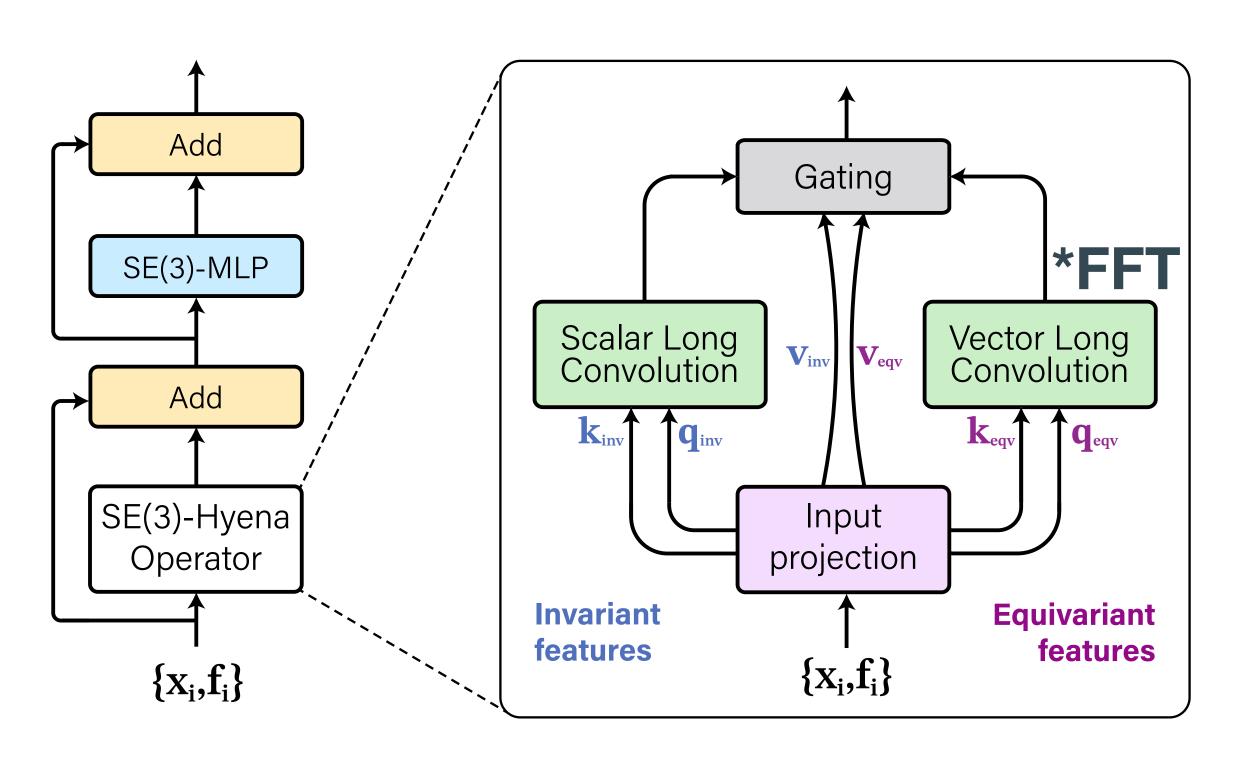
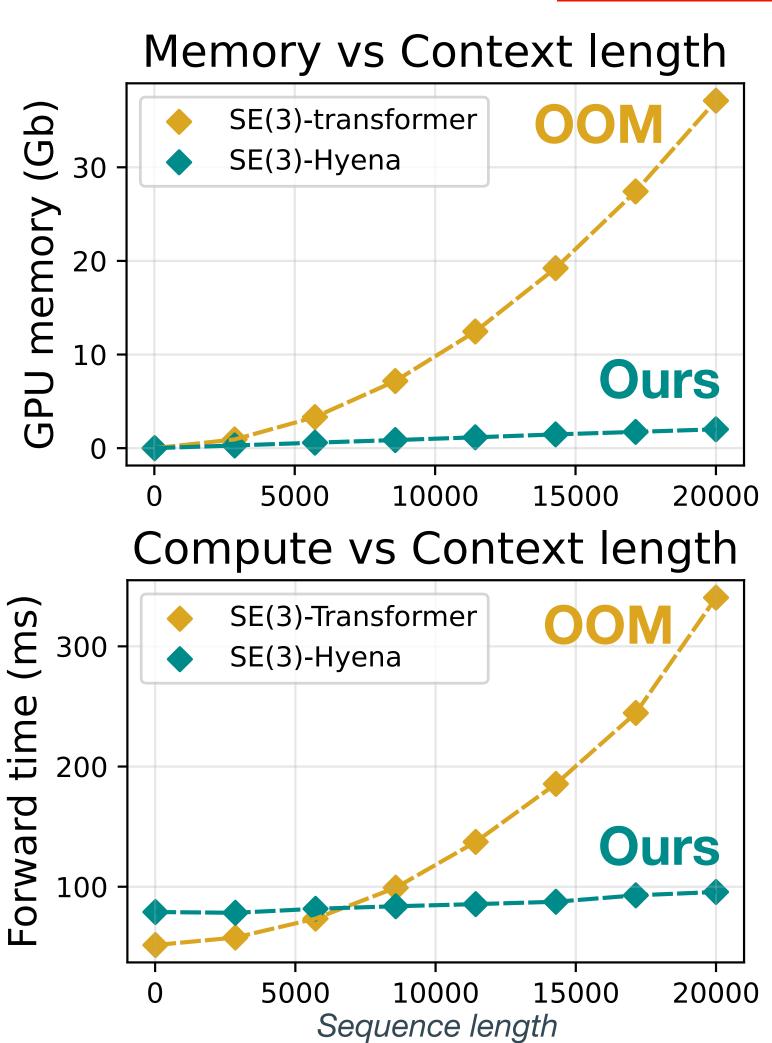
SE(3)-Hyena Operator for Scalable Equivariant Learning

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- Processing global geometry is crucial in biology, chemistry, materials, graphics, etc...
- Quadratic self-attention is prohibitively expensive
- We develop first long-convolutional equivariant network with O(NlogN) complexity



Equivariantly process up to 3.5M tokens with global (all-to-all) context on a single A10 GPU.

Input projection:

Input features:

x: equivariant vector tokens $\{\mathbf x_i, \mathbf f_i\}_{i=1}^N$ f: invariant scalar tokens

Eqv. MLP gives data-controlled filter:

$$\mathbf{z}_{i}^{eqv},\mathbf{z}_{i}^{inv}=\phi\left(\mathbf{x}_{i},\mathbf{f}_{i}
ight)$$

26

2⁷

Sequence length

 $[\mathbf{q}_i^{eqv}, \mathbf{k}_i^{eqv}, \mathbf{v}_i^{eqv}]$ query, key, value for each token

Simple implementation: 50 lines of code

Equivariant and invariant long convolution:

Invariant scalar long convolution:

$$(\mathbf{q} \circledast \mathbf{k})_i = \sum_{j=1}^N q_i k_{j-i} = (\mathbf{F}^H \mathbf{\Lambda}_k \mathbf{F} \mathbf{q})_i$$

Equivariant vector long convolution:

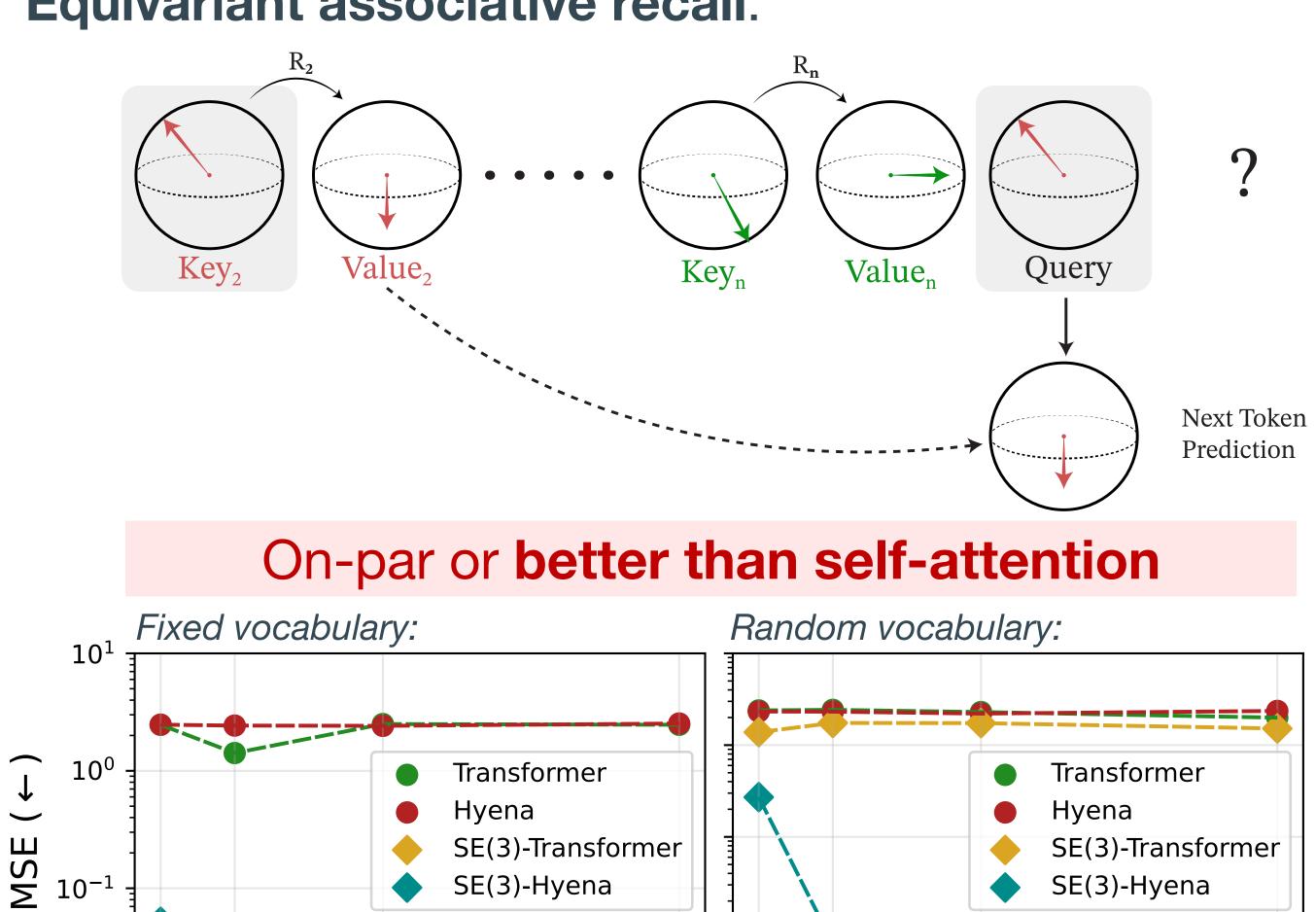
$$(\overrightarrow{\mathbf{q}}\circledast_{ imes}\overrightarrow{\mathbf{k}})_i=\sum_{i=1}^N\overrightarrow{\mathbf{q}}_i imes\overrightarrow{\mathbf{k}}_{j-i}$$

$$(\overrightarrow{\mathbf{q}} \circledast_{ imes} \overrightarrow{\mathbf{k}})_i = \sum_{j=1}^N \overrightarrow{\mathbf{q}}_i imes \overrightarrow{\mathbf{k}}_{j-i} \ (\overrightarrow{\mathbf{q}} \circledast_{ imes} \overrightarrow{\mathbf{k}})_i[l] = arepsilon_{lhp} \sum_{j=1}^N \overrightarrow{\mathbf{q}}_i[h] imes \overrightarrow{\mathbf{k}}_{j-i}[p]$$

Scalar long convolution

FFT

Equivariant associative recall:

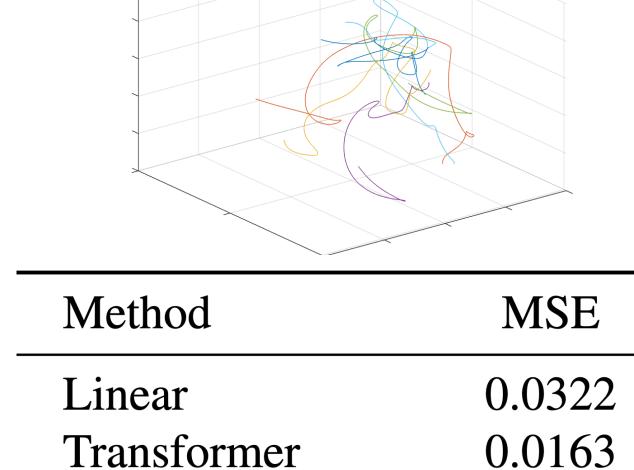


2⁶

Sequence length

2⁵

Equivariant n-body system:



Method	MSE
Linear	0.0322
Transformer	0.0163
Hyena	0.0150
SE(3)-Transformer	0.0019
SE(3)-Hyena	0.0018

Paper:

