Simplicial Neural Networks

Predicting Collaborations with Simplicial Complexes

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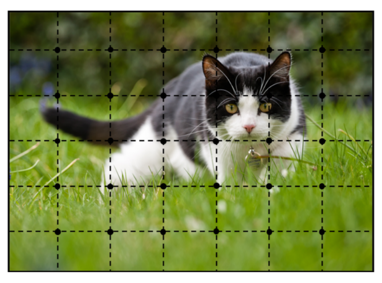
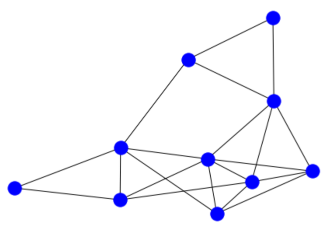
Motivation: beyond graphs

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

CNN — Input: Pixels on a grid ⟼ **GNN** — Input: Signal on graph's nodes

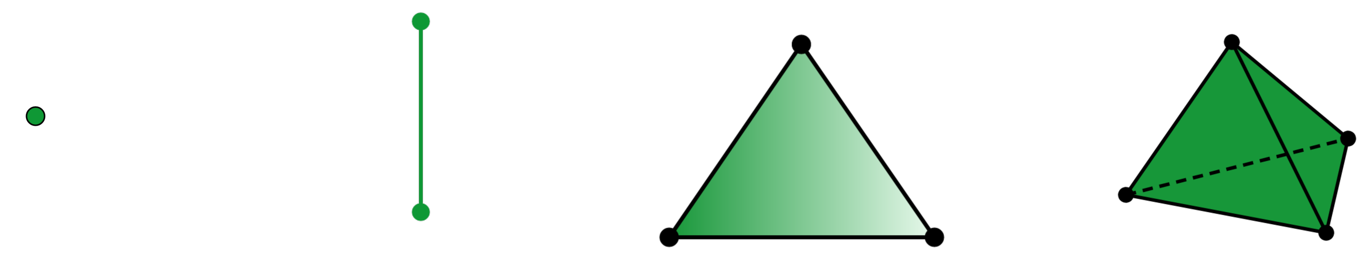




Convolutional kernels ⟶ Graph Laplacian

Graphs are intrinsically limited to modeling pairwise relationships. We extend GNNs from graphs to **simplicial complexes**, mathematical objects that can encode k-fold interactions.

Basic building blocks of a space: simplices



0-simplex 1-simplex 2-simplex 3-simplex

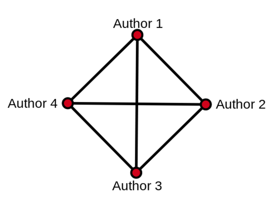
We construct simplicial complexes by gluing together simplices of various dimensions. Graphs are simplicial complexes constructed only with 0- and 1-simplices.

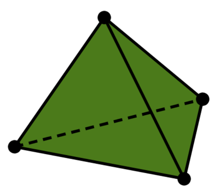
From collaborations to simplicial complexes

Simplicial complexes allow us to better represent collaborative networks where the interaction between k individuals can be described by a $(k-1)$-simplex.

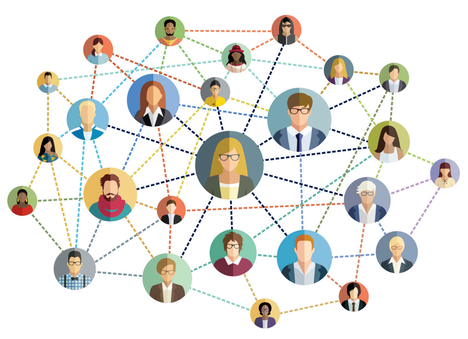
From collaborations to simplices

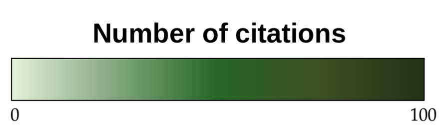
k individuals collaborating ⟶ $(k-1)$-simplex





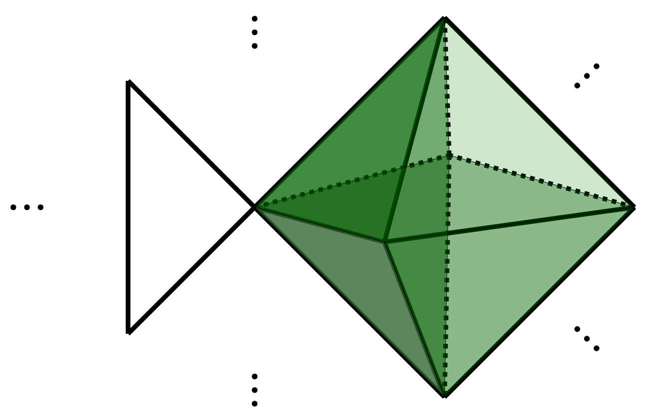
Collaborative Simplicial Complex





Collaborative network Collaboration values

Collaborative Complex



Missing collaboration values

A common problem in machine learning is assigning values to missing collaborations in a network. We frame this problem as simplicial-based semi-supervised learning, where values are predicted using a convolutional neural network whose filters smooth out the signal over the simplices.

Simplicial Neural Networks

Graph Laplacian

Given a graph G with vertices $\{v_1, \ldots, v_n\}$ its Laplacian $\mathscr{L}_0$ is the matrix whose elements are given by

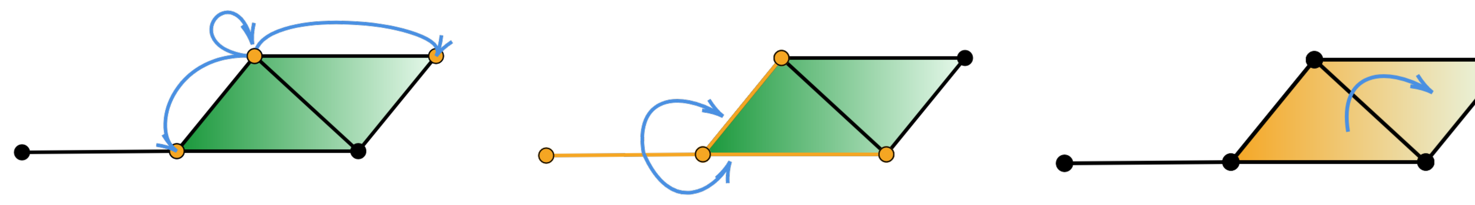
$$\mathscr{L}_0^{i,j} = \begin{cases} \deg(v_i) & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } v_i \text{ is adjacent to } v_j \\ 0 & \text{otherwise} \end{cases}$$

Intuitively, the Laplacian smoothly diffuses values on the vertices to their neighbors.

Laplacians for simplicial complexes

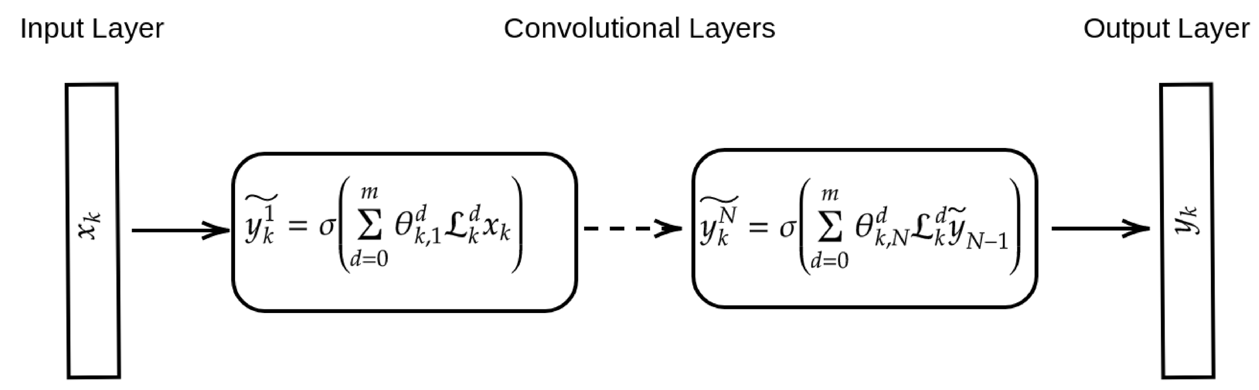
The graph Laplacian can be extended to Laplacians, $\mathscr{L}_k$, for simplices of any dimension k [2]. The k-Laplacian can be seen as a function propagating the values, y_k, on the k-simplices.

$\mathscr{L}_0$: 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

In simplicial neural networks the convolutional filters are low-degree polynomials in the Laplacian with learnable coefficients. They can be interpreted as functions propagating the collaboration values 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 d-th power of the k-Laplacian is d-localizing. Therefore, the entire filtering operation costs $\mathscr{O}(d|\mathrm{E}|) \ll \mathscr{O}(n^2)$ operations.

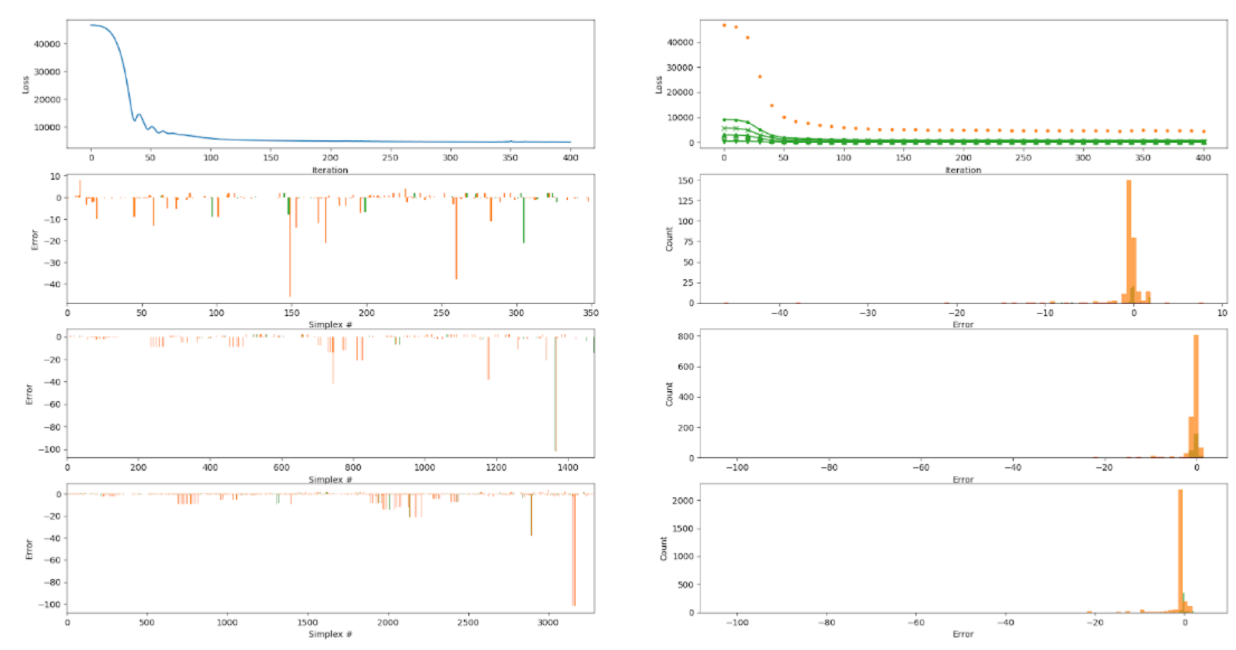
Learning the values of the collaborations

We consider the problem of assigning values to collaborations, where values are available for only a small subset of the simplices.

Data

From the the Semantic Scholar Dataset we build a collaborative complex, based on co-authorships, with 352 0-simplices, 1474 1-simplices and 3285 2-simplices. The collaboration values on the simplices are given by the total number of citations of the collaboration it represents.

First Results



Unknown values	20%
Dimension 0: training accuracy	77.7%
Dimension 0: test accuracy	73.21%
Dimension 1: training accuracy	81.34%
Dimension 1: test accuracy	83.05%
Dimension 2: training accuracy	78.66%
Dimension 2: test accuracy	78.1%

Conclusions and future work

Simplicial neural networks (SNN) are a promising tool for learning values on k-fold interactions. In our future work we will use SNN on vector field data and compare our method with other existing techniques.

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.