CLIFFORD GROUP EQUIVARIANT SIMPLICIAL MESSAGE PASSING NETWORKS

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ABSTRACT

We introduce Clifford Group Equivariant Simplicial Message Passing Networks, a method for steerable $\mathrm{E}(n)$-equivariant message passing on simplicial complexes. Our method integrates the expressivity of Clifford group-equivariant layers with simplicial message passing, which is topologically more intricate than regular graph message passing. Clifford algebras include higher-order objects such as bivectors and trivectors, which express geometric features (e.g., areas, volumes) derived from vectors. Using this knowledge, we represent simplex features through geometric products of their vertices. To achieve efficient simplicial message passing, we share the parameters of the message network across different dimensions. Additionally, we restrict the final message to an aggregation of the incoming messages from different dimensions, leading to what we term *shared* simplicial message passing. Experimental results show that our method is able to outperform both equivariant and simplicial graph neural networks on a variety of geometric tasks.

1 INTRODUCTION

Graph Neural Networks (GNNs) have become powerful in learning from relational data across various fields (Fan et al., 2019; Zitnik & Leskovec, 2017; Battaglia et al., 2016) due to their capacity to handle complex relational structures. Limitations in their expressive power for distinguishing non-isomorphic graphs (Geerts & Reutter, 2022) have been addressed by developing simplicial message-passing networks (Bodnar et al., 2021), which show both theoretical and practical enhancements in expressive power. Geometric graphs embedded in spaces like metric spaces or manifolds, with features that undergo transformations, have driven advances in the field (Satorras et al., 2021; Huang et al., 2022; Thölke & Fabritiis, 2022; Finzi et al., 2020; Brandstetter et al., 2022; Batzner et al., 2022), including the use of Clifford algebra in Clifford Group Equivariant Neural Networks (CGENNs) for enhanced expressivity (Ruhe et al., 2023). We extend this work by introducing Clifford Group Equivariant Simplicial Message Passing Networks (CSMPNs) (Liu et al., 2024), which leverage Clifford algebra to incorporate higher-order elements and achieve better performance on geometric tasks across diverse domains and dimensions, surpassing both equivariant and traditional message-passing GNNs.

2 BACKGROUND

We briefly introduce Clifford group equivariant neural networks and simplicial complexes. For in-depth coverage, see Liu et al. (2024); Eijkelboom et al. (2023); Ruhe et al. (2023); Bodnar et al. (2021).

2.1 CLIFFORD GROUP EQUIVARIANT NEURAL NETWORKS

We focus on the Clifford algebra $\mathrm{Cl}(\mathbb{R}^d, q)$ for a vector space $\mathbb{R}^d$ with a quadratic form q. Elements of the algebra, or multivectors, include scalars, vectors, bivectors, representing various geometric

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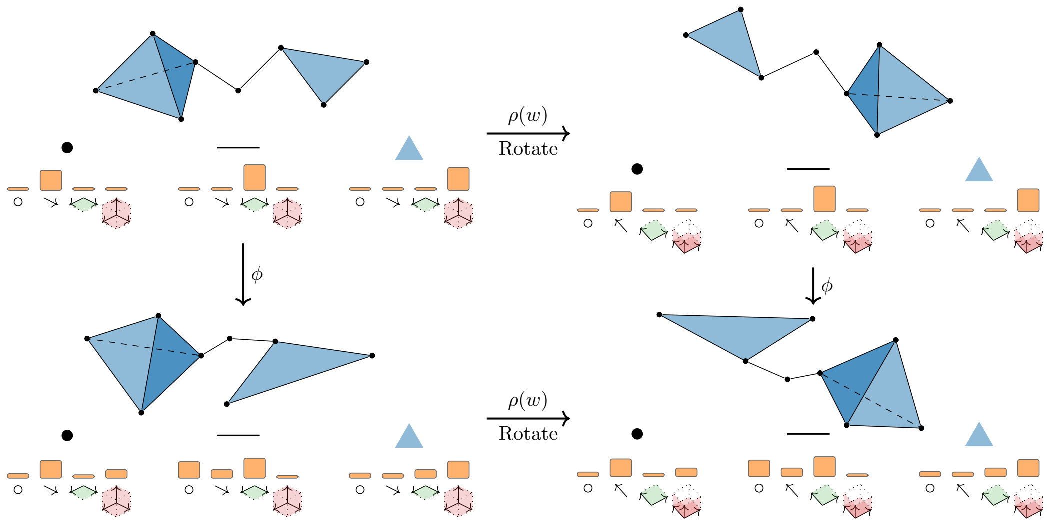

Figure 1: Illustration of our proposed architecture. Top left: a set of vertices (and edges) is lifted to a simplicial complex. We highlight three simplex types: vertices (0-simplices, ●), edges (1-simplices, —), and triangles (2-simplices, ▲). In this case, the vertex feature is vector-valued and embedded as the grade 1 part of a Clifford algebra element: a *multivector*. In three dimensions, a multivector has scalar (○), vector (↗), bivector ( ) and trivector ( ) components. Higher-order simplices are initialized using the geometric product of their constituent vertices. As such, edges in the top left visualization are bivector-valued, and triangles are trivector-valued. The simplicial message-passing framework, denoted by ϕ, refines the multivector-valued simplices, as portrayed in the bottom-left, by passing messages between simplices of different order. Crucially, ϕ maintains *equivariance* to the Clifford group's orthogonal action $\rho(w)$, representing a rotation here. In doing so, our method is ensured to respect the geometric symmetries of the input data.

quantities. For a detailed discussion on Clifford algebra, refer to Ruhe et al. (2023). The Clifford group $\Gamma(\mathbb{R}^d, q)$ consists of invertible multivectors preserving the quadratic form, leading to orthogonal automorphisms, which can be seens as the transformations in corresponding Clifford spaces.

Ruhe et al. (2023) demonstrate that polynomials in multivectors and their grade projections are Clifford group equivariant. Based on these two equivariance properties, Ruhe et al. (2023) build geometrically expressive Clifford group equivariant layers.

2.2 Simplicial Complexes

A simplicial complex K is a collection of subsets, called simplices, closed under taking subsets. The 1-skeleton of K is a graph, making complexes a generalization of graphs. Simplicial adjacencies (Bodnar et al., 2021) define how simplices are connected to form a simplicial complex. Simplicial message passing extends regular message passing to these higher-dimensional structures. The theorems by Bodnar et al. (2021) state that simplicial message passing networks are more powerful than the 1-Weisfeiler-Lehman test for graph isomorphism and obtain competitive results on various realistic graph learning tasks.

3 Clifford Group Equivariant Simplicial Message Passing Networks

3.1 Creating Geometric Simplicial Complexes

Constructing a simplicial complex K from a set V, part of a graph $G = (V, E)$, can be done in several ways. The naive approach forms a simplex for every subset of V, leading to a large number of simplices, $\binom{|V|}{n+1}$ for n-simplices, which is often impractical.

To address this, various methods lift a point set to a simplicial complex more efficiently. These include the Vietoris-Rips and Čech complexes, clique lifts from graph structures, manual constructions, and algorithmic approaches like the mapper procedure (Hajij et al., 2018). The Vietoris-Rips complex, for instance, is built by including simplices among ϵ-close vertices for a given $\epsilon > 0$. A manual lift might involve constructing a mesh by defining vertices, edges, and faces, or using domain-specific knowledge, such as the bond angle in a water molecule.

In our work, we employ the Vietoris-Rips and manual lifts, limiting the maximal simplex dimension to 2 for computational efficiency.

3.2 Embedding Simplicial Data in the Clifford Algebra

We detail the embedding of scalar and vector node features into the Clifford algebra and the creation of simplex features. Node features $h^v \in \mathbb{R}^k \oplus \left(\mathbb{R}^d\right)^l$ include scalars, like mass or charge, and vectors like position or velocity. Scalars embed into $\mathrm{Cl}^{(0)}(\mathbb{R}^d, q) = \mathbb{R}$ and vectors into $\mathrm{Cl}^{(1)}(\mathbb{R}^d, q) = \mathbb{R}^d$. Higher-order features are embedded in corresponding Clifford subspaces, resulting in $h^v \in \mathrm{Cl}(\mathbb{R}^d, q)^m$.

We now consider a simplicial complex K lifted from V. Our goal is, analogously to the node features, to obtain a Clifford feature h^σ for each simplex $\sigma \in K$. For the singletons $\{v_i\} \in K$, we can directly put $h^{\{v_i\}} := h^{v_i}$. For the edges $\{v_i, v_j\} \in K$, we can put $h^{\{v_i,v_j\}} := h^{v_i} h^{v_j}$, denoting the geometric product of the two Clifford features. This process extends to triangles and higher-dimensional simplices, multiplying Clifford features of all vertices with geometric product. In Figure 1, we depict this embedding, illustrating how edge and triangle simplices relate to bivector- and trivector-valued features. Since there are multiple ways to embed simplices, we *learn* the embedding through Clifford group-equivariant layers, i.e., we take the Clifford simplicial features as input to learnable Clifford group-equivariant layers and use the outputs as the learnable Clifford simplicial features. These can be decomposed into parameterized linear combinations as well as parameterized geometric products, resulting in analogous embeddings to the ones described above, but including learnable parameters. To ensure permutation-invariant embeddings, one can aggregate permutations of geometric products. A more intricate approach involves passing messages between the vertices of a k-simplex. The aggregated readout is then used as the initialized feature for the k-simplex.

Eijkelboom et al. Eijkelboom et al. (2023) manually define embeddings using distances and angles. Our approach, leveraging both additive and multiplicative methods, learns to embed covariant information from multiple nodes and generalizes to higher-dimensional spaces.

3.3 Equivariant Shared Simplicial Message Passing

For all $\sigma \in K$, we now have a Clifford feature $h^\sigma \in \mathrm{Cl}(\mathbb{R}^d, q)^m$. We propose two techniques that enable efficient (equivariant) message passing on simplicial complexes. In doing so, we require access to a parameterized message function ϕ^m and an update function ϕ^h. First, the message m^σ will be an equivariant aggregation of all information (processed by a neural network) from several adjacencies of different dimensions as defined in Bodnar et al. (2021) [1]. In contrast to, e.g., Eijkelboom et al. (2023); Bodnar et al. (2021), who iteratively run message passing for different adjacency types, we can leverage existing parallel implementations of classical message passing. In other words, we consider the adjacency matrix of the simplicial complex's corresponding *hypergraph*, where we have several *meta-vertices* that represent the different types of simplices. This corresponds to considering the 0-simplices of the *barycentric subdivision* of the simplicial complex, which is a common way for refining simplicial complexes (Ghrist, 2014). This idea is visualized in Figure 2.

Secondly, instead of considering a different parameterization for each type of communication, we define a single message function ϕ^m that can handle all types of communication. However, by conditioning ϕ^m on the type of message, it can still leverage the simplicial complex. In doing so,

[1] Intriguingly, Bodnar et al. (2021) prove that only the boundary and upper adjacencies are required for full expressivity. However, we only use the boundary, coboundary, and upper adjacencies to keep consistent with Eijkelboom et al. (2023).

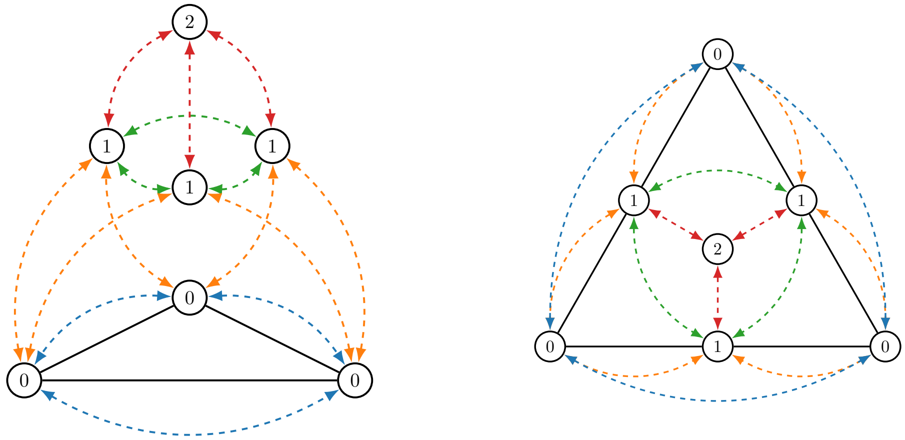

Figure 2: Left: we show how a simple graph (three fully-connected nodes) is lifted to a simplicial complex. Using simplicial message passing, we allow communication between objects of different dimensions. That is, between vertices ($0 \leftrightarrow 0$) blue dashed arrow, nodes and edges ($0 \to 1$ and $1 \to 0$) orange dashed arrow, edges ($1 \leftrightarrow 1$) green dashed arrow, and between edges and triangles ($1 \to 2$ and $2 \to 1$) red dashed arrow. Right: same as left, but a top-down view. It illustrates the hypergraph associated with the complex with several *meta-vertices* representing the simplices of various dimensionality. Instead of running message passing separately for all different communication types, we share the parameters of a single neural network operating on the extended graph. By conditioning on the message type, it is still able to leverage the simplicial complex.

we efficiently share parameters between different types of communication, which is in contrast with previous methods that defined a different neural network for each type of communication.

To make the overall method equivariant, we utilize Clifford group equivariant neural networks from Ruhe et al. (2023). Then, as long as the simplicial embedding, the aggregation operation (e.g., a summation), and ϕ^m and ϕ^h are equivariant, the overall method is Clifford group equivariant. This then makes it equivariant to rotations, reflections, and other orthogonal transformations in any dimension. The algorithm is summarized in Algorithm 1. Note that it generalizes typical message passing, which only considers messages from the upper adjacencies between 0-simplices, i.e. nodes.

Algorithm 1 Shared Simplicial Message Passing

Require: $K, \forall \sigma \in K : h^\sigma, \phi^m, \phi^h$

Repeat:

$$m^\sigma \leftarrow \operatorname{Agg}_{\substack{\tau \in B(\sigma) \\ \tau \in C(\sigma) \\ \tau \in N_\uparrow(\sigma) \\ \tau \in N_\downarrow(\sigma)}} \phi^m(h^\sigma, h^\tau, \dim \sigma, \dim \tau)$$

$$h^\sigma \leftarrow \phi^h\left(h^\sigma, m^\sigma, \dim \sigma\right)$$

4 Experiments

We selected a diverse set of geometric experiments encompassing different data types across various domains, focusing on both invariant and equivariant predictions. To ensure fair comparisons, we carefully balanced the parameter scales between our proposed CSMPN and the baseline models in all experiments.

4.1 5D Convex Hulls

In a five-dimensional space, we estimate the volume of convex hulls formed by eight points sampled from a standard distribution, inspired by Ruhe et al. (2023). This $\mathrm{E}(5)$-invariant task showcases the effectiveness of our model, CSMPN, which leverages simplicial structures for enhanced performance, outperforming traditional approaches by emphasizing the simplicial network's advantages.

	MSE (↓)
MPNN (Gilmer et al., 2017)	0.212
GVP-GNN (Jing et al., 2021)	0.097
VN (Deng et al., 2021)	0.046
EGNN (Satorras et al., 2021)	0.011
CEGNN (Ruhe et al., 2023)	0.013
EMPSN (Eijkelboom et al., 2023)	0.007
CSMPN	**0.002**

Table 1: MSE (↓) of the tested models on the convex hulls experiment.

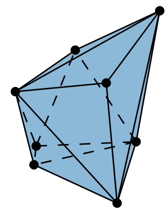

Figure 3: In the convex hulls experiment, the task is to estimate the volume of the convex hull of eight *five-dimensional* random points. Here, we display a three-dimensional example, which is easier to visualize.

Method	MSE (↓)
Radial Field (Köhler et al., 2020)	197.0
TFN (Thomas et al., 2018)	66.9
SE(3)-Tr (Fuchs et al., 2020)	60.9
GNN (Gilmer et al., 2017)	67.3
EGNN (200K) (Satorras et al., 2021)	31.7
GMN (200K) (Huang et al., 2022)	17.7
EMPSN (200K)	15.1
CEGNN (200K)	9.41
CSMPNs (200K)	**7.55**

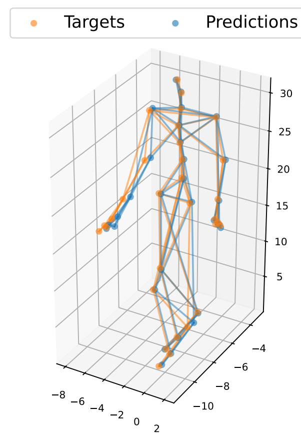

Table 2: Left: MSE (10^{-2}) of the tested models on the CMU motion capture dataset. Right: Depiction (not cherry-picked) of an instance (the ground-truth target positions) vs. a CSMPN prediction.

4.2 CMU Motion Capture

We evaluate our models on the CMU Human Motion Capture dataset (Gross & Shi, 2001), demonstrating the superiority of CSMPN over other equivariant architectures utilizing regular graphs. Focusing on predicting positions of 31 nodes representing human body parts during walking, we manually transform regular graphs into simplicial complexes to better capture human anatomy. Our results, compared against baselines including those from Huang et al. (2022), highlight the effectiveness of simplicial message passing ($\mathrm{E}(n)$ Equivariant Message Passing Simplicial Network (EMPSN)) and the added accuracy achieved with Clifford layers (in CGENN and further optimized in CSMPN).

	Aspirin	Benzene	Ethanol	Malonaldehyde
EqMotion (300K) (Xu et al., 2023)	5.95 / 8.38	1.18 / 1.73	5.05 / 7.02	5.85 / 9.02
EMPSN (300K)	9.53 / 12.63	**1.03 / 1.12**	8.80 / 9.76	7.83 / 10.85
CGENN (300K)	**3.70 / 5.63**	**1.03** / 1.59	4.53 / 6.35	4.20 / 6.55
CSMPN (300K)	3.82 / 5.75	**1.03** / 1.60	**4.44 / 6.30**	**3.88 / 5.94**

Table 3: ADE / FDE (10^{-2}) (↓) of the tested models on the MD17 atomic motion dataset.

	Attack	Defense
DAG-Net (200K) (Monti et al., 2020)	8.98 / 14.08	6.87 / 9.76
CGENN (200K)	9.17 / 14.51	6.64 / 9.42
CSMPN (200K)	**8.88 / 14.06**	**6.44 / 9.22**

Table 4: ADE / FDE (↓) of the tested models on the VUSport NBA player trajectory dataset.

4.3 MD17 Atomic Motion Prediction

We explore the molecular dynamics within the MD17 dataset Chmiela et al. (2017), focusing on predicting atom motions rather than the traditional energy prediction task. Selecting four molecules—aspirin, benzene, ethanol, and malonaldehyde—we aim to evaluate the efficacy of CSMPN in modeling the dynamics by forecasting future atom positions from initial positions of heavy atoms across ten time frames for each molecule. The construction of regular graphs for aspirin is based on k-nearest neighbors ($k = 3$), whereas other molecules utilize fully connected graphs, subsequently lifted to simplicial complexes via clique complexes.

Performance is assessed using Average Displacement Error / Final Displacement Error (ADE / FDE) metrics, with results indicating that simplicial message passing, particularly through EMPSN, significantly enhances predictive accuracy. Clifford layers contribute to further improvements, except in benzene's case, suggesting a beneficial inductive bias from the restricted expressivity of EMPSN for rigid, planar molecules. CSMPN demonstrates superior performance across most assessments, with notable advancements in ethanol and malonaldehyde predictions. Model comparisons ensure equal simplicial structures and parameter counts, maintaining architectural similarities between CGENN and CSMPN models.

4.4 NBA Players 2D Trajectory Prediction

In this study, we assess the capabilities of CSMPN using the STATS SportVU NBA Dataset (STATS Perform, 2023), which records two-dimensional tracking positions of NBA players during regular seasons. Our preprocessing follows the method of Monti et al. (2020), treating each player's position as a two-dimensional point. We focus on predicting player movements in both offensive and defensive scenarios over forty future frames, based on ten observed frames. The challenge lies in accounting for motion uncertainty and player interactions.

In our approach, each player is represented as a node in a fully-connected graph, with an additional fixed reference point to indicate the basketball court's orientation. We construct the simplicial complex using the Vietoris-Rips method with infinite ϵ and limit the maximum simplex dimension to 2. Our model's performance is compared against several baselines, including CGENN and those mentioned by Monti et al. (2020), with results detailed in Table 4.

5 Conclusion

We introduce Clifford Group Equivariant Simplicial Message Passing Networks (CSMPNs), Clifford algebra-based neural networks that are $\mathrm{E}(n)$-equivariant and operate on simplicial complexes. Our method merges the expressiveness of Clifford group equivariant networks with simplicial message passing, combining vertex combinations into higher-dimensional simplices. To enhance efficiency, we simplify message passing to hypergraph-based techniques, sharing parameters across simplex orders to maintain complex topology. Experimental results demonstrate CSMPNs outperforming both equivariant and simplicial graph neural networks across various tasks, though performance is comparable in some cases. Future research may investigate specific scenarios where simplicial geometric message passing excels. While increased computational cost is a limitation, sharing parameters across simplex orders represents significant progress, with further improvements anticipated.

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