Equivariant Maps for Hierarchical Structures

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Abstract

In many real-world settings, we are interested in learning invariant and equivariant functions over nested or multiresolution structures, such as a set of sequences, a graph of graphs, or a multiresolution image. While equivariant linear maps and by extension multilayer perceptrons (MLPs) for many of the individual basic structures are known, a formalism for dealing with a hierarchy of symmetry transformations is lacking. Observing that the transformation group for a nested structure corresponds to the “wreath product” of the symmetry groups of the building blocks, we show how to obtain the equivariant map for hierarchical data-structures using an intuitive combination of the equivariant maps for the individual blocks. To demonstrate the effectiveness of this type of model, we use a hierarchy of translation and permutation symmetries for learning on point cloud data, and report state-of-the-art on SEMANTIC3D and S3DIS, two of the largest real-world benchmarks for 3D semantic segmentation.

1 Introduction

In designing deep models for structured data, equivariance (invariance) of the model to transformation groups has proven to be a powerful inductive bias, which enables sample efficient learning. A widely used family of equivariant deep models constrain the feed-forward layer so that specific transformations of the input lead to the corresponding transformations of the output. A canonical example is the convolution layer, in which the constrained MLP is equivariant to translation operations. Many recent works have extended this idea to design equivariant networks for more exotic structures such as sets, exchangeable tensors and graphs, as well as relational and geometric structures.

This paper considers a nested hierarchy of such structures, or more generally, any hierarchical composition of transformation symmetries. These hierarchies naturally appear in many settings: for example, the interaction between nodes in a social graph may be a sequence or a set of events. Or in diffusion tensor imaging of the brain, each subject may be modeled as a set of sequences, where each sequence is a fibre bundle in the brain. The application we consider in this paper models point clouds as 3D images, where each voxel is a set of points with coordinates relative to the center of that voxel.

To get an intuition for a hierarchy of symmetry transformations, consider the example of a sequence of sequences – e.g., a text document can be viewed as a sequence of sentences, where each sentence is itself a sequence of words. Here, each inner sequence as well as the outer sequence is assumed to possess an “independent” translation symmetry. Contrast this with symmetries of an image (2D translation), where all inner sequences (say row pixels) translate together, so we have a total of two translations. This is the key difference between the wreath product of two translation groups (former) and their direct product (latter). It is the wreath product that appears in nested structures. As is evident from this example, the wreath product results in a significantly larger set of transformations, and therefore provides a stronger inductive bias.

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Figure 1: Wreath product can express the symmetries of hierarchical structures: wreath product of three groups $U \ltimes K \ltimes H$ acting on the set of elements $P \times Q \times R$, can be seen as independent copies of groups, $H$, $K$ and $U$ at different level of hierarchy acting on copies of $P$, $Q$ and $R$. Intuitively, a linear map $W_{U \ltimes K \ltimes H} : R^{PQR} \rightarrow R^{PQR}$ equivariant to $U \ltimes K \ltimes H$, performs pooling over leaves under each inner node, applies equivariant map for each inner structure (i.e., $W_U$, $W_K$ and $W_H$ respectively), and broadcasting the output back to the leaves. A $U \ltimes K \ltimes H$-equivariant map can be constructed as the sum of these three contributions, from equivariant maps at each level of hierarchy.

We are interested in application of equivariant/invariant deep learning to this type of nested structure. The building blocks of equivariant and invariant MLPs are equivariant linear maps of the feedforward layer; see Fig. 1. In particular, we show how to obtain the closed form of the equivariant linear map for the hierarchical structure from equivariant maps for the individual symmetry group. We observe that the number of independent linear operators grows with the “sum” of independent operators for individual building blocks. In contrast, this number grows with the “product” of independent operators on blocks when using direct product, confirming the stronger bias in the wreath product setting.

In the following, after discussing related works in Section 2, we give a short background on equivariant MLPs in Section 3. Section 4 starts by giving the closed form of equivariant maps for direct product of groups before moving to the more difficult case of wreath product in Section 4.2. Finally, Section 5 applies this idea to impose a hierarchical structure on 3D point clouds. We show that the equivariant map for this hierarchical structure achieves state-of-the-art performance on the largest benchmark datasets for 3D semantic segmentation.

2 Related Works

Group theory has a long history in signal processing [22], where in particular Fourier transformation and group convolution for Abelian groups have found tremendous success over the past decades. However, among non-commutative groups, wreath product constructions have been the subject of few works. Rockmore [39] give efficient procedures for fast Fourier transforms for wreath products. In a series of related works Foote et al. [15], Mirchandani et al. [34] investigate the wreath product for multi-resolution signal processing. The focus of their work is on the wreath product of cyclic groups for compression and filtering of image data.

Group theory has also found many applications in machine learning [25], and in particular deep learning. Design of invariant MLPs for general groups goes back to Shawe-Taylor [41]. More recently, several works investigate the design of equivariant networks for general finite [38] and infinite groups [7, 10, 26]. In particular, use of the wreath product for design of networks equivariant to a hierarchy of symmetries is briefly discussed in [38]. Equivariant networks have found many applications in learning on various structures, from image and text [31], to sets [36, 50], exchangeable matrices [21], graphs [1, 28, 32], and relational data [18], to signals on spheres [9, 27]. A large body of works investigate equivariance to Euclidean isometries; e.g., [11, 44, 46].

When it comes to equivariant models for compositional structures, contributions have been sparse, with most theoretical work focusing on semidirect product (or more generally using induced representations from a subgroup) to model tensor-fields on homogeneous spaces [8, 10]. Direct product of symmetric groups have been used to model interactions across sets of entities [21] and in generalizations to relational data [18]. In a recent work [33] study equivariant networks for sets of symmetric elements; however, they use direct product rather than wreath product discussed here. In the following we specifically contrast the use of direct product with wreath product for compositional structures.
3 Preliminaries

3.1 Group Action

A group \( G = \{g\} \) is a set equipped with a binary operation, such that the set is closed under this operation, \( gh \in G \), the operation is associative, \( g(gh) = (gh)h \), there exists identity element \( e \in G \), and a unique inverse for each \( g \in G \) satisfying \( gg^{-1} = e \). The action of \( G \) on a finite set \( \mathbb{N} \) is a function \( \alpha : G \times \mathbb{N} \rightarrow \mathbb{N} \) that transforms the elements of \( \mathbb{N} \), for each choice of \( g \in G \); for short we write \( g \cdot n \) instead of \( \alpha(g, n) \). Group actions preserve the group structure, meaning that the transformation associated with the identity element is identity \( e \cdot n = n \), and composition of two actions is equal to the action of the composition of group elements \( g(h) \cdot n = g \cdot (h \cdot n) \). Such a set, with a \( G \)-action defined on it is called a \( G \)-set. The group action on \( \mathbb{N} \) naturally extends to \( x \in \mathbb{R}^{|\mathbb{N}|} \), where it defines a permutation of indices \( g \cdot (x_1, \ldots, x_N) \equiv (x_{g1}, \ldots, x_{gN}) \). We often use a permutation matrix \( G^{(g)} \in \{0, 1\}^{N \times N} \) to represent this action – that is \( G^{(g)} x = g \cdot x \).

3.2 Equivariant Multilayer Perceptrons

A function \( \phi : \mathbb{R}^N \rightarrow \mathbb{R}^M \) is equivariant to a given actions of group \( G \) iff \( \phi(G^{(g)} x) = \tilde{G}^{(g)} \phi(x) \) for any \( x \in \mathbb{R}^N \) and \( g \in G \). That is, a symmetry transformation of the input results in the corresponding symmetry transformation of the output. Note that the action on the input and output may in general be different. In particular, when \( \tilde{G}^{(g)} = I_M \) for all \( g \) – that is, the action on the output is trivial – equivariance reduces to invariance. Here, \( I_M \) is the \( M \times M \) identity matrix. For simplicity and motivated by practical design choices, in the following we assume the same action on the input and output.

For a feedforward layer \( \phi : x \mapsto \sigma(Wx) \), where \( \sigma \) is a point-wise non-linearity and \( W \in \mathbb{R}^{N \times N} \), the equivariance condition above simplifies to commutativity condition \( G^{(g)} W = W G^{(g)} \forall g \in G \). This imposes a symmetry on \( W \) in the form of parameter-sharing [38][47]. While we can use computational means to solve this equation for any finite group, an efficient implementation requires a closed form solution. Several recent works derive the closed form solutions for interesting groups and structures. Note that in general the feedforward layer may have multiple input and output channels, with identical \( G \)-action on each channel. This only require replicating the parameter-sharing pattern in \( W \), for each combination of input and output channel. An Equivariant MLP is a stack of equivariant feed-forward layers, where the composition of equivariant layers is also equivariant. Therefore, our task in building MLPs equivariant to finite group actions is reduced to finding equivariant linear maps in the form of parameter-sharing matrices satisfying \( G^{(g)} W = W G^{(g)} \forall g \in G \); see Fig.4.a.a.1.a.2 for \( W \) that are equivariant to circular translation (a.1) and symmetric group \( S_4 \); the group of all permutations of 4 objects (a.2).

4 Equivariant Map for Product Groups

In this section we formalize the imprimitive action of the wreath product, which is used in describing the symmetries of hierarchical structures. We then introduce the closed form of linear maps equivariant to the wreath product of two groups. With hierarchies of more than two levels, one only needs to iterate this construction. To put this approach in perspective and to make the distinction clear, first we present the simpler case of direct product.

4.1 Equivariant Linear Maps for Direct Product of Groups

The easiest way to combine two groups is through their direct product \( G = \mathcal{H} \times \mathcal{K} \). Here, the underlying set is the Cartesian product of the input sets and group operation is \( (h, k)(h', k') \equiv (hh', kk') \). If \( \mathcal{P} \) is an \( \mathcal{H} \)-set and \( \mathcal{Q} \) a \( \mathcal{K} \)-set then the group \( G = \mathcal{H} \times \mathcal{K} \) naturally acts on \( \mathbb{N} = \mathcal{P} \times \mathcal{Q} \) using \( (h, k) \cdot (p, q) \equiv (hp, kq) \); see Fig.2.

This type of product is useful in modeling the Cartesian product of structures. The following claim characterises the equivariant map for direct product of two groups using the equivariant map for building blocks.

\[ (h, p, k, q) \]
\[ (h \cdot p, k \cdot q) \]

Figure 2: Direct product action.
Claim 1. Let $G^{(s)}$ represent $\mathcal{H}$-action, and let $W_{\mathcal{H}} \in \mathbb{R}^{P \times P}$ be an equivariant linear map for this action. Similarly, let $W_{\mathcal{K}} : \mathbb{R}^{Q \times Q}$ be equivariant to $\mathcal{K}$-action given by $G^{(t)}$ for $h \in \mathcal{K}$. Then, the product group $G = \mathcal{H} \times \mathcal{K}$ naturally acts on $\mathbb{R}^N = \mathbb{R}^{PQ}$ using $G^{(s \otimes t)} = G^{(s)} \otimes G^{(t)}$, and the Kronecker product $W_G = W_{\mathcal{H}} \otimes W_{\mathcal{K}}$, is a $G$-equivariant linear map.

Note that the claim is not restricted to permutation action. The proof follows from the mixed-product property of the Kronecker product and the equivariance of $W_{\mathcal{H}}$ and $W_{\mathcal{K}}$:

$$G^{(s)} W^G = (G^{(s)} \otimes G^{(t)})(W_{\mathcal{H}} \otimes W_{\mathcal{K}}) = (G^{(s)} W_{\mathcal{H}}) \otimes (G^{(t)} W_{\mathcal{K}})$$

$$= (W_{\mathcal{H}} G^{(s)}) \otimes (W_{\mathcal{K}} G^{(t)}) = (W_{\mathcal{H}} \otimes W_{\mathcal{K}})(G^{(s)} \otimes G^{(t)}) = W_G G^{(s \otimes t)} \quad \forall g \in G.$$

An implication of the tensor product form of $W_{\mathcal{H} \times \mathcal{K}}$ is that the number of independent linear operators of the product map (free parameters in the parameter-sharing) is the product of the independent operators of the building blocks.

Example 1 (Convolution in Higher Dimensions). $D$-dimensional convolution is a Kronecker (tensor) product of one-dimensional convolutions. The number of parameters grows with the product of kernel width across all dimensions; Fig. 2(a.1) shows the parameter-sharing for circular 1D convolution $W_{C_4}$, and (b.1) shows the parameter-sharing for the direct product $W_{C_4 \times C_4}$.

Example 2 (Exchangeable Tensors). Hartford et al. [27] introduce a layer for modeling interactions across multiple sets of entities, e.g., a user-movie rating matrix. Their model can be derived as the Kronecker product of 2-parameter equivariant layer for sets [50]. The number of parameters is therefore $2^D$ for a rank $D$ exchangeable tensor. Fig. 4(b.1) shows the 2-parameter model $W_{\mathbb{S}_4}$ for sets, and (c.1) shows the parameter-sharing for the direct product $W_{\mathbb{S}_3 \times \mathbb{S}_4}$.

4.2 Wreath Product Action and Equivariance to a Hierarchy of Symmetries

Let us start with an informal definition. Suppose as before $\mathbb{P}$ and $\mathbb{Q}$ are respectively an $\mathcal{H}$-set and a $\mathcal{K}$-set. We can attach one copy of $\mathbb{Q}$ to each element of $\mathbb{P}$. Each of these inner sets or fibers have their own copy of $\mathcal{K}$ acting on them. Action of $\mathcal{H}$ on $\mathbb{P}$ simply permutes these fibers. Therefore the combination of all $\mathcal{K}$ actions on all inner sets combined with $\mathcal{H}$-action on the outer set defines the action of the wreath product on $\mathbb{P} \times \mathbb{Q}$. Fig. 3 demonstrates how one point $(p, q)$ moves under this action. Next few paragraphs formalize this.

Semidirect Product. Formally, wreath product is defined using semidirect product which is a generalization of direct product. In part due to its use in building networks equivariant to Euclidean isometries, application of semidirect product in building equivariant networks is explored in several recent works; see [10] and citations therein. In semidirect product, the underlying set (of group members) is again the product set. However the group operation is more involved. The (external) semi-direct product $G = \mathcal{K} \rtimes_{\gamma} \mathcal{H}$, requires a homomorphism $\gamma : \mathcal{K} \to \text{Aut}(\mathcal{H})$ that for each choice of $h \in \mathcal{H}$, re-labels the elements of $\mathcal{H}$ while preserving its group structure. Using $\gamma$, the binary operation for the product group $G = \mathcal{K} \rtimes_{\gamma} \mathcal{H}$ is defined as $(h, k)(h', k') = (hh', k\gamma_h(k'))$. A canonical example is the semidirect product of translations ($\mathcal{H}$) and rotations ($\mathcal{H}$), which identifies the group of all rigid motions in the Euclidean space. Here, each rotation defines an automorphism of translations (e.g., moving north becomes moving east after $90^\circ$ clockwise rotation).

Now we are ready to define the wreath product of two groups. As before, let $\mathcal{H}$ and $\mathcal{K}$ denote two finite groups, and let $\mathbb{P}$ be an $\mathcal{H}$-set. Define $\mathcal{B}$ as the direct product of $\mathbb{P} = |\mathcal{P}|$ copies of $\mathcal{R}$, and index these copies by $p \in \mathbb{P}$: $\mathcal{B} = \mathcal{R}_1 \times \ldots \times \mathcal{R}_p \times \ldots \times \mathcal{R}_p$. Each member of this group is a tuple

\begin{equation}
\text{Imprimitive action of wreath product.}
\end{equation}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure3}
\caption{Imprimitive action of wreath product.}
\end{figure}

\footnote{The tensor product of reducible representation of two distinct finite groups is an irreducible representation for the product group. Therefore this construction of equivariant maps can be used with a decomposition into irreducible representations for the general linear case.

\footnote{\begin{equation}
(A \otimes B)(C \otimes D) = (AC) \otimes (BD)
\end{equation}}
Equi. blocks  
\( (a.1) \ C_4 \)  

Equi. maps for product \((\times)\) and hierarchical \((\iota)\) structures  
\( (a.2) \ S_4 \)

\( \delta = (k_1, \ldots, k_P) \). Since \( P \) is an \( H \)-set, \( H \) also naturally acts on \( B \) by permuting the fibers \( K_p \).

The semidirect product \( B \rtimes H \) defined using this automorphism of \( B \) is called the wreath product, and written as \( B \ltimes H \). Each member of the product group can be identified by the pair \((\bar{h}, \delta)\), where \( \delta \) as a member of the base group itself is a \( P \)-tuple. This shows that the order of the wreath product group is \( |H|^P |H| \) which can be much larger than the direct product group \( K \times H \), whose order is \( |K||H| \).

### 4.2.1 Imprimitive Action of Wreath Product

If in addition to \( P \) being an \( H \)-set, \( H \) action on \( Q \) is also defined, the wreath product group acts on \( P \times Q \) (making it comparable to the direct product). Specifically, \((h, 1, \ldots, 1) \in H \ltimes H \) acts on \((p, q) \in P \times Q \) as follows:

\[
(h, h_1, \ldots, h_P) \cdot (p, q) = (h \cdot p, h_{h_1} \cdot q).
\]

Intuitively, \( H \) permutes the copies of \( K \) acting on each \( Q \), and itself acts on \( P \). We can think of \( P \) as the outer structure and \( Q \) as the inner structure; see ??.

**Example 3** (Sequence of Sequences). Consider our early example where both \( H = C_P \) and \( K = C_Q \) are cyclic groups with regular action on \( P \cong H, \ Q \cong K \). Each member of the wreath product \( C_P \ltimes C_Q \) acts by translating each inner sequence using some \( c \in C_Q \), while \( c' \in C_P \) translates the outer sequence by \( c' \).

Let the \( P \times P \) permutation matrix \( G^{(h)} \) represent the action of \( h \in H \), and the \( Q \times Q \) matrices \( G^{(k_1)}, \ldots, G^{(k_P)} \) represent the action of \( k_p \) on \( Q \). Then the action of \( g \in H \ltimes H \) on (the vectorized) \( P \times Q \) is the following \( PQ \times PQ \) permutation matrix:

\[
G^{(g)} = \left[ \begin{array}{cccc}
G^{(h_1)}_{1,1} & \cdots & \cdots & G^{(h_1)}_{1,k_1} \\
\vdots & \ddots & \ddots & \vdots \\
G^{(h_P)}_{P,1} & \cdots & \cdots & G^{(h_P)}_{P,k_P}
\end{array} \right] = \sum_{p=1}^{P} 1_{p,h_p} \otimes G^{(k_p)}.
\]

(1)

where \( 1_{p,h_p} \) is a \( P \times P \) matrix whose only nonzero element is at row \( p \) and column \( h \cdot p \) with the value of 1; and \( G^{(k_p)}_{p,p'} \) is the element at row \( p \) and column \( p' \) of the permutation matrix \( G^{(k_p)} \). In the summation formulation, the Kronecker product \( 1_{p,h_p} \otimes G^{(k_p)} \) puts a copy of permutation matrix \( G^{(k_p)} \) as a block of \( G^{(g)} \). Note that the resulting permutation matrix is different from the Kronecker product; in this case we have \( P + 1 \) (permutation) matrices participating in creating \( G^{(g)} \), compared with two matrices in the vanilla Kronecker product.
4.2.2 Equivariant Map

Consider a hierarchical structure, potentially with more than two levels of hierarchy, such as a set of sequences of images. Moreover, suppose that we have an equivariant map for each individual structure. The question answered by the following theorem is: how to use the equivariant map for each level to construct the equivariant map for the entire hierarchy? For now, we only consider two levels of hierarchy; extension to more levels follows naturally, and is discussed later.

**Theorem 4.1.** Let \( \mathbf{W}_H \in \mathbb{R}^{P \times P} \) be the matrix of an \( H \)-equivariant map, and let \( \mathbf{W}_K \in \mathbb{R}^{Q \times Q} \) be equivariant to \( K \)-action. Then

\[
\mathbf{W}_{HK} = \mathbf{W}_H \otimes (1_Q 1_P^T) + 1_P \otimes \mathbf{W}_K, \quad \text{where} \quad 1_Q = [1, \ldots, 1]^T
\]

is a \( PQ \times PQ \) matrix of a linear map equivariant to the imprimitive action of \( H \times K \) on \( \mathbb{P} \times \mathbb{Q} \). Here, \( 1_P \) is the \( P \times P \) identity matrix.

Proof is in Appendix A. Assuming sets of independent equivariant linear operators \( \{\mathbf{W}_H\} \) and \( \{\mathbf{W}_K\} \), from Eq. (2) it is evident that the number of independent linear operators equivariant to \( H \times K \) is the sum of those of the building blocks. These operators may be combined using any parameter to create a parameterized linear map, which in turn can be expressed using parameter-sharing in a vanilla feedforward layer. This in contrast with direct product in which the number of free parameters has a product form.

**Example 4** (Various Hierarchies of Sets and Sequences). Consider two of the most widely used equivariant maps, translation equivariant convolution \( \mathbf{W}_{C_P} \), and \( \delta_Q \)-equivariant map which has the form \( \mathbf{W}_{\delta_Q} = w_I 1_Q + w_2 1_P \). There are four combinations of these structures in a two level hierarchical structure: 1) set of sets \( \delta_Q \circ \delta_P \); 2) sequence of sequences \( C_Q \circ C_P \); 3) set of sequences \( C_Q \circ \delta_P \); 4) sequence of sets \( \delta_Q \circ C_P \). Fig. 4(b.2-e.2) shows the parameter-sharing matrix for these hierarchical structures, assuming a full kernel in 1D circular convolution.

The reader is invited to contrast the three parameter layer for sets of sets, with the four parameter layer for interactions across sets in Fig. 4(c.1,c.2). Similarly, a model for sequence of sequences has far fewer parameters than a model for an image, as seen in Fig. 4(b.1,b.2).

4.2.3 Deeper Hierarchies and Combinations with Direct Product

With more than two levels, the symmetry group involves more than one wreath product, which means that the equivariant map for the hierarchy is given by a recursive application of Theorem 4.1. For example, the equivariant map for \( (H \times K) \circ \mathcal{U} \), in which \( \mathcal{U} \) acts on \( \mathbb{R} \), and \( \mathbf{W}_{\mathcal{U}} \) is the corresponding equivariant map, is given by \( \mathbf{W}_{(HK)\mathcal{U}} = \mathbf{W}_{\mathcal{U}} \otimes (1_{PQ} 1_P^T) + 1_P \otimes \mathbf{W}_{HK} \), where \( \mathbf{W}_{HK} \) is in turn given by Eq. (2). Note that wreath product is associative, and so the iterative construction above leads to the same equivariant map as \( \mathbf{W}_{(HK)\mathcal{U}} \).

We can also mix and match this construction with that of direct product in Claim 1, for example, to produce the map for exchangeable tensors (product of sets), where each interaction is in the form of an image (hierarchy) – i.e., the group is \( (C_R \times C_V) \circ (\delta_P \times \delta_Q) \).

4.3 Efficient Implementation

With equivariant maps for direct product of groups, efficient implementation of \( \mathbf{W}_{HK} \) using efficient implementation for individual blocks \( \mathbf{W}_H \) and \( \mathbf{W}_K \) is non-trivial – e.g., consider 2D convolution. In contrast, it is possible to use a black-box implementation of the parameter-sharing layers for \( \mathbf{W}_H \) and \( \mathbf{W}_K \) to construct \( \mathbf{W}_{HK} \). To this end, let \( x \in \mathbb{R}^{PQ} \) be the input signal, and \( \text{mat}(x) \in \mathbb{R}^{P \times Q} \) denote its matrix form; for example in a set of sets, each column is an inner set in this matrix form. Throughout, we are assuming a single input-output channel, relying on the idea that having multiple channels simply corresponds to replicating the linear map for each input-output channel combination. Then we can rewrite Eq. (2) as

\[
\mathbf{W}_{HK} x = \text{vec} \left( \left( \mathbf{W}_H \left( \text{mat}(x) 1_Q \right) \right) 1_P^T + \text{mat}(x) \mathbf{W}_K \right),
\]

(3)
where the first multiplication mat(x) 1_Q pools over columns (inner structures), and after application of the \( \mathcal{H} \)-equivariant map \( W_{\mathcal{H}} \) to the pooled value, the result is broadcasted back using right-multiplication by 1_Q. The second term simply transforms each inner structure using \( W_{\mathcal{H}} \). The overall operation turns out to be simple and intuitive: the inner equivariant map is applied to individual inner structures, and the outer equivariant map is applied to pooled values and broadcasted back.

**Example 5** (Equivariant Map for Multiresolution Image). Consider a coarse pixelization of an image into small patches. Eq. (3) gives the following recipe for a layer equivariant to independent translations within each patch as well as global translation of the coarse image: 1) apply convolution to each patch independently; 2) pool over each patch, apply convolution to the coarse image, and broadcast back to individual pixels in each patch. 3) add the contribution of these two operations. Notice how pooling over regions, a widely used operation in image processing, appears naturally in this approach. One could also easily extend this to more levels of hierarchy for larger images.

5 Application: Point-Cloud Segmentation

In this section we consider a simple application of the theory above to large-scale point-cloud segmentation. The layer is the 3D version of equivariant linear map for sequence of sets, which is visualized in Fig. 4(d.2). Using a hierarchical structure is beneficial compared to both the set model and 3D convolution. In particular, the set model lacks any prior of the Euclidean nature of the data, while the 3D convolution, in order to preserve resolution requires a fine-grained voxelization where each point appears in one voxel.

The past few years have seen a growing body of work on learning with point cloud data; see [19] for a survey. Many methods use hierarchical aggregation and pooling; this includes the use of furthest point clustering for pooling in POINN++ [27], use of concentric spheres for pooling in SHELLNET, or KD-tree guided pooling in [24]. Several works extend convolution operation to maintain both translation and permutation equivariance in one way or another [3, 4, 45]; see also [6, 17]. Here, objective is not to introduce a radically new procedure, but to show the effectiveness of approach discussed in previous sections in deep model design from first principles. Indeed, we are able to achieve state-of-the-art in several benchmarks for large point-clouds.

5.1 Equivariance to a Hierarchy of Translations and Permutations

Let \( X \in \mathbb{R}^{N \times C} \) be the input point cloud, where \( N \) is the number of points and \( C \) is the number of input channels (for concreteness, in this section we are including the channel dimension in our formulae.) In addition to 3D coordinates, these channels may include RGB values, normal vectors or any other auxiliary information. Consider a voxelization of the point cloud with a resolution \( D \) voxels per dimension, and consider the hierarchy of translation symmetry across voxels and permutation symmetry within each voxel. We may also replace 3D coordinates with relative coordinates within each voxel. Let \( \Pi \in \{0, 1\}^{D^3 \times N} \) with one non-zero per column identify the voxel membership. Then the combination of equivariant set layer \( X W_{1} + \Pi^T X W_{2} \) [50] with 3D convolution using the pool-broadcast interpretation given in Eq. (3), results in the following wreath-product equivariant linear layer

\[
\phi(X) = X W_{1} + \Pi^T (W_{3} \ast (\Pi X)),
\]

where \( W_{1} \in \mathbb{R}^{C \times C'}, \ast \) denotes the convolution operation, \( W_{2} \in \mathbb{R}^{K^3 \times C \times C'} \) is the convolution kernel, with kernel width \( K \), and \( C' \) output channels. Here, multiplication with \( \Pi \) and \( \Pi^T \) performs the pooling and broadcasting from/to points within voxels, respectively. Note that we have dropped the “set” operation \( \Pi^T ((\Pi X) W_{2}) \) that pools over each voxel, multiplies by the weight and broadcasts back to the points. This is because it can be absorbed in the convolution operation, and therefore it is redundant. In the equation above pooling operation can replace summation (implicit in matrix multiplication) with any other commutative operation; see [35, 48, 51], we use mean-pooling for the experiments. While the layer of Eq. (4) already achieves state-of-the-art in the experiments, we also consider adding an (equivariant) attention mechanism for further improvement; see Appendix B for details.
Table 1: Performance of various models on point cloud segmentation benchmarks.

| Model                | SEMANTIC-8 OA | S3DIS OA | VKITTI OA | mIoU | mIoU | mAcc |
|----------------------|---------------|----------|-----------|------|------|------|
| DEEPSETS             | 89.3          | 60.5     | 67.3      | 42.7 | 74.2 | 42.9 |
| POINTNET++           | 85.7          | 63.1     | 81.0      | 54.5 | 79.7 | 34.4 |
| SPG                  | 92.9          | 76.2     | 85.5      | 62.1 | 84.3 | 67.3 |
| CONVPOINT            | 93.4          | 76.5     | 88.8      | 68.2 | -    | -    |
| KP-FCNN              | -             | -        | -         | -    | 70.6 | -    |
| RSNet                | -             | -        | -         | -    | 56.5 | -    |
| PCCN                 | -             | -        | -         | -    | 58.3 | -    |
| SNAPNET              | 91.0          | 67.4     | -         | -    | -    | -    |
| ENGELMANN ET AL. 2018 | -         | -        | -         | -    | 79.7 | 57.6 |
| ENGELMANN ET AL. 2017 | -         | -        | -         | -    | 80.6 | 54.1 |
| WREATH PRODUCT NET  | 93.9          | 75.4     | 90.6      | 71.2 | 88.4 | 68.9 |
| WREATH PRODUCT NET + ATTN | 94.6 | 77.1 | 95.8 | 80.1 | 90.7 | 69.5 |

5.2 Empirical Results

We evaluate our model on two of the largest real world point cloud segmentation benchmarks, SEMANTIC3D [20] and the Stanford Large-Scale 3D Indoor Spaces (S3DIS) [2], as well as a dataset of virtual point cloud scenes, the VKITTI benchmark [16]. In all cases we report new state-of-the-art. The architecture of WREATH PRODUCT NET is a stack of equivariant layer Eq. (4) plus ReLU nonlinearity and residual connections. WREATH PRODUCT NET + ATTN also adds the attention mechanism. Details on architecture and training, as well as further analysis of results appear in Appendix C.

Outdoor Scene Segmentation - SEMANTIC3D [20] is the largest LiDAR benchmark dataset, consisting of 15 training point clouds and 15 tests point clouds with withheld labels, amassing altogether over 4 billion labeled points from a variety of urban and rural scenes. In particular, rather than working with the smaller reduced-8 variation, we run our experiments on the full dataset (SEMANTIC-8) [5]. Table 1 reports mIoU unweighted mean intersection over union metric (mIoU), as well as the overall accuracy (OA) for various methods.

Indoor Scene Segmentation - Stanford Large-Scale 3D Indoor Spaces (S3DIS) [2] consists of various 3D RGB point cloud scans from an assortment of room types on six different floor in three buildings on the Stanford campus, totaling almost 600 million points. Table 1 show that we achieve the best overall accuracy as well as mean intersection over union. This is in spite of the fact that our competition use extensive data-augmentation also for this dataset. In addition to random jittering and subsampling employed by both KPConv and CONVPOINT, KPConv also uses random dropout of RGB data.

Virtual Scene Segmentation - Virtual KITTI (VKITTI) [16] contains 35 monocular photorealistic synthetic videos with fully annotated pixel-level labels for each frame and 13 semantic classes in total. Following [12], we project the 2D depth information within these synthetic frames into 3D space, thereby obtaining semantically annotated 3D point clouds. Note that vKITTI is significantly smaller than either SEMANTIC3D or S3DIS, containing only 15 millions points in total.

Conclusion

This paper presents a procedure to design neural networks equivariant to hierarchical symmetries and nested structures. We describe how wreath product can formulate the symmetries in these settings, contrast its use case with direct product, and identify linear maps equivariant to the wreath product of groups as a function of equivariant maps for the building blocks, using additional pool-and-broadcast operations. We consider one of the many use cases of this approach to design a deep model for large-scale semantic segmentation of point cloud data, where we are able to achieve state-of-the-art using a simple architecture.

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We have released a PYTORCH implementation of our models. at ANONYMOUS.

The leader-board can be viewed at http://www.semantic3d.net/view_results.php?chl=1.

8
**Broader Impact**

As deep learning finds its way in various real-world applications, the practitioners are finding more constraints in representing their data in formats and structures amenable to existing deep architectures. The list of basic structures such as images, sets, and graphs that we can approach using deep models has been growing over the past few years. The theoretical contribution of this paper substantially expands this list by enabling deep learning on a hierarchy of structures. This could potentially unlock new applications in data-poor and structure-rich settings. The task we consider in our experiments is deep learning with large point-cloud data, which is finding growing applications, from autonomous vehicles to geographical surveys. While this is not a new task, our empirical results demonstrate the effectiveness of the proposed methodology in dealing with hierarchy in data structure.

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A Proof of Theorem 4.1

Proof. We show that both of the two terms in Eq. (2) are equivariant to \( \mathcal{K} \triangleright \mathcal{H} \)-action as expressed by the permutation matrix of Eq. (1).

Part 1. We show that \( G^{(g)} \) commutes with the first term in Eq. (2) for any \( g \in \mathcal{K} \triangleright \mathcal{H} \):

\[
\left( W_{\mathcal{H}} \otimes (1_Q 1_Q^\top) \right) G^{(g)} = \left( W_{\mathcal{H}} \otimes (1_Q 1_Q^\top) \right) \left( \sum_{p=1}^P 1_{p, k-p} \otimes G^{(g_p)} \right)
\]

\[
= \sum_{p=1}^P \left( W_{\mathcal{H}} 1_{p, k-p} \right) \otimes ((1_Q 1_Q^\top) G^{(g_p)}).
\]

\[
= W_{\mathcal{H}} \left( \sum_{p=1}^P 1_{p, k-p} \right) \otimes (1_Q 1_Q^\top)
\]

\[
= (W_{\mathcal{H}} G^{(g)}) \otimes (1_Q 1_Q^\top) = (G^{(g)} W_{\mathcal{H}}) \otimes (1_Q 1_Q^\top)
\]

\[
= \sum_{p=1}^P (1_{p, k-p} W_{\mathcal{H}}) \otimes ((1_Q 1_Q^\top) G^{(g_p)})
\]

\[
= \sum_{p=1}^P (1_{p, k-p} \otimes G^{(g_p)})(W_{\mathcal{H}} \otimes (1_Q 1_Q^\top))
\]

\[
= \left( \sum_{p=1}^P 1_{p, k-p} \otimes G^{(g_p)} \right) \left( W_{\mathcal{H}} \otimes (1_Q 1_Q^\top) \right) = G^{(g)} \left( W_{\mathcal{H}} \otimes (1_Q 1_Q^\top) \right).
\]

In Eq. (5) we substitute from Eq. (1). In Eq. (6) we pulled the summation out, and then used the mixed product property of Kronecker product. We also note that a permutation of the uniformly constant matrix \( 1_Q 1_Q^\top \) is constant. In Eq. (7), since the summation can be restricted to the first term we pull out \( W_{\mathcal{H}} \). In Eq. (8) we use the fact that the summation of the previous line is the permutation matrix \( G^{(g)} \) and apply the key assumption that \( W_{\mathcal{H}} \) and \( W_{\mathcal{H}} \) are equivariant to \( \mathcal{H} \) and \( \mathcal{K} \)-action respectively. The following lines repeat the procedure so far in reverse order to commute \( G^{(g)} \) and

\[
(W_{\mathcal{H}} \otimes (1_Q 1_Q^\top)).
\]

Part 2. For the second term, again we use the mixed-product property and equivariance of the input maps

\[
(I_P \otimes W_{\mathcal{H}}) G^{(g)} = (I_P \otimes W_{\mathcal{H}}) \left( \sum_{p=1}^P 1_{p, k-p} \otimes G^{(g_p)} \right)
\]

\[
= \sum_{p=1}^P (I_P 1_{p, k-p}) \otimes (W_{\mathcal{H}} G^{(g_p)})
\]

\[
= \sum_{p=1}^P (1_{p, k-p} I_P) \otimes (G^{(g_p)} W_{\mathcal{H}})
\]

\[
= \sum_{p=1}^P (1_{p, k-p} \otimes G^{(g_p)})(I_P \otimes W_{\mathcal{H}}) = G^{(g)} (I_P \otimes W_{\mathcal{H}})
\]

where in Eq. (12) we used the fact that the identity matrix commutes with any matrix, as well as the equivariance of \( G^{(g_p)} \). Eqs. (13) and (15) simply use the mixed product property. Putting the two parts together shows the equivariance of the first and second term in Eq. (2), completing the proof. \( \square \)
B Adaptive Pooling and Attention

While the layer of Eq. (4) performs competitively, to improve its performance we add a novel attention mechanism. To this end we complement the pool-and-broadcast scheme of Eq. (4) with an adaptive pooling mechanism using a learned $\tilde{\Pi} : \mathbb{R}^N \rightarrow \Delta_L$ in Eq. (4), where $\Delta_L$ is the $L$-dimensional probability simplex. Here, one may interpret $L$ as the number of latent classes, analogous to $D^3$ voxels. The pooling matrix $\tilde{\Pi}$, is a function of input through a linear map $W_3^{(\ell)} \in \mathbb{R}^{C \times L}$ followed by $\text{Softmax} : \mathbb{R}^L \rightarrow (0, 1)^L$, so that the probability of each point belonging to different classes sums to one – that is

$$\tilde{\Pi}_n = \text{Softmax} ((XW_3)_n) \forall n \in [N]. \quad (16)$$

We then use a linear function that models the interaction between latent classes, for each pair of channels. This is done using a rank four tensor $W_4 \in \mathbb{R}^{L \times L \times C \times C}$. As before the result is broadcasted back using $\tilde{\Pi}_n$, giving us the adaptive pooling layer, in which the output for channel $c$ is given by

$$\phi(X)_c = \sum_{c' = 1}^{C'} \tilde{\Pi}^T W_4_{c,c'} \tilde{\Pi} X_c. \quad (17)$$

Intuitively this layer can decide which subset of nodes to pool, and therefore acts like an equivariant attention mechanism. In experiments, we see further improvement in results when adding this nonlinear layer to the linear layer of Eq. (4).

C Details on Experiments

C.1 Architecture and Data Processing

Our results are produced using minor architectural variations and limited hyperparameter search. Concretely, our best-performing models on semantic3D and s3dis involve 56 residual-style blocks, where each block comprises of 2 equivariant linear maps of Eq. (4). Each map involves a single 3D convolution operator with periodic padding and a $3 \times 3 \times 3$ kernel. We use an identity map to facilitate skip connections within these blocks. The number channels is fixed 64, except the final block, which maps to the number of segmentation classes (8 for semantic3D and 13 for s3dis).

When incorporating adaptive pooling, we utilize 5, 10, 15, 25 and 50 latent classes for blocks 1-19, 19-29, 30-39, 40-49 and 50-56, respectively and inclusively. Our best-performing model on vkitti uses 5, 10, 15, and 20 latent classes for blocks 1-9, 10-14, 15-19, and 20-22, respectively and inclusively.

Additionally, while previous works rely on stochastic point cloud subsampling during pre-processing and reprojection during post-processing, we simply split large point clouds into subsets of 1 million points each to ameliorate memory issues. We then compute a $9 \times 9 \times 9$ voxelization over each sample, and train on mini-batches of 4 such samples. To generate predictions, we stitch predictions on these smaller samples together.

C.2 Datasets: Training, Validation and Test

Outdoor Scene Segmentation - semantic3D semantic3D [20] We hold out 4 of the available 15 training point clouds to use as a validation set, as in [30]. Table 2 reports the overall accuracy (OA), and mean intersection over union (mIoU) for our method and the competition. We achieve both the best overall accuracy as well as the best mean intersection over union.

Indoor Scene Segmentation - Stanford Large-Scale 3D Indoor Spaces (s3dis) The s3dis dataset [2] consists of various 3D RGB point cloud scans from an assortment of room types on six different floor in three buildings on the Stanford campus, totaling almost 600 million points. Following previous works by [12, 30, 36, 37, 42], we perform 6-fold cross validation with microaveraging, computing all metrics once over the merged predictions of all test folds.
Table 2: Performance of various models on the full semantic3d dataset (semantic-8). Higher is better, bolded is best. mIoU is unweighted mean intersection over union metric. OA is overall accuracy. Per class splits show mIoU.

| Method               | OA  | mIoU | Man-Made Terrain | Natural Vegetation | High Vegetation | Low Vegetation | Buildings | Hardscape | Scanning Artifacts | Cars |
|----------------------|-----|------|------------------|-------------------|----------------|---------------|-----------|-----------|-------------------|------|
| DEEPSET [30]         | 89.3| 60.5 | 90.8             | 76.3              | 41.9           | 22.1          | 94.0      | 46.5      | 26.8              | 85.4 |
| POINTNET [36]        | 85.7| 63.1 | 81.9             | 78.1              | 64.3           | 51.7          | 75.9      | 36.4      | 43.7              | 72.6 |
| SNAPPOINT [23]       | 91.0| 67.4 | 89.6             | 79.5              | 74.8           | 56.1          | 80.9      | 36.5      | 34.3              | 77.2 |
| SPG [50]             | 92.9| 76.2 | 91.5             | 75.6              | 78.3           | 71.7          | 94.4      | 56.8      | 52.9              | 88.4 |
| CONVPOINT [41]       | 93.4| 76.5 | 92.1             | 80.6              | 76.0           | 71.9          | 95.6      | 47.3      | 61.1              | 87.7 |

WREATH PRODUCT NET + ATTN (ours) 93.9 75.4 93.4 84.0 76.4 68.2 96.8 45.6 47.4 91.9 93.4
WREATH PRODUCT NET + ATTN (ours) 94.6 77.1 95.2 87.1 75.3 67.1 96.1 51.3 51.0 93.4

Table 3: Performance of various models on the s3dis dataset (micro-averaged over all 6 folds). Higher is better, bolded is best. mIoU is unweighted mean intersection over union metric. OA is overall accuracy. Per class splits show mIoU.

C.3 Virtual Scene Segmentation - Virtual KITTI

The VKITTI dataset [16] contains 35 monocular photo-realistic synthetic videos with fully annotated pixel-level labels for each frame and 13 semantic classes in total. Following [12], we project the 2D depth information within these synthetic frames into 3D space, thereby obtaining semantically annotated 3D point clouds. Similar to the training and evaluation scheme in [12, 29], we separate the original set of sequences into 6 non-overlapping subsequences and use a 6 fold cross-validation protocol (with micro-averaging similar to the methodology on s3DIS).

| Method               | OA  | mIoU | Ceiling | Floor | Wall | Beam | Column | Window | Door | Chair | Table | Bookcase | Sofa | Board | Clutter |
|----------------------|-----|------|---------|-------|------|------|--------|--------|------|-------|-------|----------|-----|-------|---------|
| DEEPSET [30]         | 87.3| 42.7 | 81.1    | 72.4  | 67.2 | 16.9 | 25.8   | 44.2   | 48.5 | 51.0  | 49.8  | 21.7     | 24.4| 17.2  | 34.6    |
| POINTNET [36]        | 78.5| 47.6 | 80.0    | 88.7  | 69.3 | 42.4 | 23.1   | 47.5   | 51.6 | 42.0  | 84.1  | 38.2     | 9.6 | 29.4  | 35.2    |
| KP-CNN [41]          | N/A | 56.5 | 92.8    | 78.6  | 32.8 | 34.4 | 51.6   | 68.1   | 60.1 | 59.7  | 50.2  | 16.4     | 44.9| 52.0  | 52.0    |
| CONVPOINT [41]       | 85.3| 62.1 | 89.9    | 95.1  | 76.4 | 62.8 | 47.1   | 55.3   | 64.8 | 73.5  | 60.2  | 43.5     | 4.7 | 52.9  | 52.9    |
| WREATH PRODUCT NET   | 90.6| 71.2 | 94.3    | 96.3  | 80.6 | 65.0 | 76.2   | 82.1   | 71.9 | 64.5  | 62.7  | 90.2     | 68.8| 63.5  | 59.9    |
| WREATH PRODUCT NET + ATTN (ours) | 95.8| 88.1 | 97.8    | 97.8  | 80.6 | 72.3 | 82.0   | 75.6   | 75.1 | 72.8  | 73.1  | 71.4     | 82.1| 77.2  | 77.2    |

Table 4: Performance of various models on the VKITTI dataset (micro-averaged over all 6 folds). Higher is better, best results are in bold. mIoU is unweighted mean intersection over union metric. OA is overall accuracy. mAcc is mean accuracy.

| Method               | OA  | mIoU | mAcc  |
|----------------------|-----|------|-------|
| DEEPSET [30]         | 74.2| 42.9 | 36.8  |
| POINTNET [36]        | 79.7| 34.4 | 47.0  |
| ENGELMANN ET AL. 2018 [13] | 79.7| 57.6 | 35.6  |
| ENGELMANN ET AL. 2018 [13] + 3P-KNN [59] | 87.8| 54.1 | 41.6  |
| SPG [50]             | 84.3| 67.3 | 52.0  |
| WREATH PRODUCT NET   | 88.4| 68.9 | 58.6  |
| WREATH PRODUCT NET + ATTN (ours) | 90.7| 69.5 | 59.2  |

Note that VKITTI is significantly smaller than either semantic3D or s3DIS, containing only 15 millions points in total. We hypothesize that these smaller, and sparser point clouds provide little geometric signal outside vegetation and road structure. This partially explains our only incremental improvement over the state of the art (see Table 4). However, we expect future simulations of point cloud scenes to become increasingly dense, in line with increasingly powerful LiDAR scanners for real world applications [14, 40], where our simple baselines can potentially produce significant gain both in accuracy and computation.