Geometric building blocks: a reproduction study on E(n) Equivariant Message Passing Simplicial Networks

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1 Introduction

Over the past few years, deep learning research has seen significant progress in solving graph learning tasks. A crucial aspect of such problems is maintaining equivariance to transformations, such as rotations and translations, allowing for instance to reliably predict physical properties of molecules. In this section, we will provide an overview of the predominant methods used in this domain, along with an introduction to a new method: E(n) Equivariant Simplicial Message Passing Networks (EMPSNs) [3].

Graph Neural Networks (GNNs) [12], namely their most common variant, Message Passing Neural Networks (MPNNs) [5] are instrumental when learning on graph data. Simple MPNNs however, have a number of drawbacks. Firstly they are limited in learning higher dimensional graph structures such as cliques (a set of points that are all connected to each other), since communication normally only happens from nodes to other nodes. Secondly, they suffer from over-smoothing; nodes of a graph iteratively update their features by aggregating the features of their neighbors, a process by which updated node features become increasingly similar. Previous works attempt to improve MPSNs' expressivity by considering higher dimensional simplices in the graph as learnable features [1] [7]. While these methods provide the tools for more powerful graph learning models, they do not concern themselves with equivariance.

As stated in the original EMPSN [3] paper, many real-life problems have a natural symmetry to translations, rotations, and reflections (that is, to the Euclidean group E(n)), such as object recognition or predicting molecular properties. Many approaches have been proposed to ensure E(n) equivariance: Tensor field networks [13], SE(3) Transformers [4], E(n) Equivariant Graph Neural Networks [11] among others. These works are particularly useful for working with geometric graph data, such as molecular point clouds: they use the underlying geometry of the space in which the graph is positioned to ensure E(n) equivariance. In this case however, the lack of higher-dimensional features remains a limiting factor for the reasons stated previously.

EMPSNs [3] are a novel approach to learning on geometric graphs and point clouds that is equivariant to the euclidean group E(n) (rotations, translations, and reflections). The method combines geometric and topological graph approaches to leverage both benefits. Its main contributions related to our reproduction study are the following:

1. A generalization of E(n) Equivariant Graph Neural Networks (EGNNs) which can learn features on simplicial complexes.

2. Experiments showing that the use of higher-dimensional simplex learning improves performance compared to EGNNs and MPSNs, without requiring more parameters, and proving to be competitive with SOTA methods on the QM9 dataset [10], [9].

Additionally, their results suggest that incorporating geometric information serves as an effective measure against over-smoothing.

In our work, we attempt to reproduce the results of the original EMPSN paper, and extend the method, rewriting parts of the author's code to use a common library for learning on topological domains. The library allows us to test how a different graph lifting procedure (operation that obtains higher-order simplices from graph data) compares to the one used in the original paper.

2 Background

Message passing neural networks have seen an increased popularity since their introduction [5]. In this blogpost, we will elaborate on how message passing networks are adapted to work with simplicial complexes, as proposed by [3]. We introduce the relevant definitions of message passing, simplicial complexes, equivariant message passing networks and message passing simplicial networks.

2.1 Message passing

Let $G = (V, E)$ be a graph consisting of nodes V and edges E. Then let each node $v_i \in V$ and edge $e_{ij} \in E$ have an associated node feature $\mathbf{f}_i \in \mathbb{R}^{c_n}$ and edge feature $\mathbf{a}_{ij} \in \mathbb{R}^{c_e}$, with dimensionality $c_n, c_e \in \mathbb{N}_{>0}$. In message passing, nodes have hidden states (features) we update nodes' features iteratively via the following prodedure:

$$\mathbf{m}_{ij} = \phi_m\left(\mathbf{f}_i, \mathbf{f}_j, \mathbf{a}_{ij}\right) \tag{1}$$

$$\mathbf{m}_i = \underset{j \in \mathcal{N}(i)}{\text{Agg}}\ \mathbf{m}_{ij} \tag{2}$$

$$\mathbf{f}_i' = \phi_f\left(\mathbf{f}_i, \mathbf{m}_i\right) \tag{3}$$

First, we find messages from v_j to v_i (equation 1). We then aggregate messages to v_i, with Agg being any permutation invariant function over the neighbors (equation 2). Finally we update the hidden state (features) of all nodes $\mathbf{f}_i$ (equation 3). $\mathcal{N}(i)$ denotes the set of neighbours of node v_i and ϕ_m and ϕ_f are multilayer perceptrons. This sequence of steps is one iteration, and is performed by what we call a message passing layer.

After passing our input graph's features through several successive message passing layers, a permutation invariant aggregation is applied to all final hidden states of the nodes in order to get a hidden state that represents the entire graph. *In methodology, write about the final linear layer that maps the graph feature vector into a single scalar, which represents a single physical property of a molecule*.

2.2 Simplicial complexes

A simplex in Geometry is the extension of the concept of triangles to multiple dimensions. An n-simplex consists of $n + 1$ fully connected points, i.e. a 0-simplex is a point, a 1-simplex is

a line, a 2-simplex is a triangle, a 3-simplex is a tetrahedron, a 4-simplex is a 5-cell etc. In an article entitled Architectures of Topological Deep Learning: A Survey of Message-Passing Topological Neural Networks [8], simplices are mainly referred to as cells of rank r (r-cells for short), where for example, a 1-simplex is a 1-cell. To assign features to higher-dimensional simplices in graphs, we turn to the definition of a generalized notion of graphs called abstract simplicial complexes.

We define an **abstract simplicial complex** (ASC) $\mathcal{K}$ as a collection of non-empty finite subsets of some set $\mathcal{V}$ such that for every set $\mathcal{T} \in \mathcal{K}$ and any non-empty subset $\mathcal{R} \subseteq \mathcal{T}$, it is the case that $\mathcal{R} \in \mathcal{K}$. Although an ASC is a purely combinatorial object, we can use the definition to associate a set of points of some graph $\mathcal{G}$ to a higher-order structure, using a so-called **lifting transformation**. As an example, we may consider clique complex lifting, as described in [3]: Formally, the lift results in the ASC $\mathcal{K}$ with the property that if the nodes $\{v_0, ..., v_k\}$ form a clique in $\mathcal{G}$, then the simplex $\{v_0, ..., v_k\} \in \mathcal{K}$. In other words, any clique in the graph that is comprised of k nodes becomes a k-simplex. The resulting ASC conforms to the provided definition in the sense that if an edge is in the simplicial complex, so are its nodes, if a triangle is in the complex, so are its edges and nodes, and so on. An n dimensional simplicial complex is defined as one that contains simplices of dimension/rank $\leq n$. In the scope of our study (and that of the original paper), using the cell terminology mentioned previously, we only consider 2 dimensional simplicial complexes (2-cells, or traingles are the highest rank r-cells in the complex). An illustration of clique complex lifting is provided in figure 1.

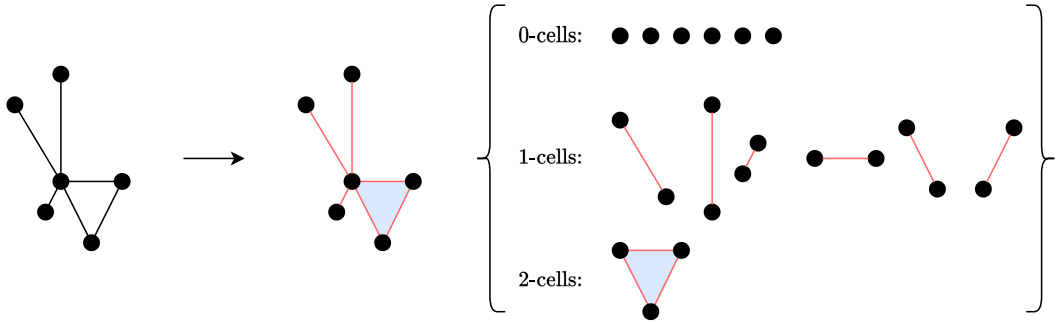

Figure 1: Illustration of clique complex lifting, in the resulting simplicial complex, we have the nodes (0-cells) of the original graph in black, the edges (1-cells) of the original graph in red and the triangles (2-cells) in blue

Unfortunately, clique complex lifting can be computationally expensive, and an alternative called the Vietori-Rips lift is described in the original paper. We start from a point cloud (points with positions in 3D euclidean space only) and we obtain a simplicial complex by assigning an r-cell to sets of points that are within a predefined distance δ away from each other. More specifically, we iterate through each point; if a sphere with radius δ around the point contains r points, they are connected, and an r-cell is assigned to that set of points. No duplicate r-cells should be present in the result. An illustration is provided in figure 2.

We may also consider alpha complex lifting; the alpha complex is a fundamental data structure from computational geometry. In the alpha complex, a subset $\sigma = \{x_{i0}, ..., x_{ik}\} \subset S$ belongs to Alpha(S, r) if there exists a point $y \in \mathbb{R}^m$ that is equidistant from every member of σ, so

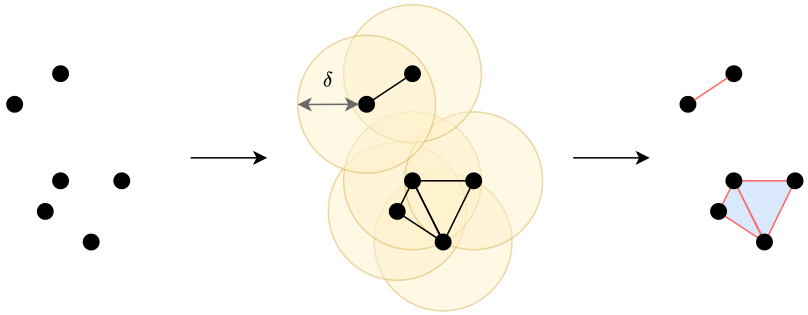

Figure 2: Vietoris-Rips lift

that

$$\rho := ||y - x_{i0}|| = ... = ||y - x_{ik}|| \leq r$$

and thus $||y - x|| \leq r \quad \forall x \in S$. Formally, the alpha complex is defined as the collection:

$$\text{Alpha}(S, r) = \left\{ \sigma \subset S : \bigcap_{x \in \sigma} V_x(r) \neq \emptyset \right\}$$

A subset σ of size $k + 1$ is called a k-dimensional simplex of Alpha(S, r). [2]

2.3 Equivariant message passing networks

Firstly, it is important to define what equivariance is. Suppose G is a group and X and Y are sets on which G acts. A function $f : X \to Y$ is called equivariant with respect to G if it commutes with the group action. In other words, applying a transformation $g \in G$ followed by the function f yields the same result as first applying f and then the transformation. Formally,

$$f(g \cdot x) = g \cdot f(x) \qquad \textit{equivariance}$$
$$f(g \cdot x) = f(x) \qquad \textit{invariance}$$

A frequently utilized model for geometric graphs is the $E(n)$ Equivariant Graph Neural Network (EGNN). This model enhances the message-passing process by incorporating positional data while maintaining equivariance to $E(n)$ [11]. This is crucial because, in certain scenarios, the nodes within a graph are located in Euclidean space, creating what is known as a geometric graph. This spatial information can be integrated into the message-passing framework to incorporate physical attributes to leverage geometric data. The message function is adapted to depend on $E(n)$ invariant information, such as the distance between two nodes. Consequently, the initial step in the message-passing process is modified as follows

$$\mathbf{m}_{ij} = \phi_m \left(\mathbf{f}_i, \mathbf{f}_j, \text{lnv} \left(\mathbf{x}_i, \mathbf{x}_j \right), \mathbf{a}_{ij} \right)$$

having that for all $g \in E(n)$

$$\text{lnv} \left(g \cdot \mathbf{x}_i, g \cdot \mathbf{x}_j \right) = \text{lnv} \left(\mathbf{x}_i, \mathbf{x}_j \right)$$

Then for every layer, the position of the nodes is updated as follows:

$$\mathbf{x}_i' = \mathbf{x}_i + C \sum_{j \neq i} \left(\mathbf{x}_i - \mathbf{x}_j \right) \phi_x \left(\mathbf{m}_{ij} \right)$$

where ϕ_x is a MLP. This positional update is typically unused for E(n)-invariant tasks such as predicting the internal energy of a molecule.

2.4 Message passing simplicial networks

We denote $\sigma \prec \tau$ when a simple σ is on the boundary of a simplex τ if an only if $\sigma \subset \tau$ and there is no δ such that $\sigma \subset \delta \subset \tau$. In other words, σ is directly on the boundary (immediately adjacent) of τ with any intermediate simplices between them. Message Passing Simplicial Networks (MPSNs) offer a message-passing framework that considers more complex forms of adjacency between objects in an abstract simplicial complex (ASC). Specifically for our paper, the following types of adjacency are identified:

- Boundary adjacencies $\mathcal{B}(\sigma) = \{\tau \mid \tau \prec \sigma\}$ (e.g. if σ is a triangle, the simplices that are boundary-adjacent to it are its nodes and edges)
- Lower-adjacencies $\mathcal{N}_{\downarrow}(\sigma) = \{\tau \mid \exists \delta, \delta \prec \tau \wedge \delta \prec \sigma\}$ (e.g. if σ is a triangle, a lower-adjacent simplex could be another triangle that shares a common edge with σ)

Then, as we saw in 2.1, the messages from adjacent simplices have to be aggregated to a simplex σ. For example, all boundary-adjacent simplex messages are aggregated as follows:

$$\mathbf{m}_{\mathcal{B}}(\sigma) = \underset{\tau \in \mathcal{B}(\sigma)}{\text{Agg}} \left(\phi_{\mathcal{B}}\left(\mathbf{f}_{\sigma}, \mathbf{f}_{\tau}\right)\right)$$

for $\phi_{\mathcal{B}}$ is a MLP. Alternatively, we incorporate the 2 message types in the updates as follows:

$$\mathbf{f}'_{\sigma} = \phi_f\left(\mathbf{f}_{\sigma}, \mathbf{m}_{\mathcal{B}}(\sigma), \mathbf{m}_{\mathcal{N}_{\downarrow}}(\sigma)\right)$$

Lastly, for a k dimensional simplicial complex $\mathcal{K}$

$$\mathbf{h}_{\mathcal{K}} := \bigoplus_{i=0}^{k} \text{Agg}_{\sigma \in `lK, |\sigma|=i+1} \mathbf{h}_{\sigma}$$

where $\mathbf{h}_{\mathcal{K}}$ is the hidden state representing the entire complex, and $\bigoplus$ is the concatenation. For clarity, if the network then updates the positions of the nodes in each layer, this makes the network E(n) equivariant; if the network solely passes the invariant information without altering the geometric locations then it's just E(n) invariant.

3 Methodology

3.1 Lifting procedure

We have reproduced the original paper's experiments performed on the QM9 dataset. QM9 is a dataset of stable small organic molecules with their with geometric, energetic and thermodynamic properties. It contains important quantum chemical properties and serves as a standard benchmark for machine learning methods or systems of identifications of the contained molecular properties.The QM9 datasets consists of molecular graphs with 19 graph level features. The nodes of the molecular graphs are atoms embedded in a three dimensional euclidean space. The goal of the methodology for QM9 is graph feature prediction, and since the features are continuous values this is a regression task. The molecular graphs present in QM9 contains no higher order topological information. To address this limitation we propose lift the graph structure to a higher-dimension to leverage certain higher-order interactions present in nature [CITE].

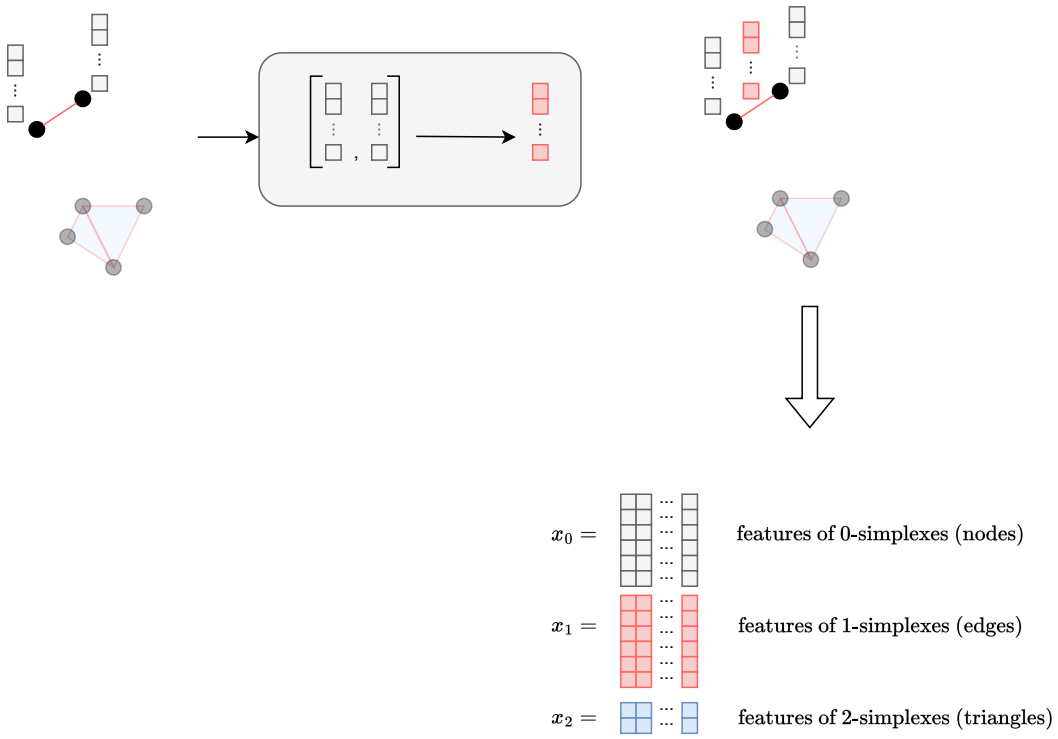

Figure 3: Computation of simplex features

To do this we *lift* the point cloud to a Vietoris-Rips complex based on a parameter δ as described in 2, which is a subset of the Cech Complex. As mentioned previously, we limit the maximum dimension of the lift to rank 2. Additionally, this work uses two types of communication among simplices: 1) from r-simplices to r-simplices and 2) from $(r-1)$-simplices to r-simplices, however we do not use 2-simplices to 2-simplices, as in [3]. In addition to the lifting of the structure to a higher order topological structure we will also lift the features to embeed each r-simplex with a certain feature vector. We experiment with three methods: 1) A sum projection of the lower boundary of the simplex, 2) a mean projection of the lower boundary simplices and 3) a mean of the 0-simplex components composing all lower boundary simplices and shown in Figure 4 as done in [3]. Additionally, we also used a lift to the Alpha Complex, a subcomplex of the Cech Complex as well. The invariant information is included as an abstract edge attribute information between a simplex boundary within a communication framework.

3.2 Deep learning architecture

This work proposes a step toward standarization in the field of TDL by using TopoX [6], a suite of Python packages that construct a base framework for constructing Complexes (Simplicial, Combinatorial, Cellular) [CITE], applications of spectral graph theory algorithms and examples of SOTA topological deep learning architecture. The lifting of the topology to a higher-order structure and the lifting of features is decoupled and easily added to any standard data loading procedure, a standardized structure for message passing as a convolutional layer and methods for

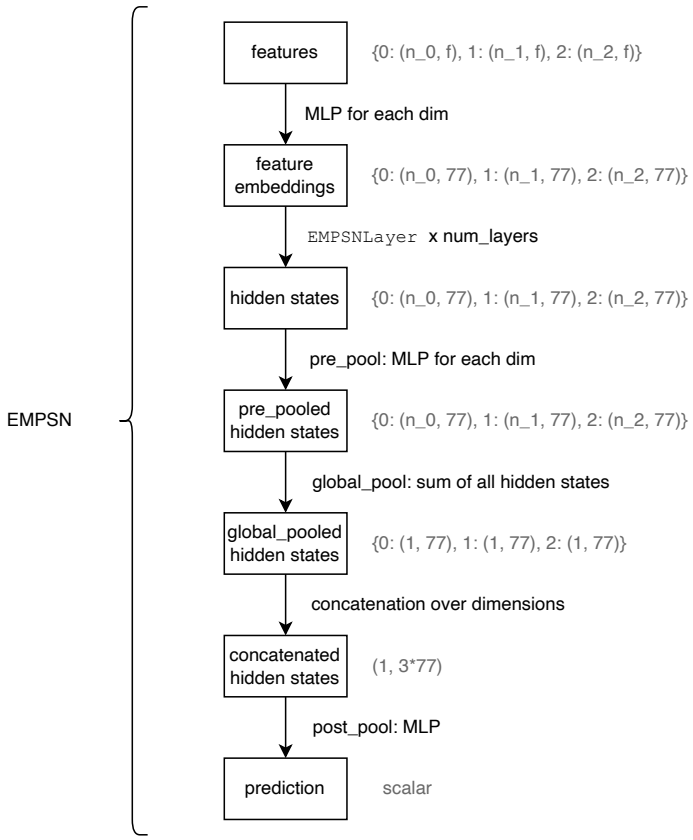

Figure 4: Network Architecture

structuring a TDL project. In turn, this approach makes for faster experimentation as it makes experiments replicable and interpretable. The construction of the invariance can evaluated both as a pre-processing step or during the forward pass to account for an equivariant architecture where the nodes in the graph update positions.

4 Original paper

The current paper applies the theory outlined above to two proof of concept studies. Since the first experiment is the focus of the paper and the code for the second experiment is not provided, we will gain more insight into the first experiment. This experiment utilizes the QM9 dataset and an Invariant MPSN with seven hidden layers and 77 hidden dimensions. The QM9 dataset is a dataset of molecules, and the task is to predict certain molecular properties that these molecules exhibit. Performance is measured using Mean absolute error (MAE), which is also the loss function for IMPSN. The initial graph structure of the molecules is dropped and a new hierarchical graph structure is created by the lifting operation, using the Vietoris-Rips lift. After the transformation the network is trained for 1000 epochs and only 1 feature is predicted per network. Due to computational cost, we have reproduced the results of the original paper

Table 1: Caption

for only 3 of these features in 4.Every run took about $\tilde{7}0$ hours to complete on a HARDWARE SPECIFICS IDK

5 Strengths and weaknesses

The invariant geometric framework combined with the topological information generated by the lifting operation is a unique strength of the proposed methodology. Additionally, the methodology is data-efficient with comparable results to state-of-the-art (SotA) methods. This strength is evident in the method's performance on the QM9 dataset. Even though the proposed methodology is not engineered for a specific scientific domain and does not employ a large network, it is comparable to, or outperforms, more specialized methods (that utilize domain-specific strategies) on certain features and consistently outperforms EGNN.

Another strength is the general applicability of this method. The proposed equivariant simplicial message passing network (EMPSN) is applicable to any geometric graph dataset. In addition, the results suggest that the incorporation of geometric information in the message passing procedure combats over-smoothing of node features, a common problem in graph neural networks (GNNs).

Although on paper, the methodology scores very well, the current implementation has several weaknesses.

A key weakness is related to the geometric realisation of the simplices. In the original paper, the author explains three E(n) equivariant features, Distance, angle, and volume, calculable for any dimensional simplex adjecency relation. In practice this set of features is not always expressive in lower dimensional simplices. Two feature values are 0, this happens when the volume of a point is calculated in the 0-0 adjecency relation. Other features values occur twice in the same boundary relation. This happens since the volume of a 1d simplex is identical to the distance between the points of that 1d simplex. In other words, the 'volume' of a line segment is the same as the distance between the points of that line segment. It leaves to be questioned why the author decided to incorporate redundant features. In the codebase, no justification can be found regarding decisions on feature selection.

What ties into the afformentioned weakness is the fact that the codebase has very poor readability and provides little context. In addition, the codebase contains ample hard-coded functionality and is tightly coupled. For example, expanding the methodology for higher order simplices would require a significant overhaul of multiple key classes and requires an understanding of their coupling. The combination of cryptic variable names, lack of documentation and extensive use of hard-coded functionality makes the codebase ill suited for adapting the methodology.

The last weakness relates to scope of the codebase. The original paper describes two experiments: one using an Invariant MPSN and one that uses the full Equivariant MPSN. Unfortunately, the code for the latter is not included in the paper, therefore the results of the Equivariant MPSN are not reproducible.

Although the concept of the proposed methodology is original and its theoretical foundation is

thoroughly explained there are multiple concerns relating to the implementaion of EMPSN that are left unanswered.

Given the fact the results in the original paper are already impressive, it raised the question how much the performance of the methodology could be improved given the afformentioned seemingly unoptimal design choices surrounding the invariant features. So far, Reproduction attempts with the original code show very similar trends, but they don't seem to score as high as the original paper implies.

6 Describe your novel contribution.

For our contribution, we decided to attempt to refactor the codebase to utilize as of much of the TopoX framework as possible. TopoX is a topological deep learning suite built on top of pytorch that facilitates standardises geometric and topological deep learning applications. The methodology of this paper is a prime candidate to utilize this framework and the stardardisation of its code can radically improve the reproducibily and modifiability of EMPSN. Besides, TopoX creators have placed a request for people to translate lifting operations into their framework. Both these additions are qualitatively useful additions to not only the current paper, streamlining and clarifying the procedures, but also the TopoX suite, by increasing code written by their standards. In addition to refactoring, we aim to experiment with the replacement of the Vietoris-Rips lift with an alpha complex lift, where the resulting simplicial complexes are alpha complexes to investigate the impact different simplicial conplexes. We acknowledge that the choice for topological complex is an important one since it is an assumption of shape of the higher order structure in the data.

7 Results of your work

Our code is located in this forked repository: https://github.com/martin-carrasco/challenge-icml-2024.git

7.1 As a summary:

- We have reformatted the code for the Vietoris-Rips lift.
- We have attempted to restructure the codebase as much as possible, using the building blocks of TopoX, specifically the ones for simplicial layers and the message passing framework. By doing so we have changed the input required for the layers from the indexing-based structure that the original authors used, into a adjacency/incidence matrix format, which is a more generalizable structure.
- we have implemented a different lifting method (alpha lift) and investigated the differences
- The main changes are in the lifting subfolder and in the models subfolder.

8 Conclusion

In this post we have investigated a novel 'proof of concept' study that investigates the use of simplicial structures combined with geometric properties as a useful avenue to study. the paper designs an equivariant or invariant message passing simplicial network. It seems that the author

is fair in his assessment of the utility. It is a compact network and the usage of invariance combined with simplices seems prudent, although the accuracy of the predictions seems to not reach the same level as the original paper. We name a couple of found strengths and weaknesses, focussing on the efficiency and generalisability. While also remarking the difficulty of the code and its implementation. By refitting the code into a promising new suite for topological deep learning, named TopoX, we hope to make the code more accessible and to contribute to the growing amount of papers using TopoX.

9 Contributions

- Nordin Belkacemi - focused on the code and theory
- Andreas Berentzen - implemented lifting code and invariance feature calculation, wrote strengths and weaknesses for the blogpost
- Martin Carrasco - main codewriter, implemented the lifting code and the EMPSN neural network
- Valeria Sepicacchi - wrote the theoretical background and helped with EMPSN code
- Jesse Wonnink - wrote rest of the blogpost and helped with EMPSN code

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