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

May 29, 2024

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) [13], 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] [8]. 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 [14], SE(3) Transformers [4], E(n) Equivariant Graph Neural Networks [12] 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 [11], [10].

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 Theoretical 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 procedure:

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

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

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

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.

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 [9], 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.

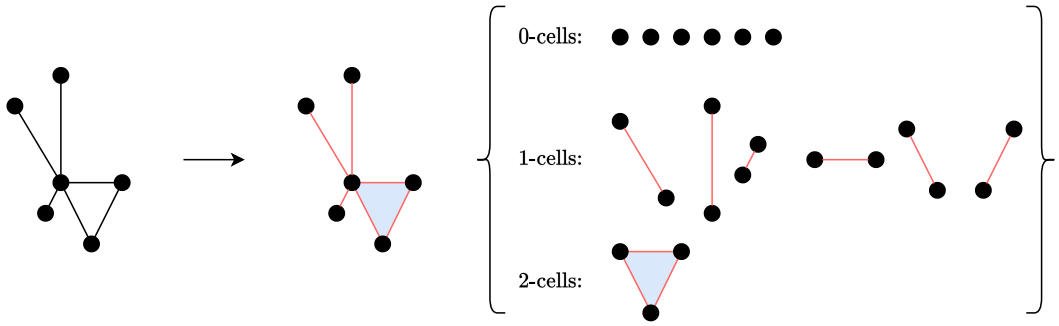

Figure 1: Illustration of clique complex lifting, in the resulting simplicial complex, we have the nodes (0-cells) of the original graph in black, the edges (1-cells) of the original graph in red and the triangles (2-cells) in blue

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

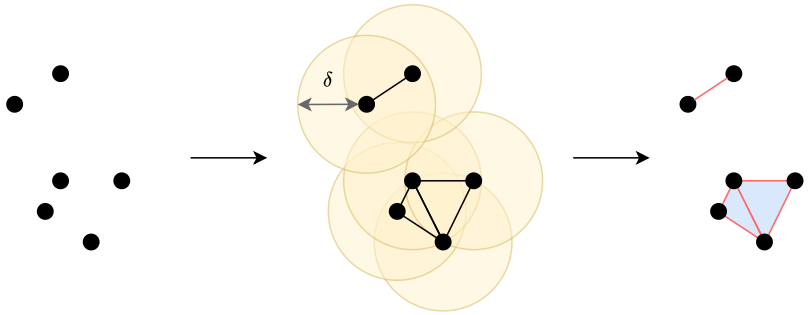

Figure 2: Vietoris-Rips lift

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 $E(n)$ [12]. 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 $\mathcal{K}$

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

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 Lifted representation of the 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 to lift the graph structure to facilitate the construction of different order simplices.

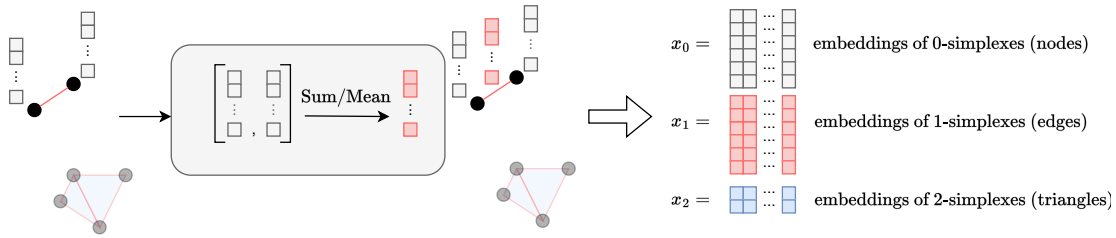

Figure 3: Computation of simplex embeddings

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. There is limit on the maximum rank of the simplices, however due to naturally occuring phenomena it can be constrained. For this particular set of experiments it is restricted to rank 2. Additionally, this work presents 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 embed 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. The invariant information is included as abstract edge attribute information between a simplex boundary within a communication framework. The simplex boundary features are shown in the table below below:

	0_0	0_1	1_1	1_2
F1	$\|\|x_{\mathbf{p}_i} - x_{\mathbf{p}_j}\|\|$	$\|\|x_{\mathbf{p}_i} - x_{\mathbf{p}_j}\|\|$	$\|\|x_{\mathbf{p}_i} - x_{\mathbf{a}}\|\|$	$\|\|x_{\mathbf{p}_i} - x_{\mathbf{a}}\|\|$
F2	0	0	$\|\|x_{\mathbf{p}_i} - x_{\mathbf{b}}\|\|$	$\|\|x_{\mathbf{p}_i} - x_{\mathbf{b}}\|\| + \|\|x_{\mathbf{p}_i} - x_{\mathbf{a}}\|\|$
F3	0	$\|\|x_{\mathbf{p}_i} - x_{\mathbf{p}_j}\|\|$	$\|\|x_{\mathbf{a}} - x_{\mathbf{b}}\|\|$	$V(S_2)$
F4	-	-	$\|\|x_{\mathbf{p}_i} - x_{\mathbf{a}}\|\|$	$\|\|x_{\mathbf{p}_i} - x_{\mathbf{a}}\|\|$
F5	-	-	$\|\|x_{\mathbf{p}_i} - x_{\mathbf{b}}\|\|$	$\angle\mathbf{p}_i + \angle\mathbf{p}_j$
F6	-	-	$\angle\mathbf{p}_i$	$\angle\mathbf{a}$

Table 1: Metadata of E(n) invariant features of simplex adjacencies

In 1 the same point variables are used as in the original paper. $V(S_2)$ denotes the volume of the second order simplex, this is calculated as the surface area of the triangle plane contained within the points contained in S_2. As can be seen, some values occur twice in a simplex adjacency relation. The second time the same value occurs is because the volume of a 1d simplex is identical to the distance between its points.

3.2 Deep learning architecture

This work proposes a step toward standardization 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) [7], applications of spectral graph theory algorithms and examples of

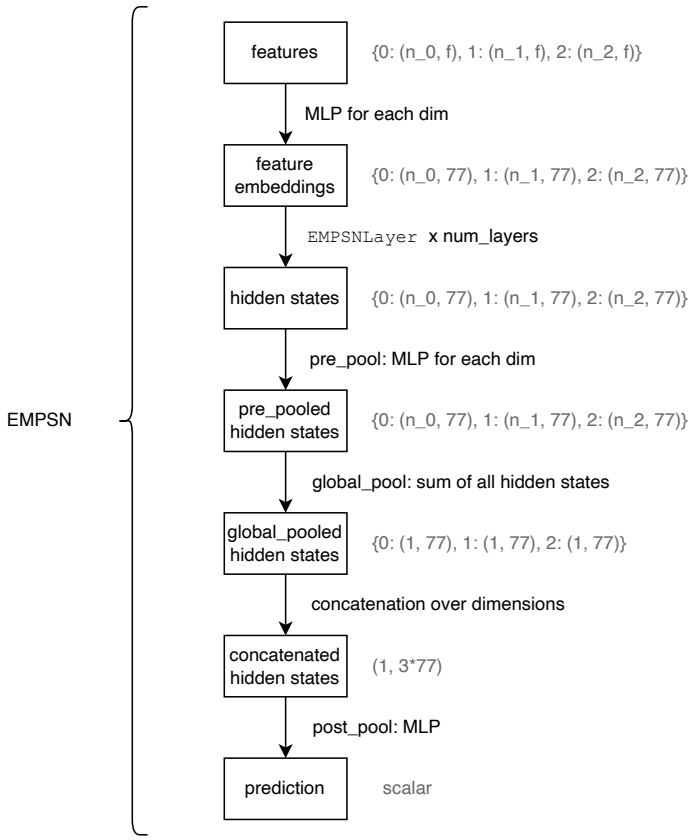

Figure 4: Network Architecture

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 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 performed as a pre-processing step or during the forward pass, the latter accounts for an equivariant architecture where the geometric information of the nodes in the graph are updated.

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.

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 it enables a data-efficient learning procedure with comparable results to state-of-the-art (SotA) methods. 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 the 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 some 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 adjacency relation. In practice, these features are not always expressive are identical in lower dimensional simplices. When analyzing the metadata of each adjacency relation, it becomes clear some features are consistently 0 or appear twice. For instance, Two of the three features of the 0-0 adjacency relation are 0, This happens when the volume of the two points is calculated. Other feature values occur twice in the same boundary relation. For instance, the volume of a 1d simplex is identical to the distance between the points of that 1d simplex. Yet both features exist in the metadata for the 1-1 adjacency relation. In total, more than one-third of the invariant features are 0 or appear twice in the same row. Since message passing only occurs between adjacency boundaries and not among different boundaries there is full flexibility in feature selection, thus it leaves to be questioned why the author decided on the original invariant feature metadata for each adjacency relation. Not In the paper nor in the codebase, a justification can be found regarding decisions on invariant feature selection.

What ties into the aforementioned 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 to 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 make adapting the methodology difficult.

The last weakness relates to the 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.

Given the fact the results in the original paper are impressive, it raises the question of how much the performance of the methodology could be further improved given the aforementioned

seemingly unoptimal design choices surrounding the invariant features. Although the concept of the proposed methodology is original and its theoretical foundation is thoroughly explained there are multiple concerns relating to the implementation of EMPSN.

6 Author contribution

Our contribution can be summed up in three main points:

1. Refactoring of the original code to follow the guidelines of the TopoX suite framework. This includes the original topological lift and the feature lifting. 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.
2. Implementation of the lifting procedure for the Alpha Complex and two different feature lifting procedures using projection sum and mean projection over lower simplices.
3. Application of the equivariance property on the MQ9 dataset

7 Experiments and Results

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

7.1 Replication

The first attempt at replication was using the authors first code. Some of the shortcomings were the difficulty of dealing with tensor stacking for mini-batching, the transformation of molecular properties and index matching on the message passing layer. Aside form the the code was able to be run out of the box.

In the original implementation, MAE drops quickly but stabilises around the 3 mark. This is far from the reported value on the paper of 0.066. This came about some fixes on the indices and was the maximum it dropped on all approaches. On the H property the MAE was on the order of thousands, way above the reported error even when taking into account the factor change of units.

7.2 TopoX refactor

We executed the refactored the original code and adapted it to the TopoX framework. This included reworking the procedures for passing messages, aggregating messages using the scatter procedure and correctly handling the invariant information along the simplices. We used communication on between each all simplices among r-simplices except on dimension and communication from lower to higher simplices for the two possible pairs. This implies that the maximum dimension was capped at 2 and the δ value was set as 3. We tried precomputing the invariances to no avail as the memory requirement becomes too high, for that we remain with the original method by calculating invariances on the forward pass for a particular batch.

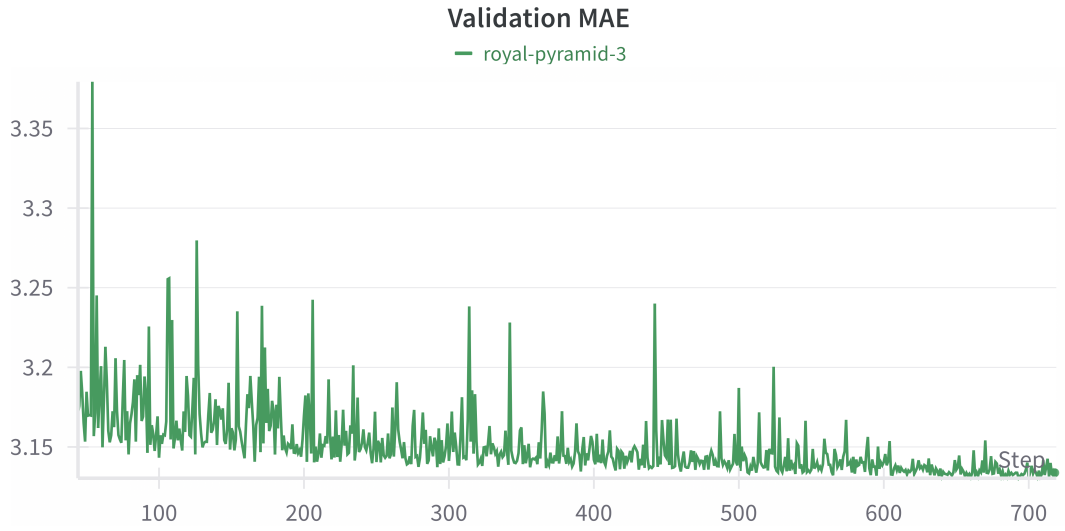

Figure 5: Validation MAE - Experiment 1

7.3 Alpha Complex

We used the same parameter for executing the Alpha Complex. The only change incurred is capping the dimensionality of the resulting lifted topology. The lifting procedure for Alpha Complex implies that the higher r-simplex is not capped. Thus, we need to satisfy some constraints in regards to our architecture: 1) the maximum dimension should be capped to 2, 2) there needs to be at least r-simplex for each r up to 2. In this case, this amounts to making sure the maximum dimension is at least 2, if not then the graph is not included in the training/validation/test dataset.

7.4 Different feature projections

Aside from the original proposal of proposition for lifting the feature to higher dimensional structures we explore two other techniques found in the literature [CITE]. Fist, the *mean projection* of the lower dimensions, which takes the average of all the simplices. Second, the default implementation of TopoX, the sum projection of the $(r-1)$-simplices composing it.

7.5 Equivariance on QM9

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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