CELL COMPLEX NEURAL NETWORKS

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Abstract. Cell complexes are topological spaces constructed from simple blocks called cells. They generalize graphs, simplicial complexes, and polyhedral complexes that form important domains for practical applications. We propose a general, combinatorial, and unifying construction for performing neural network-type computations on cell complexes. Furthermore, we introduce inter-cellular message passing schemes, message passing schemes on cell complexes that take the topology of the underlying space into account. In particular, our method generalizes many of the most popular types of graph neural networks.

1. Introduction

Motivated by the recent success of neural networks in various domains and data types, we propose cell complex neural networks (CXNs), a general unifying scheme that allows neural network-type computations on cell complexes. Specifically, we define a neural network structure on cell complexes, which are topological spaces constructed from pieces called cells with the cells homeomorphic to topological balls of varying dimensions. Cell complexes form a natural generalization of graphs, simplicial complexes, and polyhedral complexes. They provide a combinatorial formalism that allows the inclusion of complicated relationships not available to more restrictive structures such as graphs and meshes, while retaining most of intuitive structure of these simpler objects.

The simplest nontrivial types of cell complexes are graphs. From this perspective, our work can be considered as a generalization of graph neural networks (GNNs). Earlier work that generalizes regular Convolutional Neural Network (CNN) to graphs was presented in and extended in . Furthermore, a significant effort has been made towards generalizing deep learning to manifolds, most notably geometric deep learning and the work of Bronstein et al. Other work includes utilizing filters on local patches using geodesic polar coordinates and heat kernels propagation schemes, among many others. We refer the reader to recent reviews of GNNs and its variations and to for a recent survey on geometric deep learning.

Our main contributions are summarized as follows. First, we propose a general unifying and simple training scheme on cell complexes, vastly expanding the array of available domains upon which we can apply deep learning protocols. In particular, it encompasses most of the popular types of graph neural networks, and generalizes those architectures to higher-dimensional domains such as 3D meshes, simplicial complexes, and polygonal complexes. Second, the training on a cell complex is defined in an entirely combinatorial fashion, and hence naturally extends general message passing schemes currently utilized on GNNs. The combinatorial description of the proposed method allows for intuitive manipulation, conceptualization, and implementation. Third, we introduce inter-cellular message passing schemes, message passing schemes on cell complexes that take the topology of the underlying space into account. In particular, we defined a message passing scheme that is induced from the boundary and coboundary maps used to compute homology and cohomology in...
algebraic topology. Computationally, a cell complex net is defined using adjacency matrices, analogous to those used to encode the structure of a graph neural network. This means their implementation can be readily adapted from the existing graph neural networks libraries (e.g., [8]).

In Section 2 we present the background and notation that are needed to understand the proposed network. We introduce cell neural networks in Section 3. We provide more intercellular message passing schemes in 4. Finally, we discuss potential applications in Section 5.

2. Cell Complexes

A cell complex is a topological space $X$ obtained as a disjoint union of cells, each homeomorphic to the interior of a $k$-Euclidean ball for some $k$, attached together via attaching maps in a locally reasonable manner. See Figure 1 for various examples of cell complexes.

![Figure 1. Examples of cell complexes.](image)

The set of $k$-cells in $X$ is denoted $X^k$. The dimension of a cell $x \in X$ will be denoted by $d(x)$. The dimension of a cell complex is the largest dimension of one of its cells. A cell complex is called regular if every attaching map is a homeomorphism onto the closure of the image of its corresponding cell. In this article all cell complexes will be regular, and consist of finitely many cells. Regular cell complexes generalize graphs, simplicial complexes, and polyhedral complexes while retaining many desirable combinatorial and intuitive properties of these simpler structures. Recall that each cell $a$ in $X$ has two possible orientations. An oriented cell complex is a cell complex in which every cell has a chosen orientation.

The information of the attaching maps of a regular cell-complex are stored combinatorially in a sequence of matrices $\partial_k : \mathbb{R}^{[X^k]} \rightarrow \mathbb{R}^{[X^{k-1}]}$ that describes, roughly speaking, the number of times $k$-cells wrap around $(k-1)$-cells in $X$. The definition of these matrices $\partial_k$ depends on whether the cells of $X$ are oriented or not. Since our cell complexes are regular then the entries of $\partial_k$ are in $\{0, \pm 1\}$ when the complex is oriented. If the cell complex is not oriented then the entries of $\partial_k$ are in $\{0, 1\}$. The matrix $\partial_k$ is usually called the $k$-boundary matrix of $X$. Dually, we define $\partial_k^* : \mathbb{R}^{[X^{k-1}]} \rightarrow \mathbb{R}^{[X^k]}$ to be the transpose of the matrix $\partial_k$.

Let $X$ be a cell complex and let $c^n$ be an $n$-cell in $X$. We denote by $\text{facets}(c^n)$ to the set of all $(n - 1)$-cells $X$ that are incident to $c^n$. Similarly, we will denote by $\text{cofacets}(c^n)$ to the set of all $(n + 1)$-cells $X$ that are incident to $c^n$. Note that $\text{facets}(c^n)$ or $\text{cofacets}(c^n)$ might be the empty set.

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1 The technical details of the definition of cell complex are not essential in our setting. For the precise definition the reader is referred to standard texts in algebraic topology.
The sets facets($c^n$) or cofacets($c^n$) are important in our discussion and they are our tool to define the notion of adjacency between two cells with the same dimension in the context of cell complexes. We distinguish between two cases.

**The complex X is oriented.** When X is oriented then we will also store along with each cell in facets($c^n$), cofacets($c^n$) the orientation induced by $c_n$ with respect to the maps $\partial_n$, and $\partial_n^*$, respectively.

In this case we will also denote by facets$^+(c^n) \subset$ facets($c^n$), facets$^-(c^n) \subset$ facets($c^n$) to the subsets of facets($c^n$) that consists of cells that are positively oriented, negatively oriented, with respect to $c^n$, respectively. The set cofacets$^+(c^n)$ and the set cofacets$^-(c^n)$ are defined analogously.

Observe that, facets($c^n$) = facets$^+(c^n)$ $\cup$ facets$^-(c^n)$ and facets$^+(c^n)$ $\cap$ facets$^-(c^n)$ = $\emptyset$. Similarly, cofacets($c^n$) = cofacets$^+(c^n)$ $\cup$ cofacets$^-(c^n)$ and cofacets$^+(c^n)$ $\cap$ cofacets$^-(c^n)$ = $\emptyset$.

**Example 2.1.** Consider the cell complexes given in Figure 2. We compute a few examples of the sets we define above to illustrate the concept.

For Figure 2 (a) we have cofacets($v_1$) = $\{-e_1, e_2\}$, cofacets($v_2$) = $\{e_1, -e_2, -e_3, -e_4, e_5\}$, cofacets($v_3$) = $\{e_3, e_4, -e_5, e_6, e_7\}$ and cofacets($v_4$) = $\{-e_6, -e_7\}$. Moreover, facets($F_1$) = $\{e_1, -e_2\}$. Finally, cofacets($e_6$) = $\{F_3\}$ and cofacets($e_7$) = $\{-F_3\}$.

On the other hand for Figure 2 (b) we have cofacets($e_1$) = $\{F_1, -F_2\}$ and cofacets($e_2$) = $\{F_1, -F_2\}$.

**Figure 2.** Examples of computing the adjacency and co-adjacency neighbors of cells in cell complexes.

If X is an oriented complex then a cell $b^n$ is said to be adjacent to an n-cell $a^n$ with respect to an (n + 1)-cell $c^{n+1}$ if $a^n \in$ facets$^+(c^{n+1})$ and $b^n \in$ facets$^-(c^{n+1})$. Similarly, an n-cell $b^n$ is said to be coadjacent to $a^n$ with respect to an (n - 1)-cell $c^{n-1}$ if $a^n \in$ cofacets$^+(c^{n-1})$ and $b^n \in$ cofacets$^-(c^{n-1})$. The set of cells that are adjacent to a cell a in X will be denoted by $N_{adj}(a)$. Similarly, The set of all coadjacent cells of a cell a in X will be denoted by $N_{co}(a)$.

**Example 2.2.** In Figure 2 (a) we have $N_{adj}(v_2) = \{v_1, v_3\}$, $N_{adj}(v_4) = \emptyset$.

For Figure 2 (b) we have, $N_{co}(F_1) = \{F_2\}$. This is because $F_1 \in$ cofacets$^+(e_1)$ and $F_2 \in$ cofacets$^-(e_1)$. On the other hand, $N_{co}(F_2) = \emptyset$. Note that in this example $N_{adj}(e_1) = N_{adj}(e_2) = \emptyset$.

See also Figure 3 for an illustrative example on adjacency and coadjacency relationships.

If $a^n, b^n$ are n-cells in X then we define the set $\mathcal{C}_O[a^n, b^n]$ to be the intersection cofacets($a^n$) $\cap$ cofacets$^*$($b^n$). The set $\mathcal{C}_O[a^n, b^n]$ describes the set of all incident n+1-cells of $b^n$ that have $a^n$ as an adjacent cell. Note that in general $\mathcal{C}_O[a^n, b^n] \neq \mathcal{C}[b^n, a^n]$. Similarly, the set $\mathcal{C}[a^n, b^n]$ is defined to be the intersection facets($a^n$) $\cap$ facets$^*$($b^n$).
Figure 3. The adjacency and coadjacency of a cell. (a) The adjacent 1-cells of the orange target 1-cells. (b) The coadjacent 2-cells of the orange 2-cell. This adjacency/coadjacency relations will be used for inter-cellular message passing schemes.

Example 2.3. In Figure 2 (a) we have $C\mathcal{O}[v_2, v_3] = \{e_3, e_4\}$ whereas $C\mathcal{O}[v_3, v_2] = \{e_4\}$. On the other hand in Figure 2 (b) we have $C\mathcal{O}[e_1, e_2] = C\mathcal{O}[e_2, e_1] = \emptyset$.

The complex $X$ is not oriented. When the complex $X$ is not oriented the notation is much easier. In this case we say that two $n$-cells $a^n$ and $b^n$ are adjacent if there exists an $(n+1)$-cell $c^{n+1}$ such that $a^n, b^n \in \text{facets}(c^{n+1})$. Similarly, we say that $a$ and $b$ are coadjacent in $X$ if there exists an $(n-1)$-cell $c^{n-1}$ with $a^n, b^n \in \text{cofacets}(c^{n-1})$. The set of all adjacent cells in $X$ of a cell $a$ in $X$ will be denoted by $N_{adj}(a)$. Similarly, The set of all coadjacent cells in $X$ of a cell $a$ in $X$ will be denoted by $N_{co}(a)$.

If $a^n, b^n$ are $n$-cells in $X$ then we define the set $C\mathcal{O}[a^n, b^n]$ to be the intersection $\text{cofacets}(a^n) \cap \text{cofacets}(b^n)$. In this case the notation is symmetric, in other words, $C\mathcal{O}[a^n, b^n] = C\mathcal{O}[b^n, a^n]$. Similarly, the set $C[a^n, b^n]$ is defined to be the intersection $\text{facets}(a^n) \cap \text{facets}(b^n)$.

Observe that these notions generalize the analogues notions of adjacent and coadjacent matrices in directed and undirected graphs. Given this setting we now introduce the notion of cell complex neural networks.

3. Cell Complex Neural Networks (CXNs)

The simplest type of cell complexes are graphs. Hence to motivate cell complex neural networks we recall the definition of graph neural networks.

3.1. Graph Neural Networks. Given a graph $G = (V, E)$, a graph neural network on $G$ with depth $L > 0$ updates a feature representation for every node in the graph $L$ times. Initially, every node $i$ is given a feature vector $x_i^{(0)}$. On the $k$ stage of the computation, each node $i$ in the graph collects messages from its neighbors $j$, represented by their feature vectors $x_j^{(k-1)}$, and aggregates them together to form a new feature representation $x_i^{(k)}$ for the node $i$. More precisely, a graph neural network consists requires the following input data:

1. A graph $G = (V, E)$.
2. For each node $i \in V$ we have an initial vector $x_i^{(0)} \in \mathbb{R}^{l_0}$.
Given the above data the feed-forward algorithm on $G$ executes $L$ message passing schemes defined recursively for $0 \leq k \leq L$ by:

$$x_i^{(k)} := \alpha^k\left(x_i^{(k-1)}, E_{j \in N(i)}(\phi^k(x_i^{(k-1)}, x_j^{(k-1)}, e_{ij}))\right) \in \mathbb{R}_{l_k}^k,$$

where $e_{ij} \in \mathbb{R}^D$ is a possible optional, edge feature from the node $j$ to the node $i$, $E$ is a permutation invariant differentiable function, and $\alpha^k, \phi^k$ are trainable differentiable functions. Note that at each stage $k$ all messages share the same differentiable functions $\phi^k$ and $\alpha^k$.

Consider the graph given in Figure 4. Let’s say we want to build a graph neural network on this graph with depth 2. To illustrate the computation, we pick a vertex in the graph, save $v_1$. At first stage the surrounding neighbors of $v_1$, namely $\{v_2, v_3, v_4\}$ pass their messages to $v_1$. The information obtained from these messages are aggregated and combined together via trainable differentiable functions $\alpha^1$ and $\phi^1$. On the second stage all neighbors of $v_1$ collect the messages information from their respective neighbors in a similar fashion. This process is illustrated in Figure 4.

![Diagram](image)

**Figure 4.** An example of graph neural net of depth 2. The computation are only illustrated on the red node. In this figure we abuse the notation and we do not distinguish between a node $i$ and its associated vector $x_i^{(k)}$. The blue box represents the differentiable functions $\alpha^1$ and $\phi^1$ where as the white box represents the functions $\alpha^2$ and $\phi^2$.

### 3.2. Cell Complex Neural Network

A cell complex neural net forward propagation computation requires the following data as an input:

1. A cell complex $X$ of dimension $n$, possibly oriented;
2. For each $m$-cell $c^m$ in $X$, we have an initial vector $x_{c^m}^{(0)} \in \mathbb{R}_{r_m}^m$.

The forward propagation algorithm then performs a sequence of message passing executed between cells in $X$. Precisely, given the desired depth $L > 0$ of the net one wants to define on the complex $X$, the forward propagation algorithm on $X$ consists of $L \times n$ inter-cellular message passing schemes defined for $0 < k \leq L$:

$$x_{c^0}^{(k)} := \alpha_{0}^{(k)}\left(x_{c^0}^{(k-1)}, E_{a^0 \in N_{adj}(c^0)}(\phi_{0}^{(k)}(x_{c^0}^{(k-1)}, x_{a^0}^{(k-1)}, F_{e^1} e_0 \phi \phi_{c^0}[a^0,e^0]\{x_{a^0}^{(k-1)}\}))\right) \in \mathbb{R}_{e_{l_0}}^0,$$

$$;$$

$$x_{c^n-1}^{(k)} := \alpha_{n-1}^{(k)}\left(x_{c^n-1}^{(k-1)}, E_{a^{n-1} \in N_{adj}(c^{n-1})}(\phi_{n-1}^{(k)}(x_{c^n-1}^{(k-1)}, x_{a^n-1}^{(k-1)}, F_{e^n} e_0 \phi \phi_{c^n-1}[a^n-1,c^n-1]\{x_{a^n-1}^{(k-1)}\}))\right) \in \mathbb{R}_{e_{l_{n-1}}}^{n-1}$$. 


where \( x^{(k)}_{a_m}, x^{(k)}_{a_n}, x^{(k)}_{a_p} \in \mathbb{R}^k \), \( E, F \) are permutation invariant differentiable functions, and \( \alpha^j_k, \phi^k_j \) are trainable differentiable functions where, \( 0 \leq j \leq n - 1 \) and \( 0 < k \leq L \). Note that for each cell \( a^n \) in \( X \) the vectors \( x^{(0)}_{a^n} \) are never updated during the training of a CXN with this passing scheme. This is analogous to the optional feature vectors \( e_{i,j} \) in the context of graph neural networks. Although the formulation above is simple, it can generalize most types of the popular types of GNNs (e.g., [14, 25]).

![Diagram](image)

**Figure 5.** Two layers Cell Complex Neural Network (CXN). The computation is demonstrated with respect to the red target vertex. The information flow goes from lower cells to higher incident cells.

Figure 5 demonstrates the above construction/formulation on a simplicial complex example, which will denote by \( X \). Note that we abuse the notation in the figure and do not distinguish between a simplex \( s \) and its vector \( x^{(k)}_s \). For each vertex \( \{v_i\}_{i=1}^5 \) in \( X \), we assume we are given a vector \( x^{(0)}_{v_i} \); we have \( x^{(0)}_{v_j} \) for each edge \( \{e_j\}_{j=1}^7 \), and have \( x^{(0)}_{F_i} \) for the faces \( \{F_i\}_{i=1}^2 \). We start the computation for cells with dimension 0. Each \( v_i, 0 \leq i \leq 5 \), computes:

\[
\begin{align*}
x^{(1)}_{v_i} &:= \alpha^0_0 \left( x^{(0)}_{v_i}, E_{e_j \in \text{adj}(v_i)} (\phi^0_1 (x^{(0)}_{v_i}, x^{(0)}_{v_j}, x^{(0)}_{e_{ij}})) \right),
\end{align*}
\]

where \( e_{ij} \) is the edge that connects \( v_i \) to \( v_j \). Notice that all nodes share the same trainable functions \( \alpha^0_0 \) and \( \phi^0_1 \). Figure 5(a) shows this graph for \( v_1 \). Furthermore, each edge \( e_i \) also induces a computational graph and computes \( x^{(1)}_{e_i}, 1 \leq i \leq 7 \):

\[
\begin{align*}
x^{(1)}_{e_i} &:= \alpha^1_1 \left( x^{(0)}_{e_i}, E_{e_j \in \text{adj}(e_i)} (\phi^1_1 (x^{(0)}_{e_i}, x^{(0)}_{e_j}, x^{(0)}_{F_{ij}})) \right),
\end{align*}
\]

where \( F_{ij} \) denotes the unique face that bounds both edges \( e_i \) and \( e_j \). Notice that all edges share the same trainable functions \( \alpha^1_1 \) and \( \phi^1_1 \). On stage 2, we compute \( x^{(2)}_s \) for all simplices \( s \) of dimension 0 and 1. Figure 5 shows this computation for \( x^{(2)}_{v_1} \). Notice that the computational graphs that feed into it are the ones computed in stage 1. Also, notice how the information from this node flows from the surrounding nodes, edges and faces.

4. General Message Passing Scheme

The inter-cellular message passing scheme we suggested earlier updates the vectors on the flows from a given 0-cell a gathers the information from surrounding cells in a radial fashion.
defined by the adjacency matrices of the cell complex. While this message passing method is natural from the perspective of generalizing GNNs passing schemes, it forms a single method out of many other natural methods that can be defined in the context of GXNs. We outline some of these methods here.

4.1. Coadjacency Message Passing Scheme. The message passing method given in 3 does not update the final $n$–cells on the complex. In certain applications however it might be desirable to make the flow of information go from the lower cells to the higher cells. An example of such an application is mesh segmentation where it is desirable to update the information associated with a face on the mesh after gather local information around that face. The scheme given in 3 can be adjusted easily for this purpose. To this end, we utilize the data on the cells on the complex as before. However, the inter-cellular message passing schemes are defined as follows:

$$x^{(k)}_{c_n} := \alpha^{(k)}_{n-1} \left( x^{(k-1)}_{e_n}, E_{a_n} e_{N_{co}(c_n)} \left( \phi^{(k)}_{n-1} \left( x^{(k-1)}_{c_n}, x^{(k-1)}_{a_n}, F_{e_n} e_{N_{co}[a_n, c_n]}(x^{(k-1)}) \right) \right) \right) \in \mathbb{R}_{l}^{k_n},$$

(4.1)

$$\vdots$$

$$x^{(k)}_{c_1} := \alpha^{(k)}_{1} \left( x^{(k-1)}_{c_1}, E_{a_1} e_{N_{co}(c_1)} \left( \phi^{(k)}_{1} \left( x^{(k-1)}_{c_1}, x^{(0)}_{a_1}, F_{e_0} e_{N_{co}[a_1, c_1]}(x^{(0)}) \right) \right) \right) \in \mathbb{R}_{l}^{k_1},$$

(4.2)

Note that here the initial vector associated with zero cells in $X$ are never updated. An example of these computation is illustrated in Figure 6.

![Figure 6](image)

**Figure 6.** CXN with 2 layers. The computation is only demonstrated with respect to the light grey face. The information flow goes from higher cells to lower incident cells.

4.2. Homology and Cohomology-Based Passing Schemes. Here we briefly outline a message passing scheme that is consistent with the boundary and coboundary maps in the context of homology and cohomology of a cell complex. Let $x^k$ be a cell in a, possible oriented, cell complex $X$. Let $Bd(x)$ be set of cells $y$ of dimension $k - 1$ such that $y \in \partial(x)$ and $x$ and $y$ have compatible
orientations. Similarly, let $CoBd(x)$ denotes all cells of $y \in X$ with $x \in \partial(y)$ and both $x$ and $y$ have compatible orientations. Denote by $I$ to the union $Bd(x) \cup CoBd(x)$ we may define the passing scheme as follows:

$$x^{(k)}_{c_{m}} := \alpha^{(k)}_{m}(x_{c_{m}}^{(k-1)}, E_{a \in \mathcal{I}(x)}(\phi^{(k)}_{m,d(a)}(x_{c_{m}}^{(k-1)}, x^{(k-1)}_{a}))) \in \mathbb{R}^{l_{k}}.$$ 

Notice that the trainable function $\phi^{(k)}_{m,d(a)}$ needs to accommodate for the fact that the dimension of vector associated with $a$, namely $x^{(k)}_{a}$, may vary for different $a \in \mathcal{I}(x)$.

5. Significance & Potential Applications

CXNs allows for many applications, we outline the following potential directions:

(1) **Studying the type of the underlying space.** A central question is topology the topological type of the underlying space: given two spaces $A$ and $B$, are they equivalent up to a given topological equivalence? In practice this maybe translated to a similarity question between two structures. Indeed, TDA has been extensively utilized towards this purpose [7, 11]. On the other hand, deep learning allows studying the structure of the underlying space by building complex relationship between various elements in this spaces. Cell complexes form a general class of topological spaces that encompasses graphs, simplicial complexes and polyhedral complexes. Cell neural networks hence provide a potential tool to study structure similarity between discrete domains such as 3D shapes and discrete manifolds.2

(2) **Learning cell complex representation.** The graph representation [12] can be potentially extended to cell complexes using CXNs. In this context, a cell complex autoencoder needs to take into account cell with higher dimensions and not only the 0-cells as it is the case in the graph autoencoder. In particular, cell complexes seem natural objects for language embedding as they can be used to build complex relationship. Specifically, we can build a cell complex out of a corpus of text: words are vertices, they share an 1-cells if they are adjacent in the corpus, within a sentence, sentences form the boundaries of 3-cells, paragraphs form the boundaries of 4-cells, chapters form the boundaries of 4-cells, etc. Notice that unlike less general complexes (e.g. simplicial complexes), a $k$-cell in a cell complex may have an arbitrary number of $(k-1)$ incident cells.

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2Within this context, with their current neighborhood aggregation scheme, graph neural networks have been shown to not being able to solve the graph isomorphism problem [28].
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