 0 & 3 & -1 \\ 0 & -1 & 1 & -1 & 2 \end{pmatrix} & \begin{array}{c} \text{AB} \\ \text{AC} \\ \text{AD} \\ \text{BC} \\ \text{CD} \end{array} \end{array}$$

(c) 1-Laplacian

Figure 1: Example of co-authorship complex and its 1-Laplacian build from data

2.2 Simplicial Laplacians

We are in this paper concerned with finite simplicial complexes. In particular, it is not necessary for them to come equipped with some embedding into Euclidean space, nor do we demand that they triangulate a Riemannian manifold. To define a discrete version of the Laplacian for simplicial complexes, one simply takes the linear adjoint of the coboundary operator with respect to the inner product, defining $\delta_i^* : C^{i+1} \to C^i$ by

$$\langle \delta_i f_1, f_2 \rangle_{i+1} = \langle f_1, \delta_i^* f_2 \rangle_i \quad \forall f_1 \in C^i(K), f_2 \in C^{i+1}(K).$$

In analogy with Hodge–de Rham theory [15], we then define the *degree-i simplicial Laplacian* of a simplicial complex K as the linear operator $\mathcal{L}_i : C^i(K) \to C_i(K)$ such that

$$\mathcal{L}_i = \mathcal{L}_i^{\text{up}} + \mathcal{L}_i^{\text{down}},$$

where $\mathcal{L}_i^{\text{up}} = \delta_i^* \circ \delta_i$ and $\mathcal{L}_i^{\text{down}} = \delta_{i-1} \circ \delta_{i-1}^*$. In case $i = 0$, $\mathcal{L}_0$ corresponds to the classical graph Laplacian. Observe that there are p Laplacians for a complex of dimension p. In most practical applications, the matrices for the Laplacians are very sparse and can easily be computed as a product of sparse coboundary matrices and their transposes. Since the Laplacians encode information about the adjacency of the simplices, they can be interpreted as a message passing functions. Additionaly, the carry valuable topological information about the simplicial complex. In particular, Eckmann [14] proved that the kernel of the k-Laplacian is isomorphic to the k-(co)homology of its associated simplicial complex. In other words, the number of zero-eigenvalues tells us the number of k-dimensional holes. For a more detailed introduction on this topic we refer the reader to [13].

2.3 Simplicial Neural Networks

Our contribution is a notion of convolution for simplicial complexes using the Laplacian.

- Goal: building a convolutional NN whose input is an arbitrary p-cochain on a fixed simplicial ocmplex K

- Definition of Fourier Transform
- Convolutional Filters: low degree polynomials in the frequency domain
- Implemented using Chebyshev polynomials
- Computational cost: good the p-Laplacian is localized and sparse.
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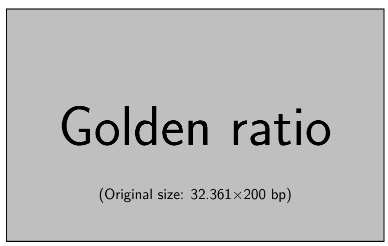

Figure 2: Maybe figures SNN

3 Experimental results

In this section we present preliminary experimental results for the simplicial neural network. The datasets we analyze have been extracted from the Semantic Scholar datasets. The data consists of XXX papers together with their authors and number of citations. We retain paper with more than 5 citations and at most 10 authors.An important step in preprocessing many kinds of input data in TDA is constructing a simplicial complex. Our work focus on *co-authorship complexes* (or *collaboration complexes*) [8], simplicial complexes where a paper with k authors is represented by a $(k-1)$-simplex. We constructed different co-authorship complexes by considering sub-samplings from the papers set of the Semantic Scholar dataset. The sub-samplings were obtained by performing random walks on the nodes of the graph which vertices corresponds to the papers and edges connect papers sharing at least one author. The co-authorship complexes obtained from each sub-sampling have corresponding k cochains given by the number of shared citations of the k-collaborations (see Figure 1).We evaluate the performance of SNNs on the task of predicting missed input data. Specifically, given a fixed co-authorship complex missing data is introduced at random on the training cochains at 4 levels: $10\%, 20\%, 30\%$, and 50%. As in a typical pipeline for this task, in our approach missing data is first replaced by some values. In our case the training input is given by the citations on the co-authorship complex where the random missing data is substituted by the median of the known data. We trained a SNN composed by 3-layers with 30 convolutional filters of degree 5. We used the L_1 norm as reconstruction loss over the known elements an the Adam optimizer with learning rate of 1×10^{-3}. The SNN was trained for 1000 iterations. We then test the performance of the network on its accuracy in predicting the missing data. A predicted citation is considered correct if

(a)

(b)

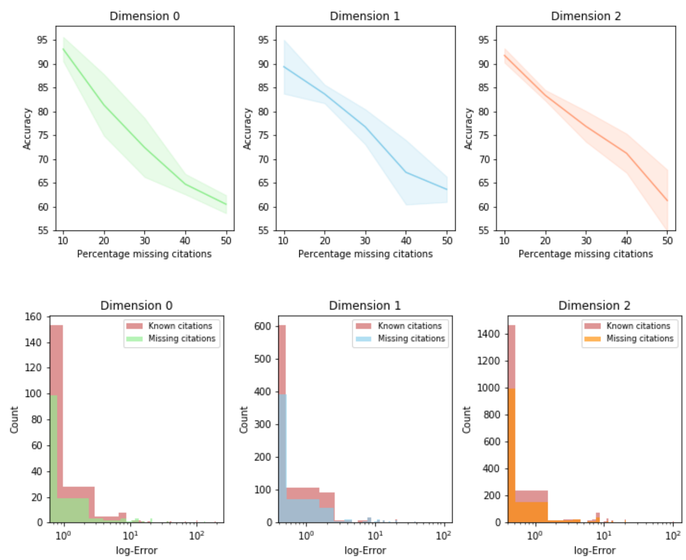

Figure 3: (a) Accuracy of SNN in predicting missing citations. (b)Distribution of the prediction's error

the predicted value differs of at most 1 from the actual number of citations. The prediction error is the absolute value of the difference between the predicted citation and the actual value of the citation. Figure 3 (a) shows the accuracy of the SNN in prediction missing citations on CC1 (Co-authorship Complex 1, Table 1). The distribution of the prediction error is shown in Figure 3. Transfer learning

Table 1: Number of simplices

Dimension	0	1	2	3	4	5	6	7	8	9	10
CC1	352	1474	3285	5019	5559	4547	2732	1175	343	61	5
CC2	1126	5059	11840	18822	21472	17896	10847	4673	1357	238	19

was used as a second assessment for our network. In particular, we test how accurately a SNN pretrained on a co-authorship complex can predict citations on a different complex. Figure 4 shows the accuracy on predicting missing citations on CC1 using the above architecture of SNN trained on CC2 (Co-authorship Complex 2, see Table 1).

[[**Stefania says:** Tell conclusion results, say something about baseline, say something about dimension 2.]]

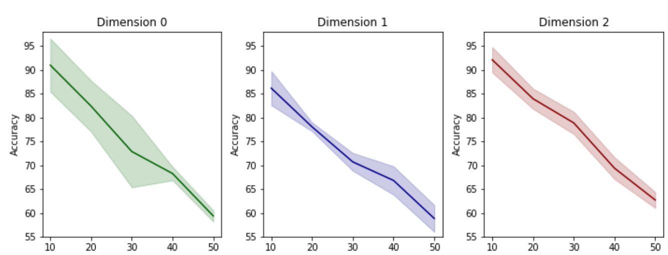

Figure 4: Accuracy in predicting missing citations with a pretrained SNN

4 Conlusion and Future Work

In this work we have introduced a new mathematical framework to design neural networks dealing with simplicial complex and showed preliminary results of their On the computational side, future works will focus on two directions: i)vector field data ii)comparing the results with state of the art techniques As well in the theoretical side we will investigate the following two problem: i) generalizing the processes of coarsening and pooling to SNNs. This will involve developing an efficient higher dimensional clustering algorithm for coarsening and to find a meaningful rearrangement of the clustered k-simplices for an efficient pooling. One possible candidate is the Mapper-algorithm. ii) studying the expressive power of SNNs (like WL-tests) [[**Stefania says:** Say somewhere the code has been implemented in Python using Pytorch?]] [[**Stefania says:** Cite paper missing input data with GNNs]]

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