Simplicial Neural Networks

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Motivation: beyond pairwise interactions

In [1] CNNs have been extended to convolutional neural networks on graphs (GNNs).

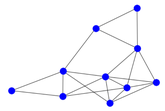
CNN

Input: Pixels on a grid

Convolutional kernels

GNN

Input: Signal on graph's nodes



Graph Laplacian

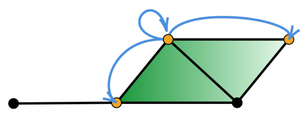
- Graphs model pairwise relationships. We extend GNNs to **simplicial complexes**, which can encode k-fold interactions.
- The input of simplicial neural networks (SNNs) are **k-cochains (functions)** on the k-simplices.
- We use the **simplicial Laplacian** to define a proper notion of convolution.

Simplicial Neural Networks

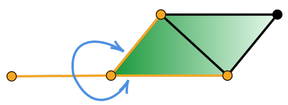
Laplacians for simplicial complexes

The graph Laplacian can be extended to Laplacians for simplices of any dimension k [2]. The k-Laplacian can be interpreted as a function propagating the values of the k-cochains, y_k, on the k-simplices.

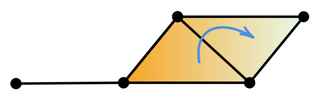
$\mathscr{L}_0$: Graph Laplacian
$y_0 = \mathscr{L}_0 x_0$



$\mathscr{L}_1$: 1-Laplacian
$y_1 = \mathscr{L}_1 x_1$

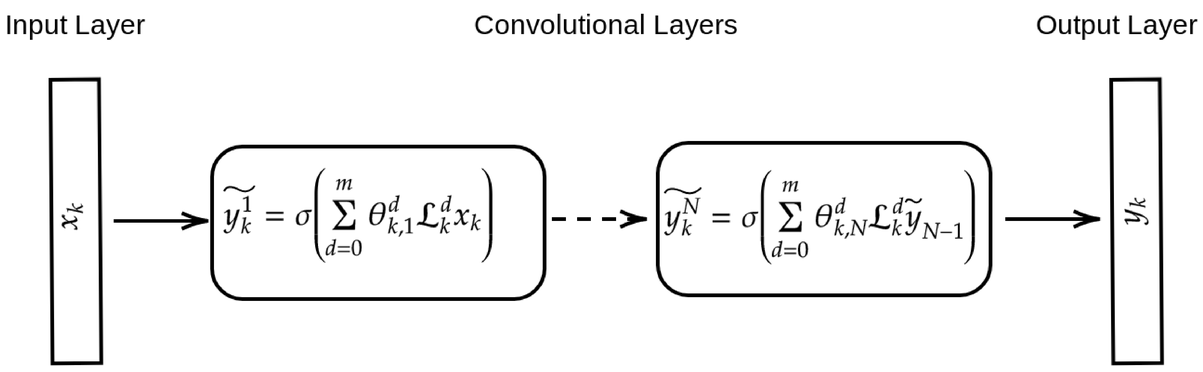


$\mathscr{L}_2$: 2-Laplacian
$y_2 = \mathscr{L}_2 x_2$



Simplicial Neural Networks (SNNs)

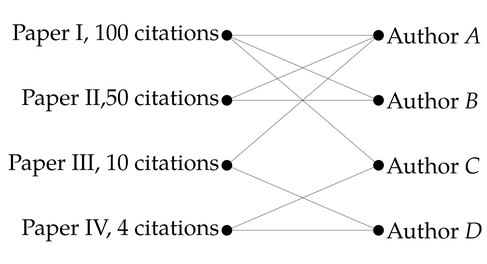
In SNNs the convolutional filters are low-degree polynomials in the Laplacian with learnable coefficients. These polynomial can be interpreted as functions propagating the values of the k-cochains at a distance not greater than their degree.

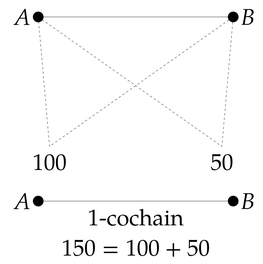


As in the graph case, one of the advantages of using such convolutional filters is that the N-th power of the k-Laplacian is N-localizing. Therefore, the entire filtering operation costs $\mathscr{O}(N|\mathrm{E}|) \ll \mathscr{O}(n^2)$ operations.

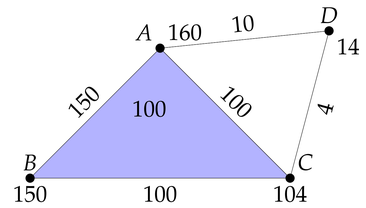
Coautorship complex: from a bipartite graph to a complex

From any bipartite graph with weights one can build a simplicial complex with k-cochains.





1-cochain
$150 = 100 + 50$

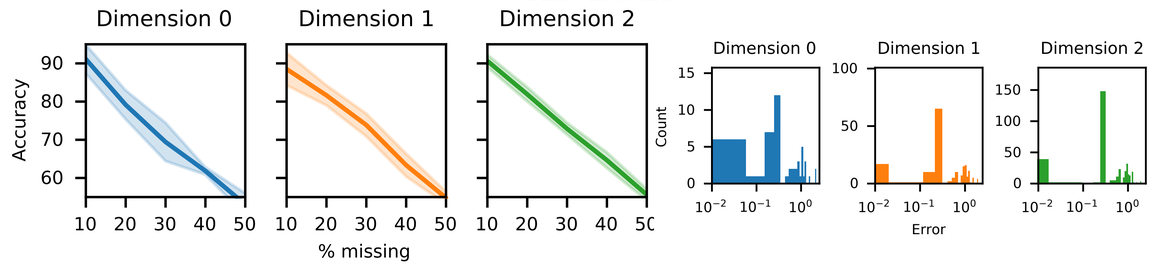


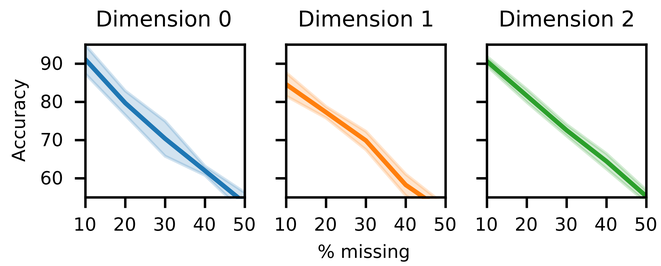
- From the the Semantic Scholar Dataset we built two different coauthorship complexes $CC1$ and $CC2$.

Imputing missing citations on the coauthoship complex

We consider the problem of **imputing missing values of citations** on the cochains ($k = 1, 2, 3$) of a coautorship complex. We train a SNN bala bla

First Results





References

[1] M. Defferrard, X. Bresson, and P. Vandergheynst, *Convolutional neural networks on graphs with fast localized spectral filtering*, Adv. in NeurIPS, 2016.
[2] D. Horak and J. Jost, *Spectra of combinatorial Laplace operators on simplicial complexes*, Adv. in Math. 2013.