Clifford Group Equivariant Simplicial Message Passing Networks

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Overview

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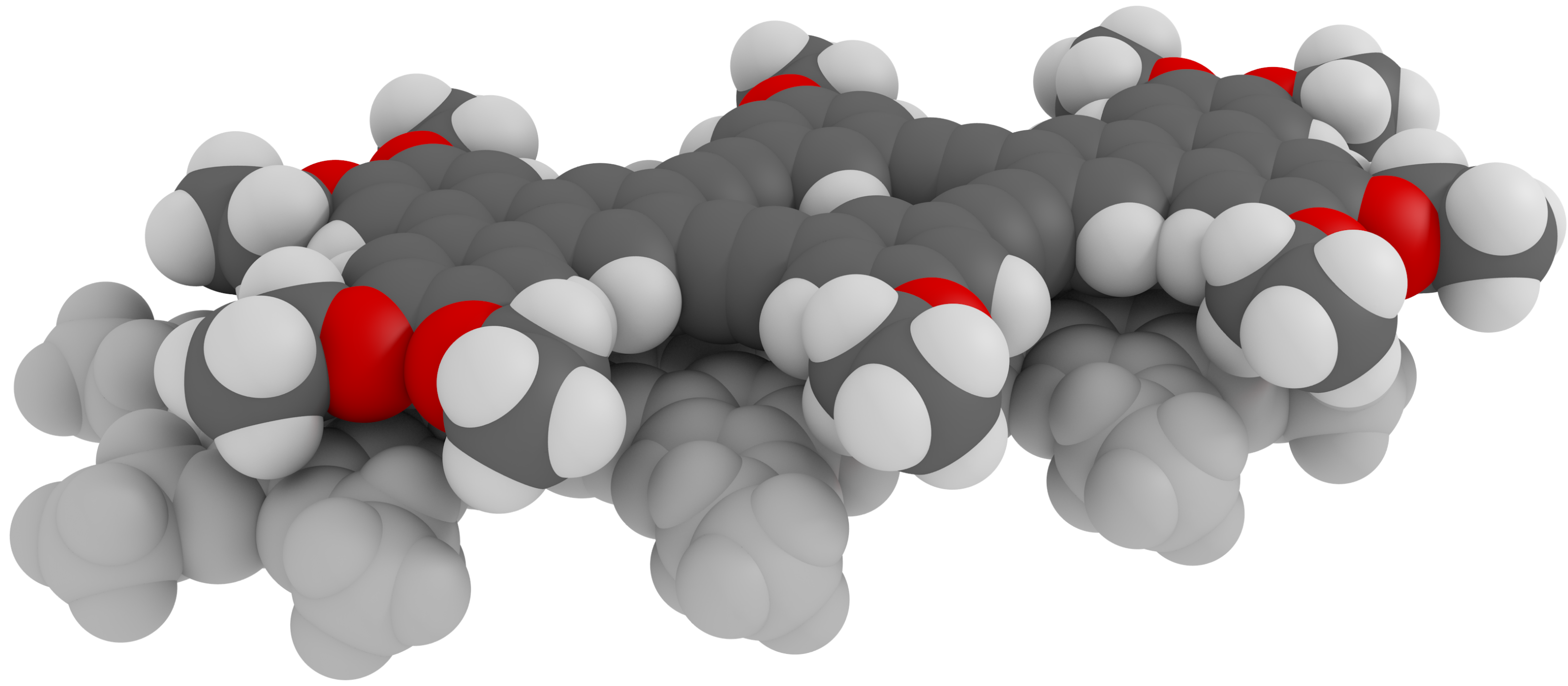
- Conclusion

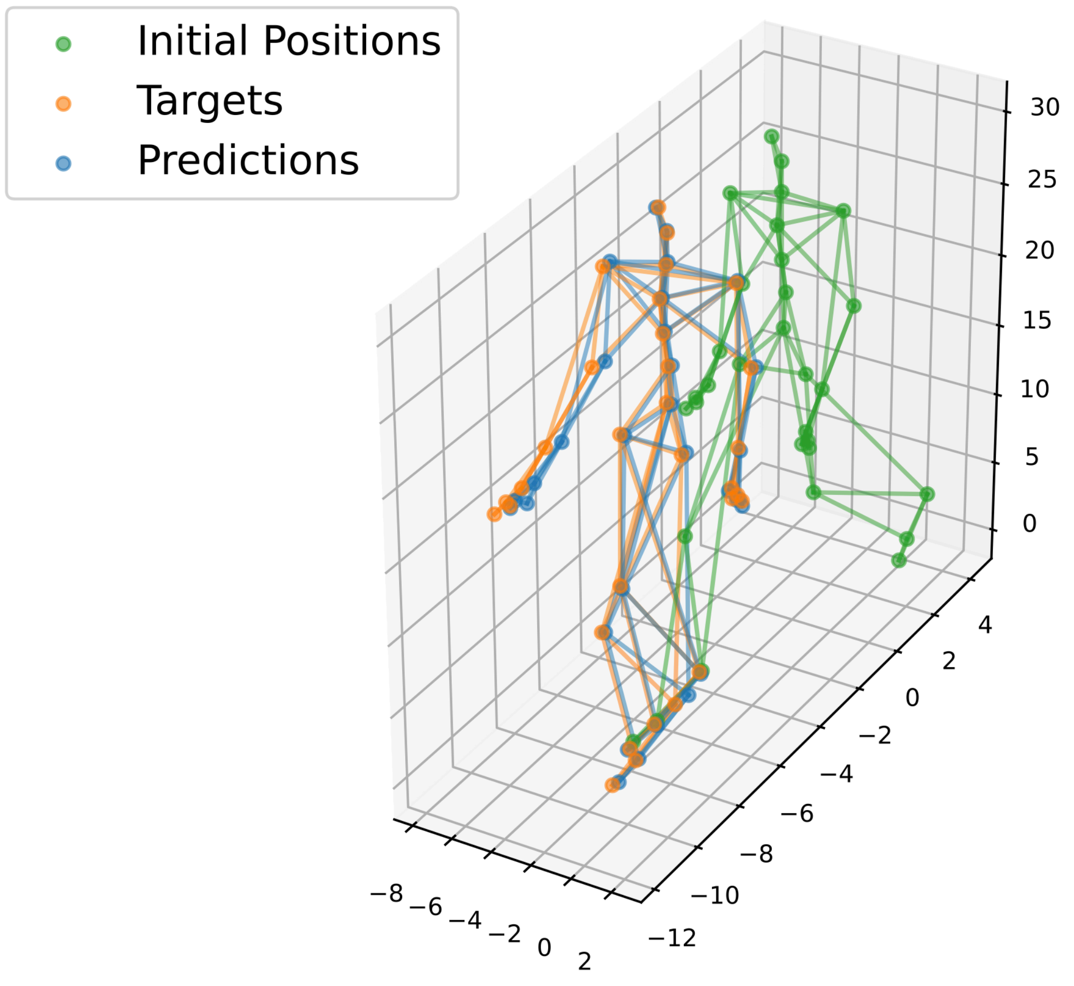
Motivation



- Many real-world data have complex geometric and topological layout, such as molecules, proteins, motions, etc…

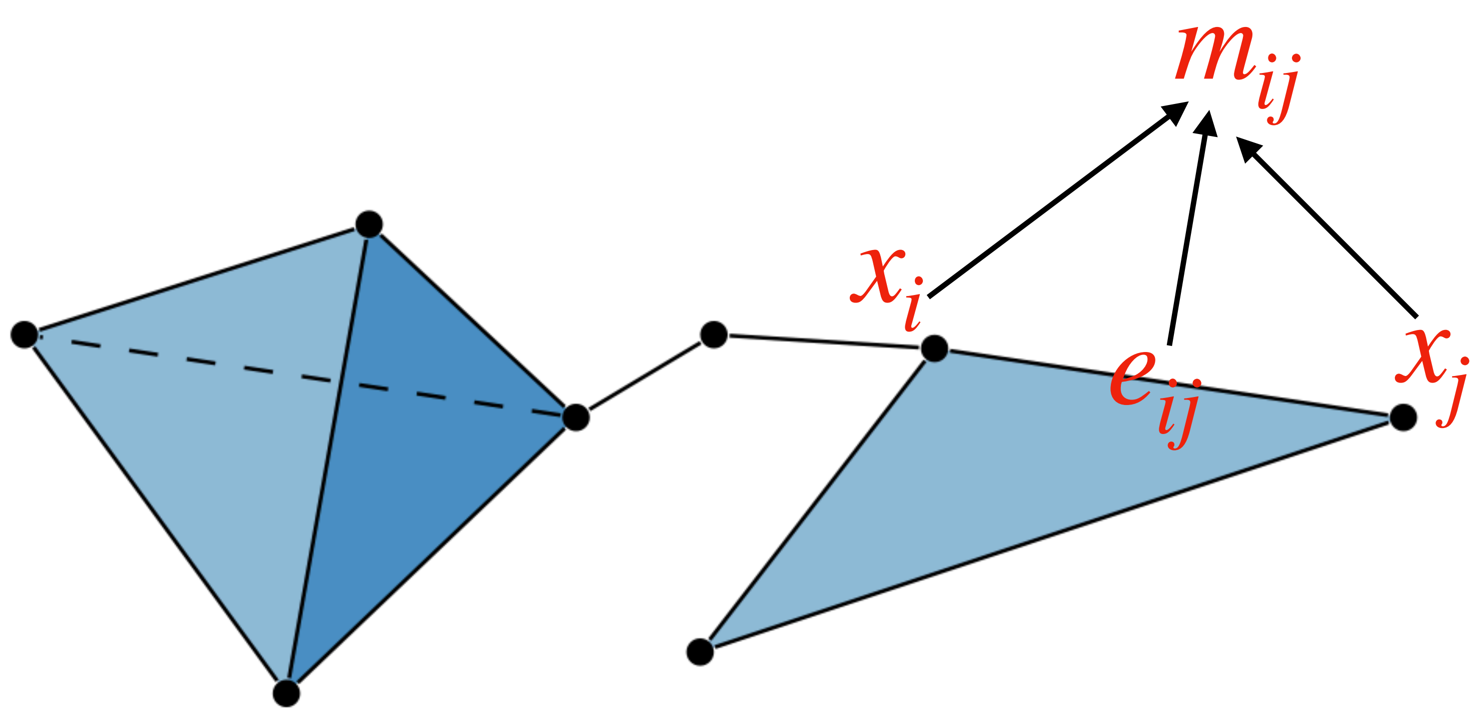
- Graph Neural Networks are mostly used to tackle these challenges but they are only capable of modelling bi-interactions at each time

- Can we find a general method to both satisfy the equivariance constraint and being able model both geometries and topologies lie in the data?



Message Passing Neural Networks (MPNNs)

- A specific type of networks that learn on irregular data, i.e. graphs
- MPNNs learn on graphs by modelling **bi-node interactions** through neural networks
  - Message function: $m_{ij} = \phi(x_i, x_j, e_{ij})$
  - Update function: $x_i^{l+1} = \psi(\sum_{j \in \mathcal{N}_i} m_{ij}) + x_i^l$

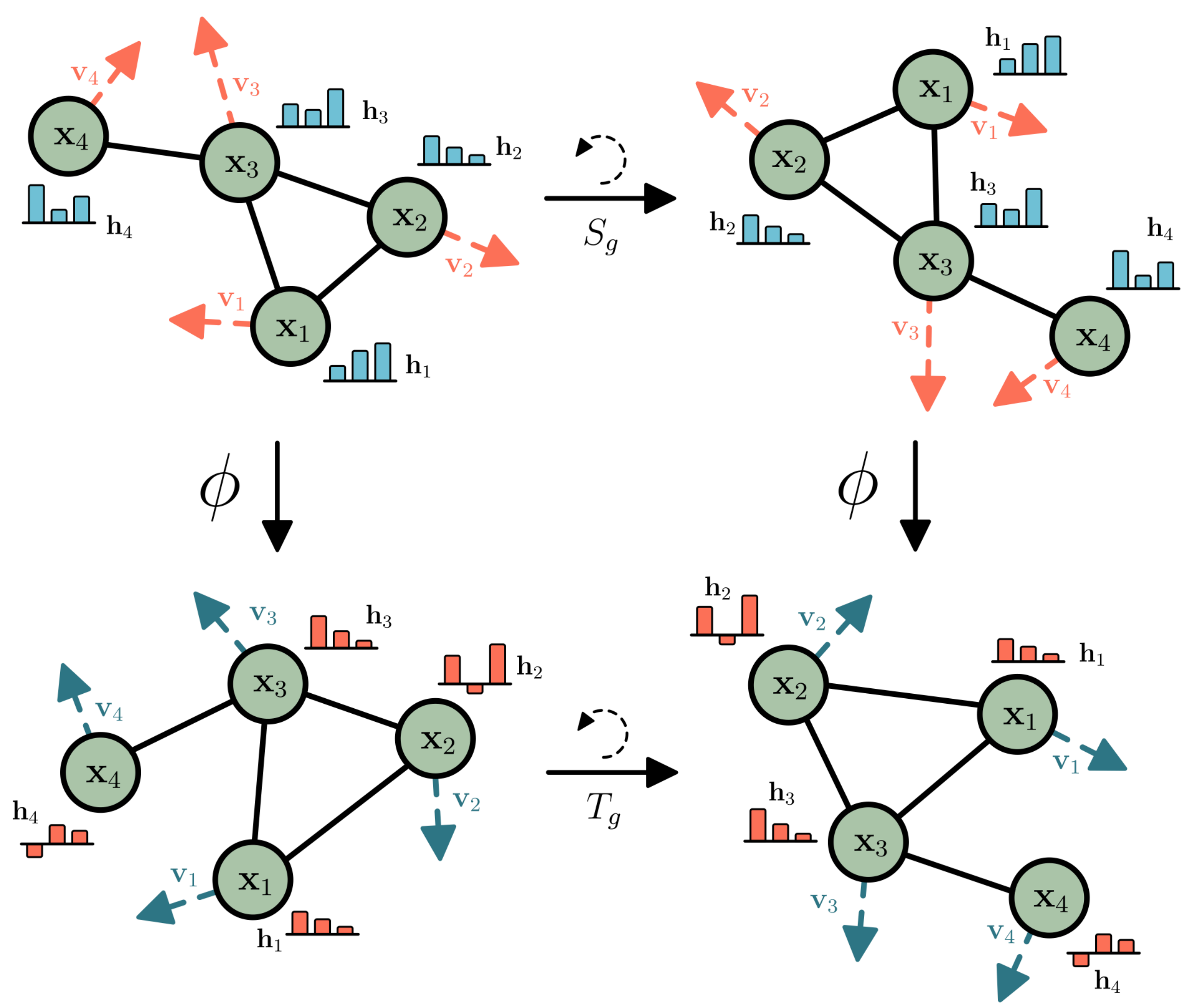


Equivariant Message Passing Networks

- Sometimes we are interested in learning and inferencing on graphs live in certain geometric space, e.g. Euclidean space, with some group of interest, e.g. orthogonal group

- Equivariance: $\forall w \in G : \rho(w)\phi(x) = \phi(\rho(w)(x))$

- Invariance: $\forall w \in G : \phi(x) = \phi(\rho(w)(x))$



(From Victor et al. 2021)

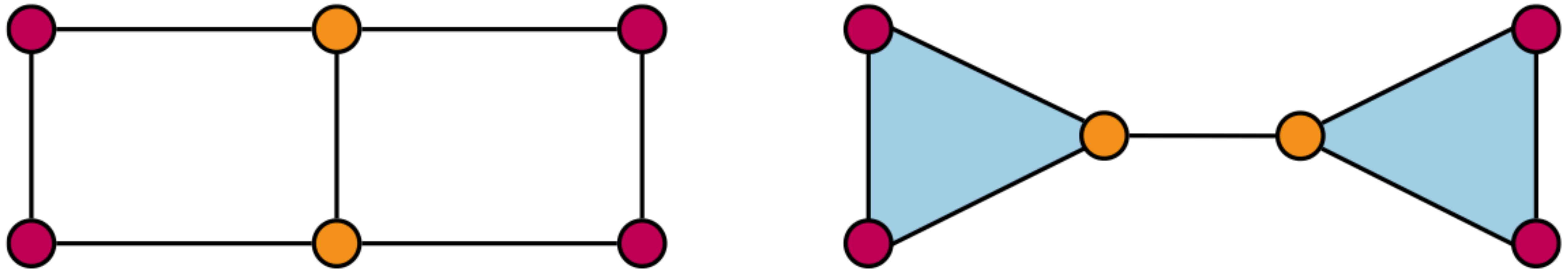
Represent Data in Clifford Space

- Euclidean Clifford Space is chosen to embed geometric data
  - Euclidean Geometric Algebra ($Cl(\mathbb{R}^3)$) is simple and memory efficient compared to Projective and Conformal counterparts
  - Clifford Networks are equivariant to Clifford groups, in $Cl(\mathbb{R}^3)$ case, orthogonal groups $O(3)$

Message Passing Simplicial Networks

- Message Passing Networks are powerful, but they cannot distinguish two graphs with the same connectivity and the same set of nodes, even the two graphs have different topology.

- By lifting graphs to simplicial complex and pass messages on simplicial complex, we can identify them again!



- Message Passing Simplicial Networks learn the topological features in simplicial complex

Simplex Complex

Definition 2.3 (Simplicial Complex)**.** *Let V be a finite set. An abstract simplicial complex K is a subset of the power set 2^V that satisfies:*

1. $\forall v \in V : \{v\} \in K$;
2. $\forall \sigma \in K : \forall \tau \subseteq \sigma, \tau \neq \emptyset : \tau \in K$.

- 0-simplex σ^0, nodes v_i
- 1-simplex σ^1, edges $\{v_i, v_j\}$
- 2-simplex σ^2, triangles $\{v_i, v_j, v_k\}$

Message Passing Simplicial Networks (MPSNs)

MPSN We propose a message passing model using the following message passing operations based on the four types of messages discussed in the previous section. For a simplex σ in a complex $\mathcal{K}$ we have:

$$m_{\mathcal{B}}^{t+1}(\sigma) = \mathrm{AGG}_{\tau \in \mathcal{B}(\sigma)} \Big(M_{\mathcal{B}}\big(h_\sigma^t, h_\tau^t\big)\Big) \quad (2)$$

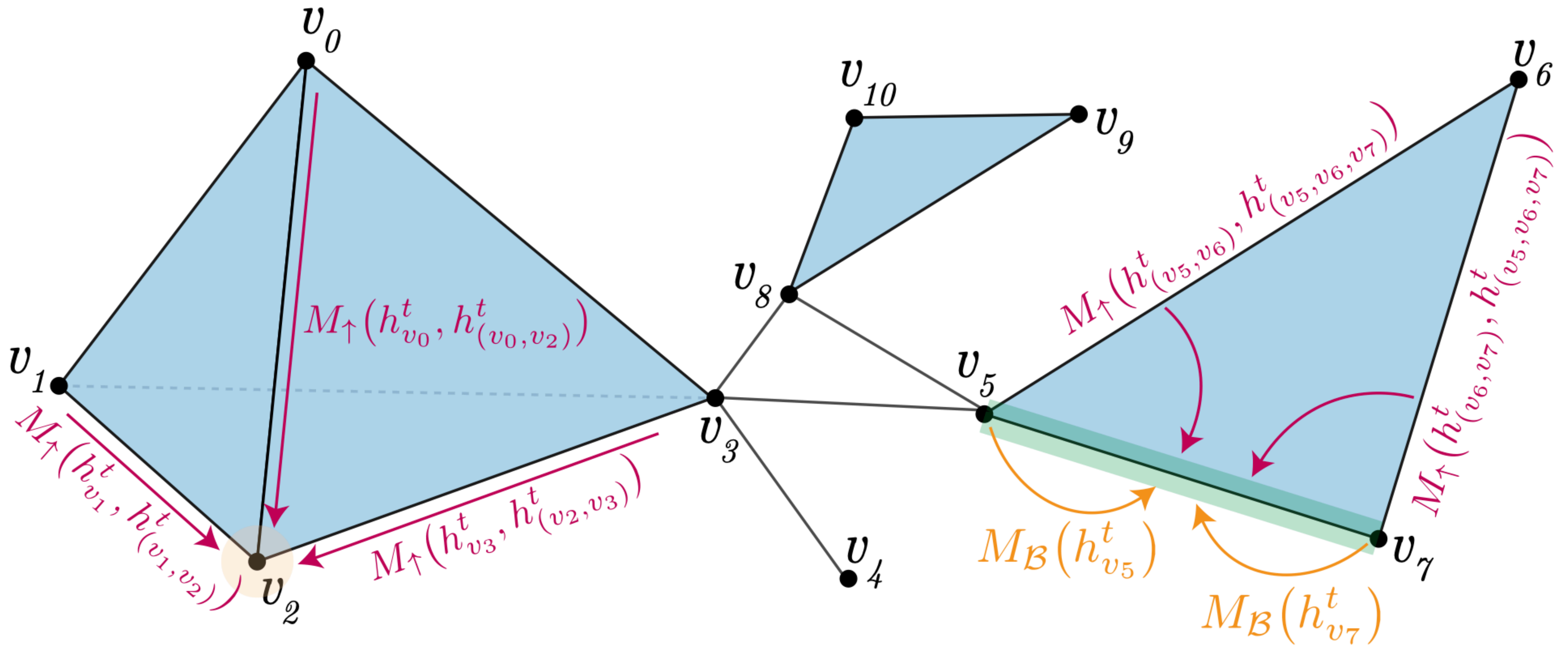
$$m_{\mathcal{C}}^{t+1}(\sigma) = \mathrm{AGG}_{\tau \in \mathcal{C}(\sigma)} \Big(M_{\mathcal{C}}\big(h_\sigma^t, h_\tau^t\big)\Big) \quad (3)$$

$$m_{\downarrow}^{t+1}(\sigma) = \mathrm{AGG}_{\tau \in \mathcal{N}_\downarrow(\sigma)} \Big(M_{\downarrow}\big(h_\sigma^t, h_\tau^t, h_{\sigma\cap\tau}^t\big)\Big) \quad (4)$$

$$m_{\uparrow}^{t+1}(\sigma) = \mathrm{AGG}_{\tau \in \mathcal{N}_\uparrow(\sigma)} \Big(M_{\uparrow}\big(h_\sigma^t, h_\tau^t, h_{\sigma\cup\tau}^t\big)\Big). \quad (5)$$

Then, the update operation takes into account these four types of incoming messages and the previous colour of the simplex:

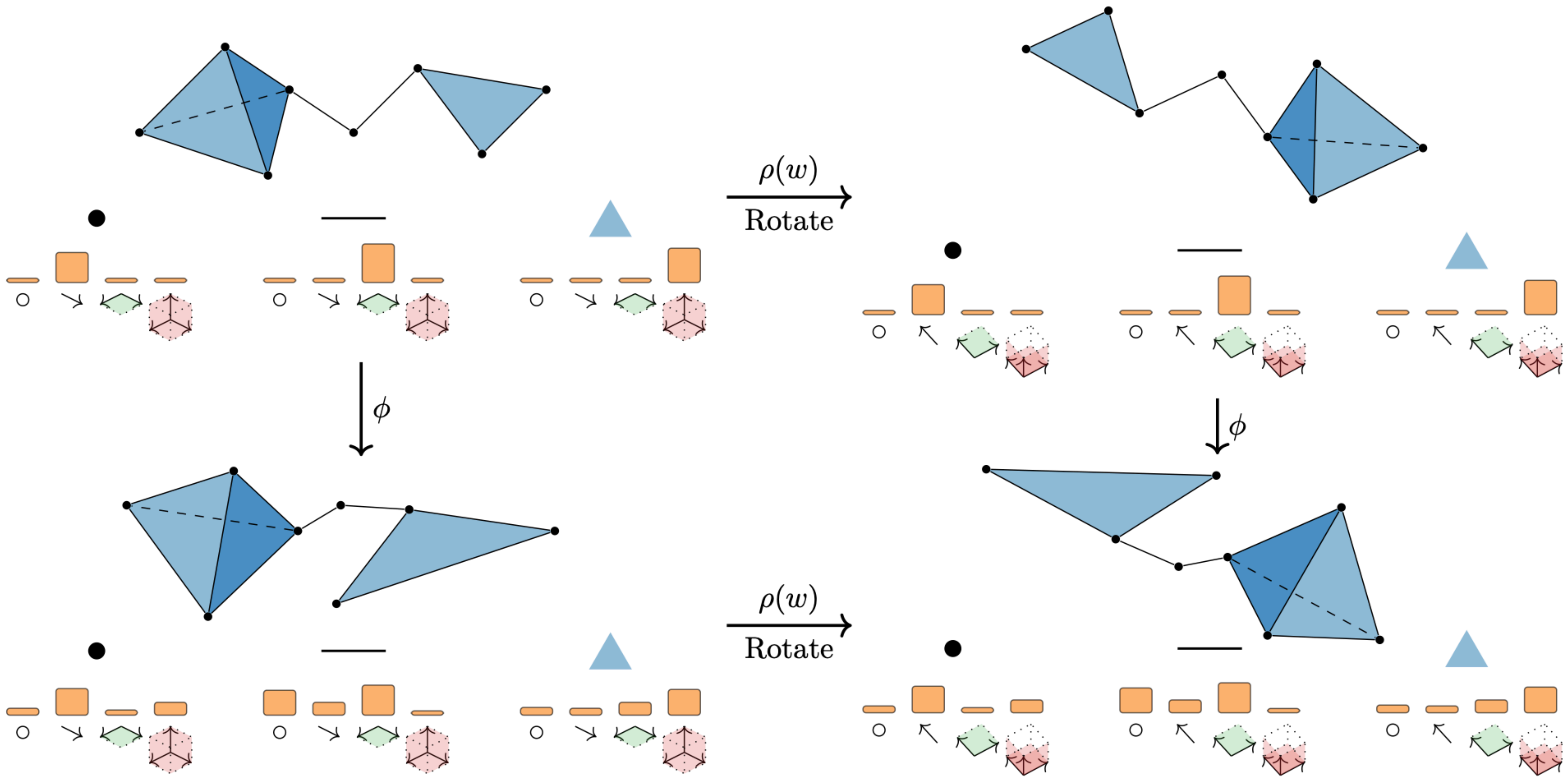
$$h_\sigma^{t+1} = U\Big(h_\sigma^t, m_{\mathcal{B}}^t(\sigma), m_{\mathcal{C}}^t(\sigma), m_{\downarrow}^{t+1}(\sigma), m_{\uparrow}^{t+1}(\sigma)\Big). \quad (6)$$



(From Bodnar et al. 2021)

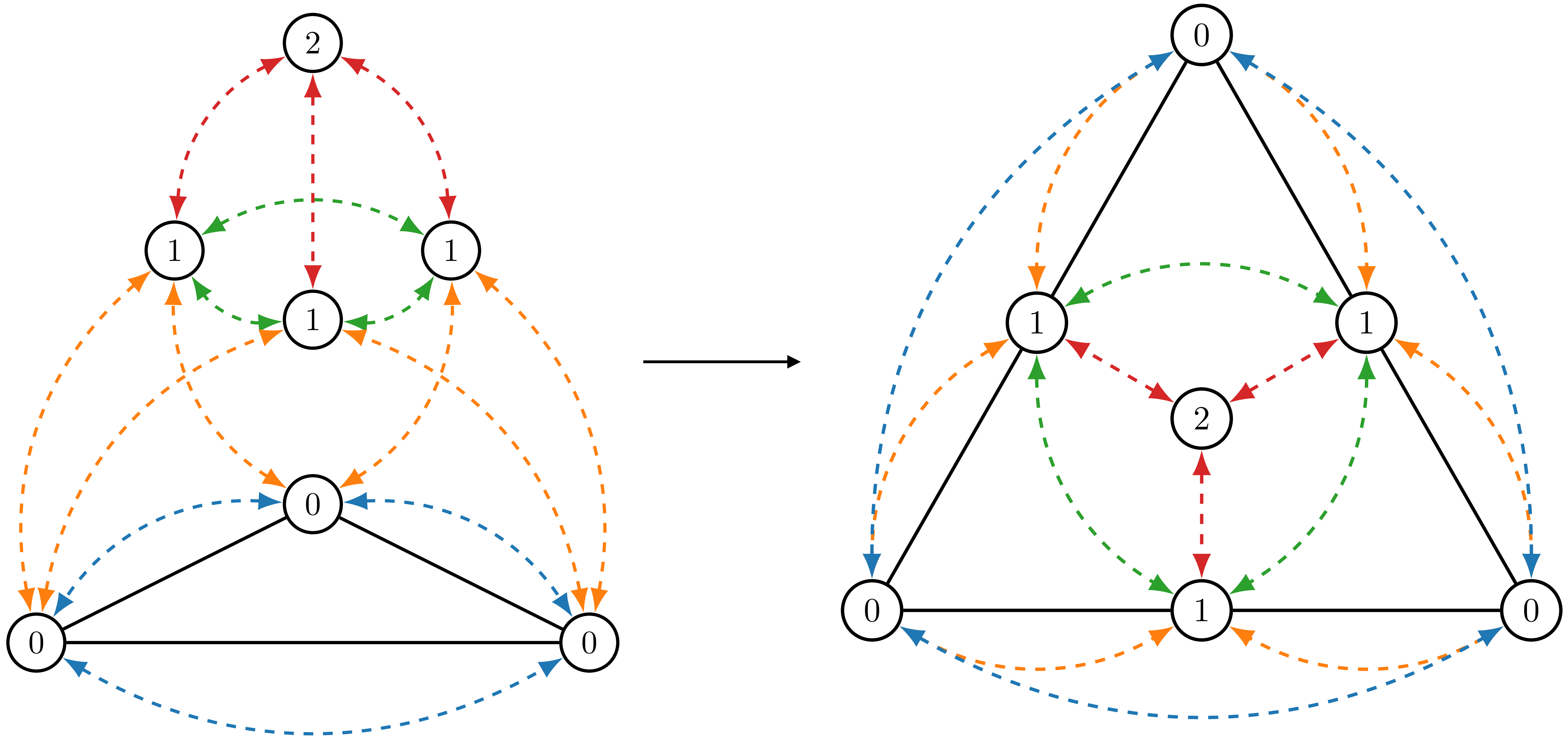
Representing data in Clifford Space and pass messages between simplifies yield a general method learning on geometric graphs:

Clifford Group Equivariant Simplicial Message Passing Networks



Shared Message Passing Networks

- In MSPNs, **every** type of communications between different dimensional simplices use different message networks.
- In this case, **6** networks are created and are forward propagated sequentially.
- We use only **1 shared** message passing network, *conditioned on communication type.*



Shared Message Passing Networks

Algorithm 1 Shared Simplicial Message Passing

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

Repeat:

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

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

Shared Message Passing Networks

- How do we get higher-order Clifford simplicial features h^σ?
  - For 0-simplex, i.e. node, we just embed node feature f^v in to Clifford space to get $h^v \in Cl(V, q)$.
  - For 1-simplex σ^1, edges $\{v_i, v_j\}$, we stack $[h^{v_i}, h^{v_j}]$ as inputs to a Clifford equivariant bilinear layer.
  - 2-simplex σ^2, triangles $\{v_i, v_j, v_k\}$, we stack $[h^{v_i}, h^{v_j}, h^{v_k}]$ as inputs to two Clifford equivariant bilinear layer.
  - This process generalizes to higher-order simplicial Clifford features.

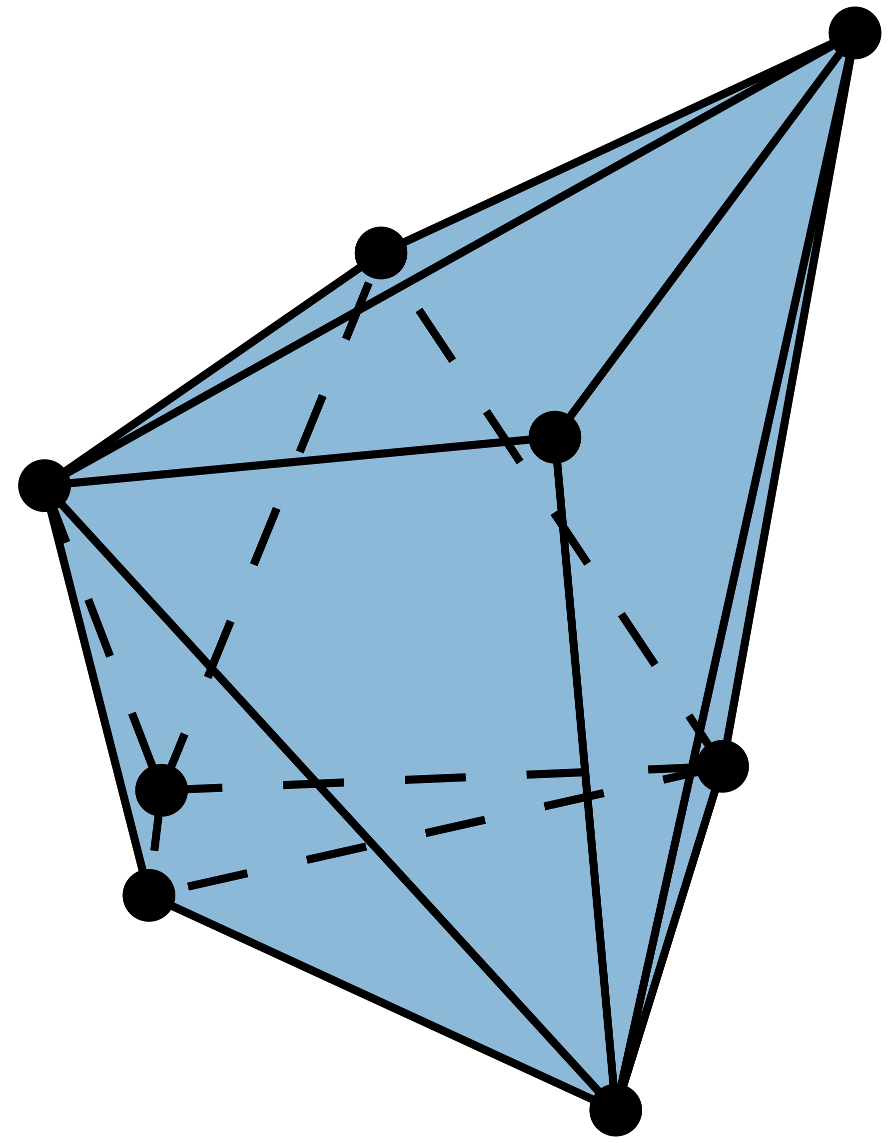
Experiments

5D Convex Hulls (O(5))

- Given eight five-dimensional points, estimate their convex hull and its volume.

	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
CGENN (Ruhe et al., 2023a)	0.013
EMPSN (Eijkelboom et al., 2023)	0.007
CSMPN	**0.002**

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

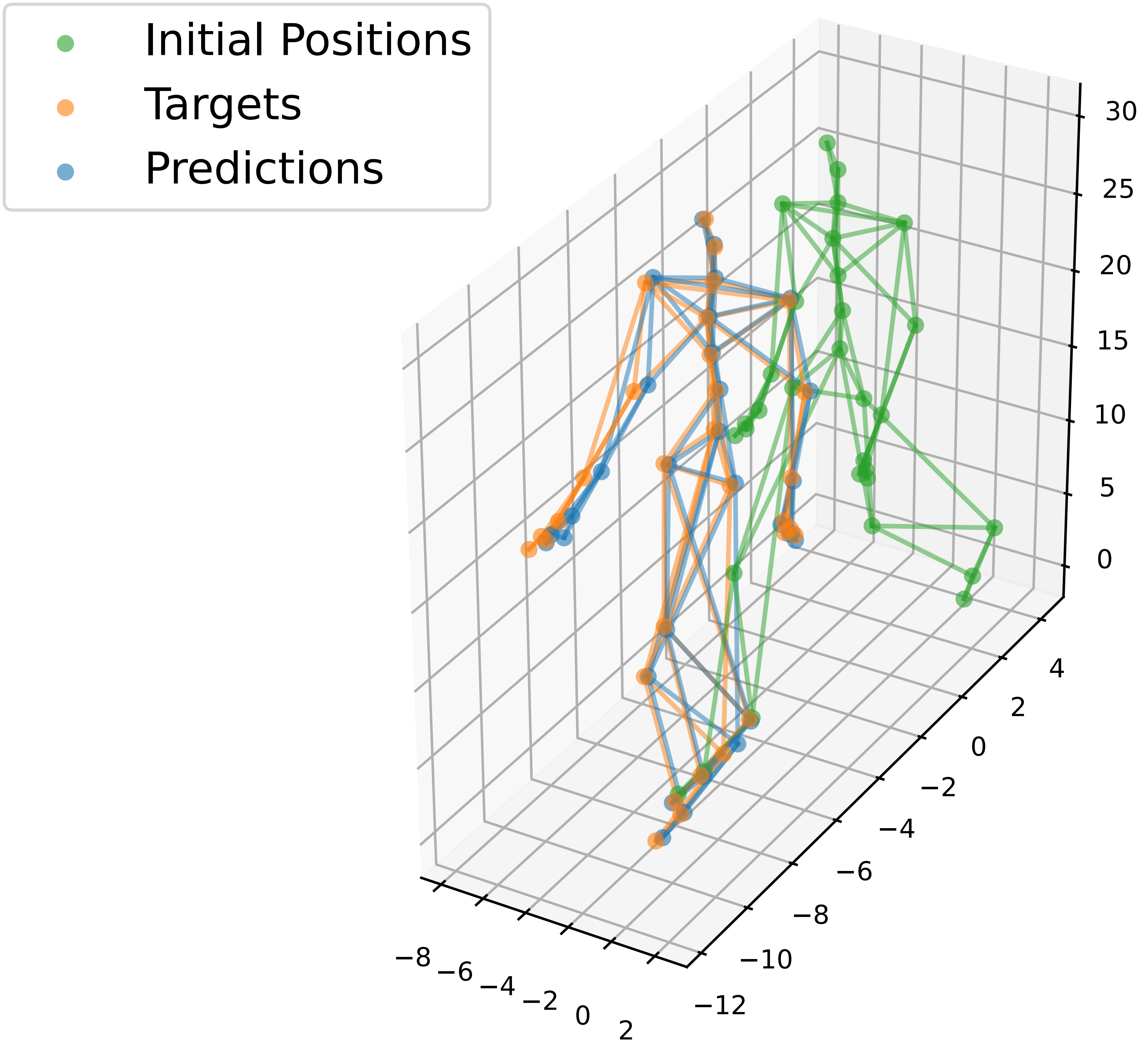


Experiments

Human Walking Motion Prediction (E(2))

- Given 31 three-dimensional points coordinates , estimate the coordinates of these points after 30 time steps.

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
CGENN (200K)	9.41
CSMPN (200K)	**7.55**



Experiments

MD17 Atomic Motion Prediction (E(3))

- Given the atomic positions at 10 separate time steps , estimate the coordinates of these atoms after serveral time steps.

	Aspirin	Benzene	Ethanol	Malonaldehyde
Radial Field (Köhler et al., 2020)	17.98 / 26.20	7.73 / 12.47	8.10 / 10.61	16.53 / 25.10
TFN (Thomas et al., 2018)	15.02 / 21.35	7.55 / 12.30	8.05 / 10.57	15.21 / 24.32
SE(3)-Tr (Fuchs et al., 2020)	15.70 / 22.39	7.62 / 12.50	8.05 / 10.86	15.44 / 24.47
EGNN (Satorras et al., 2021)	14.61 / 20.65	7.50 / 12.16	8.01 / 10.22	15.21 / 24.00
S-LSTM (Alahi et al., 2016)	13.12 / 18.14	3.06 / 3.52	7.23 / 9.85	11.93 / 18.43
NRI (Kipf et al., 2018)	12.60 / 18.50	1.89 / 2.58	6.69 / 8.78	12.79 / 19.86
NMMP (Hu et al., 2020)	10.41 / 14.67	2.21 / 3.33	6.17 / 7.86	9.50 / 14.89
GroupNet (Xu et al., 2022)	10.62 / 14.00	2.02 / 2.95	6.00 / 7.88	7.99 / 12.49
GMN-L (Huang et al., 2022)	9.76 / -	48.12 / -	4.83 / -	13.11 / -
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.

Experiments

NBA Players 2D Trajectory Prediction

- Given the player positions at 10 separate time steps , estimate the coordinates of these players for future 40 time steps.

	Attack	Defense
STGAT (Huang et al., 2019)	9.94 / 15.80	7.26 / 11.28
Social-Ways (Amirian et al., 2019)	9.91 / 15.19	7.31 / 10.21
Weak-Supervision (Zhan et al., 2019)	9.47 / 16.98	7.05 / 10.56
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.

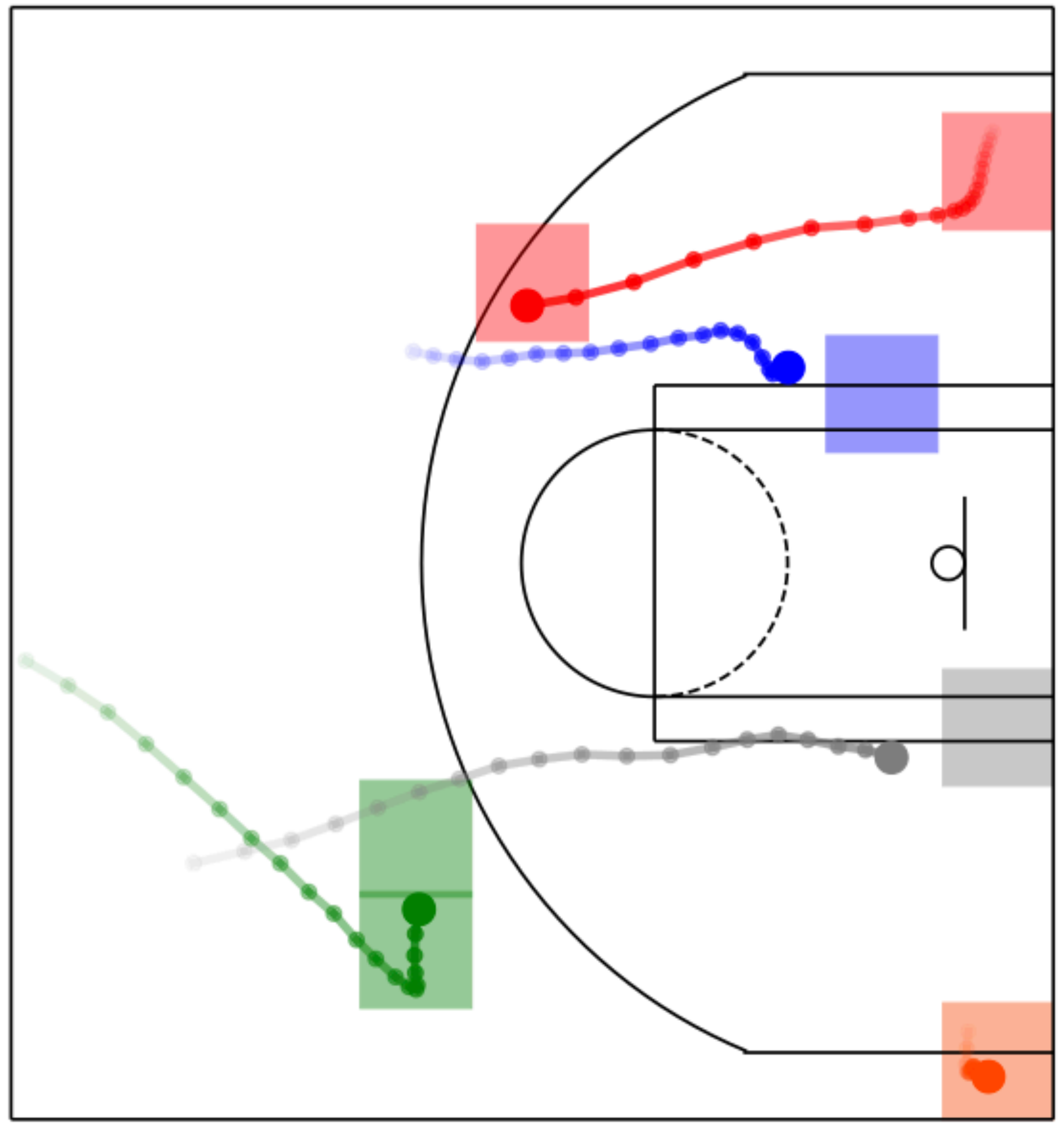


Figure from Alessio Monti, Alessia Bertugli, Simone Calderara, and Rita Cucchiara. Dag-net: Double attentive graph neural network for trajectory forecasting, 2020.

In Conclusion

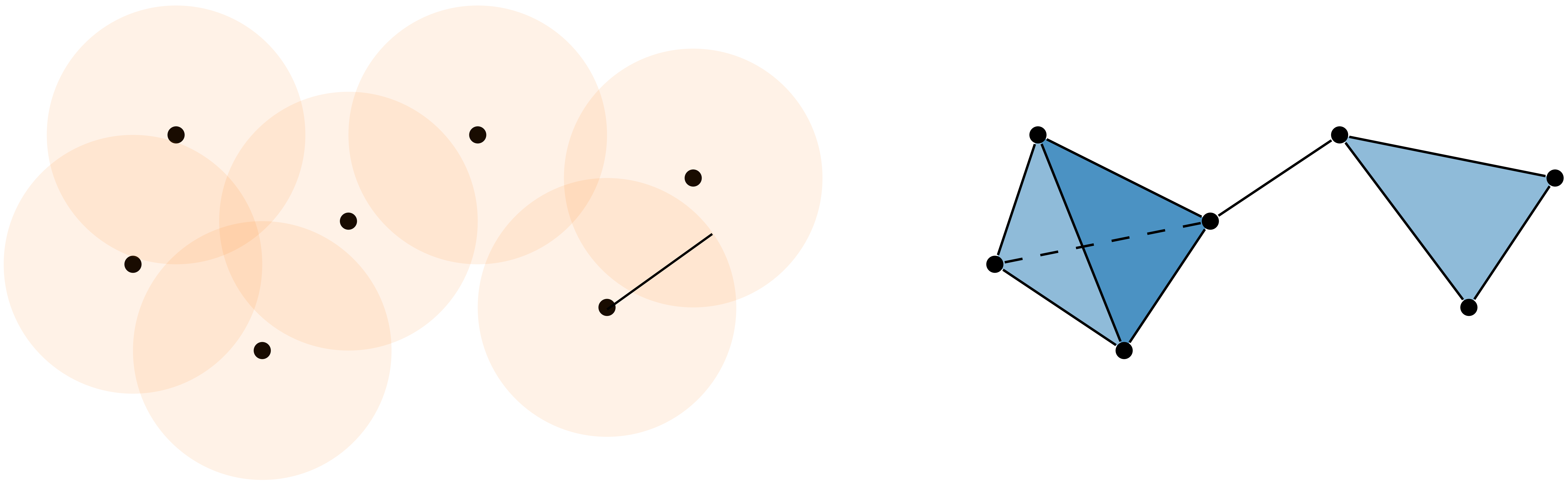
- We combine Clifford steerable equivariant models with simplicial message passing networks to capture both topological and geometric aspects of the graphs.
- Shared Message Passing Networks save the computations by sharing parameters across different dimensional simplices
- We are able to adapt to any dimensional spaces thanks to Clifford algebra.
- Limitation:
    - computational overhead, both steerable methods and simplicial message passing networks
    - We are still not sure how the model should be designed to best leverage both worlds, future direction might be researching on how to combine this two aspects of the graphs.

Thanks

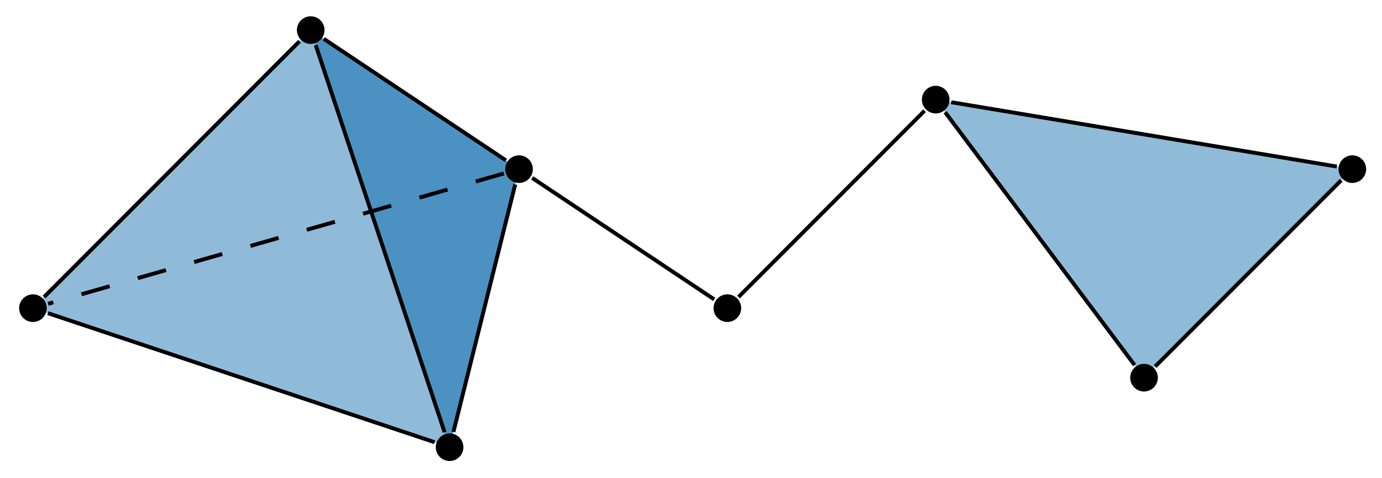
Q&A

Vietoris-Rips Lift

- Vietoris-Rips Lift

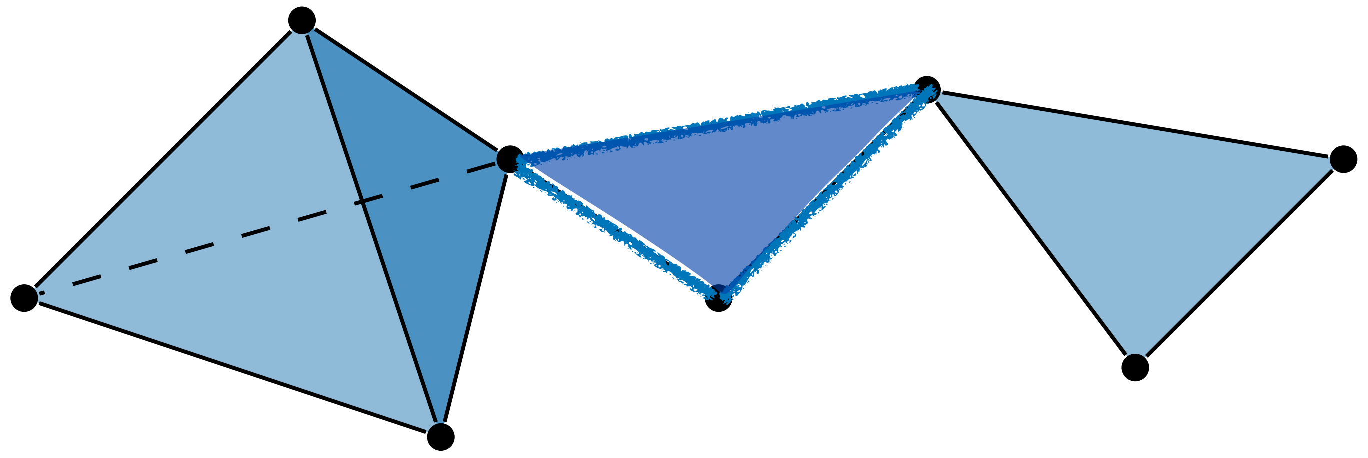


Manual Lift



Manual Lift

- Manually define the simplices by users' interests



Simplicial Lift

- OK, but how do we define the adjacency?

- Boundary Adjacency (1 -> 0, 2 -> 1)
- Coboundary Adjacency (0 -> 1, 1 -> 2)
- Upper Adjacency (0 -> 0, 1 -> 1)
- Lower Adjacency (1 -> 1)