Simplicial Neural Networks

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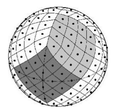
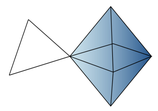
Convolution: a way to exploit the space's structure

CNNs	Group NNs	Simplicial NNs
Regular grids	Homogeneous spaces	Higher-order interactions
		
Convolutions: local and shift-invariant operations	Convolutions: local and group action-invariant operations	Convolutions: local operations considering higher-order structures

Basic building blocks of a space: simplices

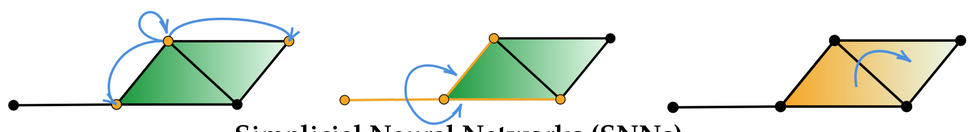
We construct simplicial complexes by gluing together simplices of various dimensions.

Simplicial Neural Networks

Laplacians for simplicial complexes

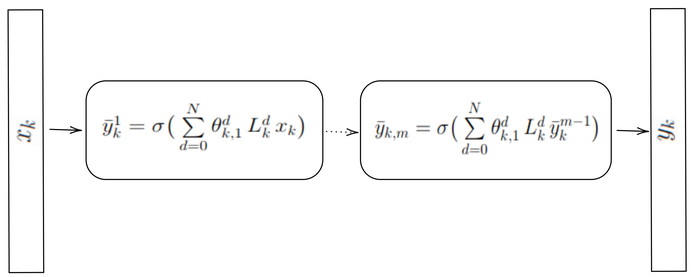
The graph Laplacian can be extended to Laplacians for simplices of any dimension k [**1**]. The k-Laplacian can be interpreted as a function propagating values of functions on the k-simplices. These functions are called k-cochains, x_k.

L_0: Graph Laplacian	L_1: 1-Laplacian	L_2: 2-Laplacian
$y_0 = L_0 x_0$	$y_1 = L_1 x_1$	$y_2 = L_2 x_2$



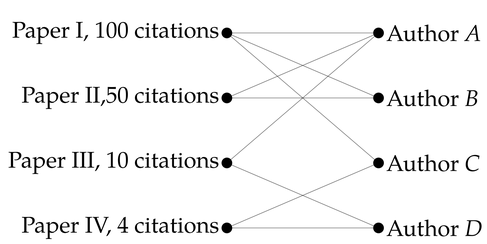
Simplicial Neural Networks (SNNs)

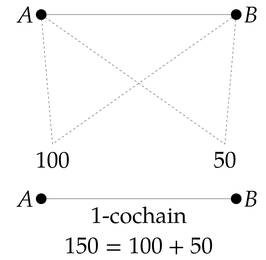
- The convolutional filters are low-degree polynomials in the Laplacian with learnable coefficients.
- The input are multiple k-cochains on the k-simplices, W_k.



1. Convolution can be implemented by N sparse matrix-vector multiplications: the computational cost is $\mathcal{O}(\xi|W_k|)$.
2. The number of weights to be learned is reduced from $\mathcal{O}(|W_k|)$ to $\mathcal{O}(1)$.
3. The operation is N-localizing: if two simplices are more than N hops apart, there is no interaction between them.

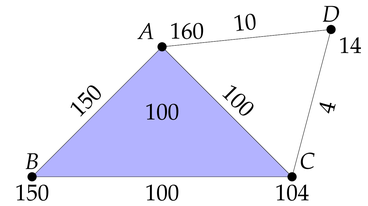
Coautorship complex: from a bipartite graph to a complex





1-cochain

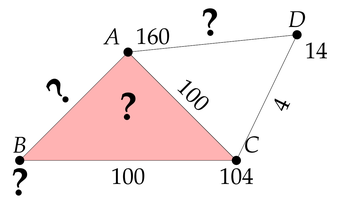
$150 = 100 + 50$



Predicting missing citations on the coauthoship complex

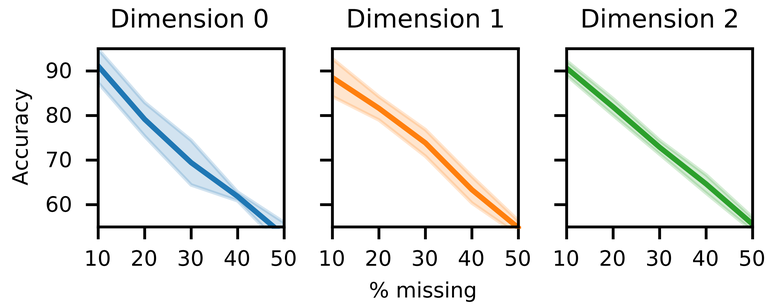
Data

Coautorship complexes are built from the Semantic Scholar dataset [**2**] where missing citations are introduced at random on the k-cochains ($k = 1, 2, 3$) at five rates: $10\%, 20\%, 30\%, 30\%$, and 50%.



First Results

Mean accuracy $\pm$ standard deviation over 5 samples in imputing missing citations.



Performance of baselines: mean accuracy $\pm$ standard deviation over 5 samples for 30% missing citations.

Method	Dimension 0	Dimension 1	Dimension 2
Global Mean	3.30 ± 0.82	5.75 ± 1.28	2.96 ± 0.49
Global Median	7.78 ± 2.70	10.44 ± 1.00	12.50 ± 0.63
Neighbors Mean	11.88 ± 5.29	24.15 ± 1.85	27.38 ± 1.18

Code: `https://github.com/stefaniaebli/simplicial_neural_networks`

References

[1] D. Horak and J. Jost, *Spectra of combinatorial Laplace operators on simplicial complexes*, Adv. in Math. 2013.

[2] W. Ammar et al. , *Construction of the Literature Graph in Semantic Scholar*, `https://www.semanticscholar.org/paper/09e3cf5704bcb16e6657f6ceed70e93373a54618`.