Simplicial Neural Networks

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Abstract

We generalize graph convolutional neural networks to data that live on a class of topological spaces called simplicial complexes. These are natural multi-dimensional generalizations 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 Neural Networks intro
- Extension to simplicial complexes.
- Simplicial complex represent collaboration on which we have data like citations.
- Preliminary results on vector field data. Where we believe this method can be applied and work?
- Cite work on hypergraphs, message passing.
- Advantage our work: low computational cost, Laplacian an operator encodes topological information has been extensively used in other application eg page ranking. In higher dimension we believe it carries additional information on the simplicial complex.

2 Proposed Technique

FIXME

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.

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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*. These vector spaces come equipped with *boundary maps*, namely linear maps defined by

$$\partial_p : C_p \to C_{p-1}$$

$$\partial_p((v_0, \ldots, v_p)) = \sum_{i=0}^{p} (-1)^i (v_0, \ldots, \hat{v}_i, \ldots, v_p)$$

[[**Stefania says:** Change above with definition of cochain. Cochain in in a grid are pixels. Any diemnsion are the features of our simplices]]

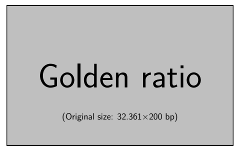

Figure 1: Simplices and cochains

2.2 Combinatorial Laplacians

We are in this paper concerned with finite simplicial complexes, and assume that they are built in a way that encodes useful information about the data being studied. In particular, it is not necessary for it to come equipped with some embedding into Euclidean space, nor do we demand that it triangulates a Riemannian manifold. Therefore dualities like the Hodge star, which is used to construct the Hodge–de Rham Laplacian in the smooth setting [2] that motivates us, are unavailable for our method. The same is true for discrete versions of the Hodge star, such as that of Hirani [1]. To define a discrete version of the Laplacian for simplicial complexes, we simply take the linear adjoint of the boundary operator with respect to the inner product, defining $\partial_i^* : C_{i-1} \to C_i$ by

$$\langle \partial_i^* \sigma, \tau \rangle_i = \langle \sigma, \partial_i \tau \rangle_{i-1} \quad \forall \sigma \in K_{i-1}, \tau \in K_i.$$

In analogy with Hodge–de Rham theory, 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

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

$$\mathcal{L}_i^{\text{up}} = \partial_{i+1} \circ \partial_{i+1}^* : C_i(K) \to C_i(K)$$

$$\mathcal{L}_i^{\text{down}} = \partial_i^* \circ \partial_i : C_i(K) \to C_i(K).$$

[[**Stefania says:** Write with co-boundary]] In case $p = 0$, $\mathcal{L}_0$ 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 boundary matrices and their transposes.

[[**Stefania says:** Laplacian encodes important topological information (just add references)]] [[**Stefania says:** Laplacian can be seen as a message passing function on the simplices]]

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

2.3 Simplicial Neural Networks

- 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.

3 Experimental results

In this section we present experimental results for the simplicial neural network on co-authorship collaboration complexes extracted from the Semantic Scholar datasets. Specifically, we focus on predicting missed input data.

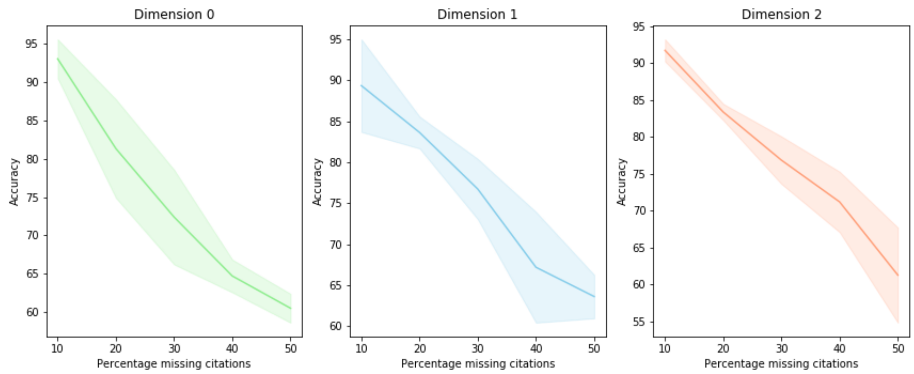

Figure 2: Accuracy of SNN in predicting missing citations

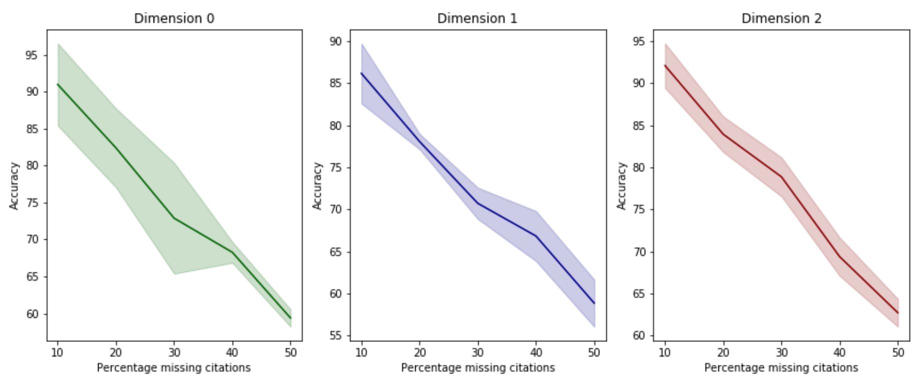

Figure 3: Accuracy in predicting missing citations with a pretrained SNN

4 Conlusion and Future Work

FIXME

- Define pooling
- Better baseline for the above work
- Preliminary results on vector field data. Where we believe this method can be applied?

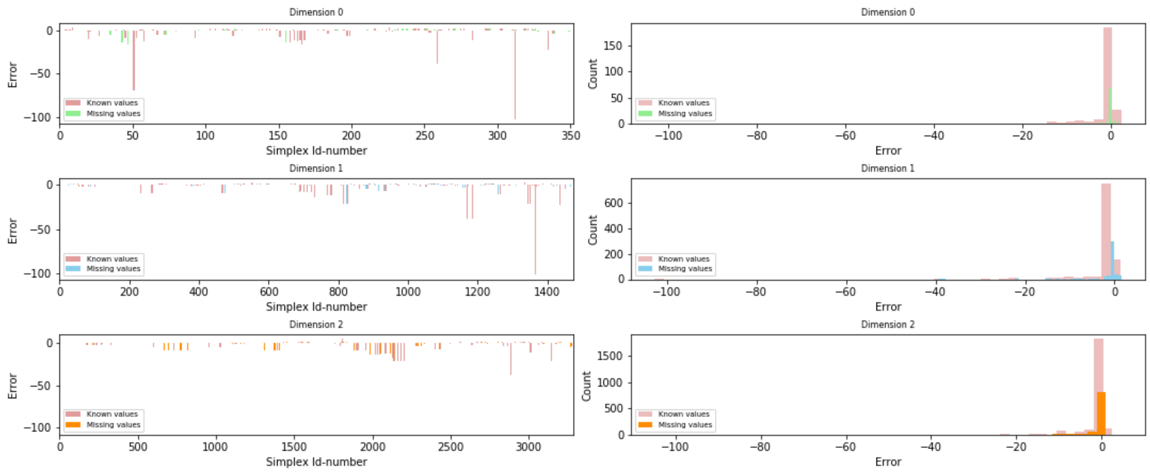

Figure 4: Distribution of the prediction's error

References

[1] Anil N. Hirani. “Discrete Exterior Calculus”. PhD thesis. California Insitute of Technology, 2003.

[2] Ib Madsen and Jørgen Tornehave. *From calculus to cohomology: de Rham cohomology and characteristic classes*. Cambridge University Press, 1997.