Geometric Algebra Transformers

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Geometric Algebra Transformer

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a universal architecture for geometric data

Geometric Algebra
Transformer

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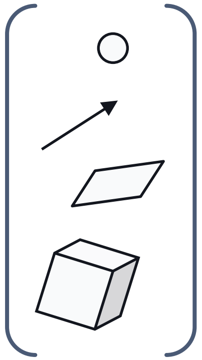

Geometric algebra
representations

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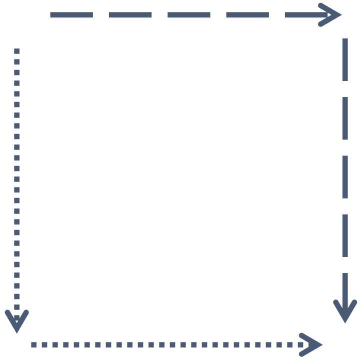

Equivariant
layers

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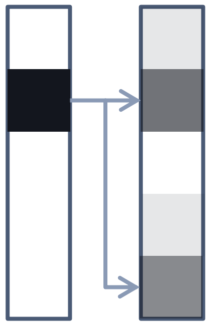

Transformer
architecture

Geometric Algebra Transformer

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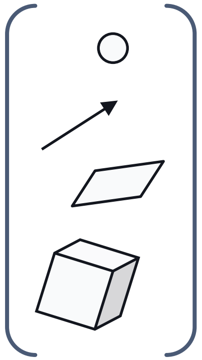

Geometric algebra representations

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Equivariant layers

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Transformer architecture

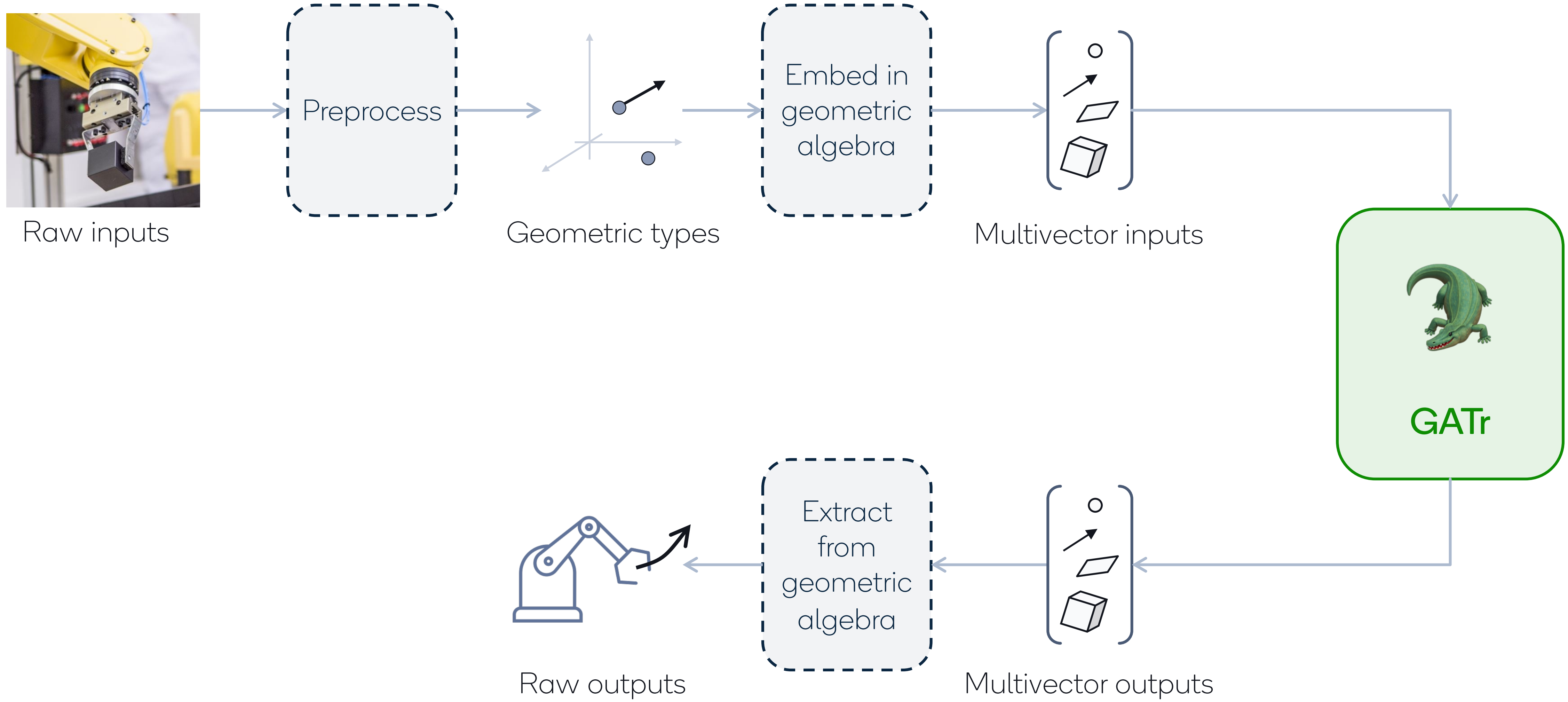
Geometric algebra:

- Multivectors, a **16-dimensional representation** of 3D geometric data
- "**Typing**": a point is not a direction of movement is not the orientation of a plane
- A dictionary for **representations of common objects and transformations**

Object / operator	Scalar	Vector		Bivector		Trivector		PS
	1	e_0	e_i	e_{0i}	e_{ij}	e_{0ij}	e_{123}	e_{0123}
Scalar $\lambda \in \mathbb{R}$	λ	0	0	0	0	0	0	0
Plane w/ normal $n \in \mathbb{R}^3$, origin shift $d \in \mathbb{R}$	0	d	n	0	0	0	0	0
Line w/ direction $n \in \mathbb{R}^3$, orthogonal shift $s \in \mathbb{R}^3$	0	0	0	s	n	0	0	0
Point $p \in \mathbb{R}^3$	0	0	0	0	0	p	1	0
Pseudoscalar $\mu \in \mathbb{R}$	0	0	0	0	0	0	0	μ
Reflection through plane w/ normal $n \in \mathbb{R}^3$, origin shift $d \in \mathbb{R}$	0	d	n	0	0	0	0	0
Translation $t \in \mathbb{R}^3$	1	0	0	$\frac{1}{2}t$	0	0	0	0
Rotation expressed as quaternion $q \in \mathbb{R}^4$	q_0	0	0	0	q_i	0	0	0
Point reflection through $p \in \mathbb{R}^3$	0	0	0	0	0	p	1	0

- **Canonical operations** on these representations

Geometric algebra representations in practice



Geometric Algebra
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Geometric algebra
representations

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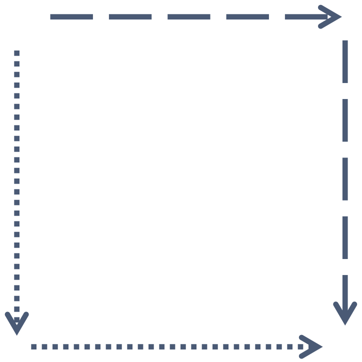

Equivariant
layers

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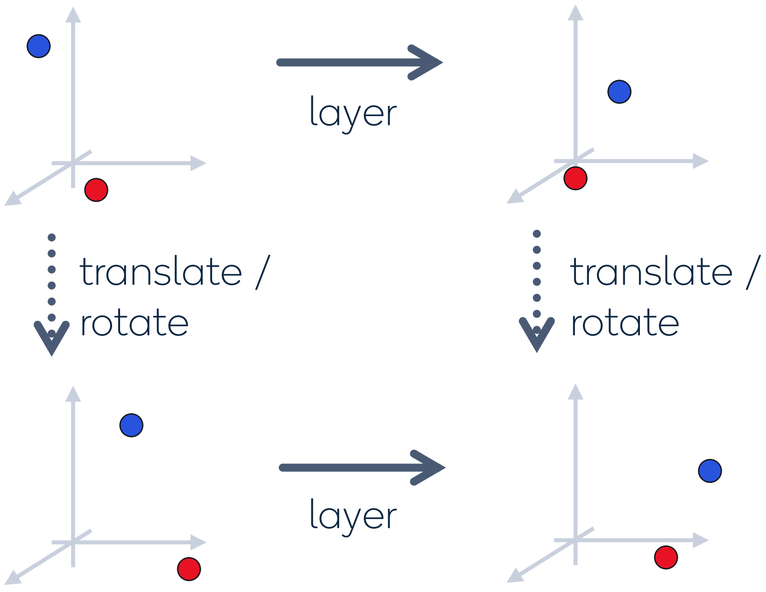
Transformer
architecture

Guiding principle: **E(3) equivariance**



We design equivariant...

- **Linear layers**
- **Nonlinearities** and **normalization layers**
- **Geometric layers**
- **Attention mechanisms**

Geometric Algebra Transformer

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Geometric algebra representations

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Equivariant layers

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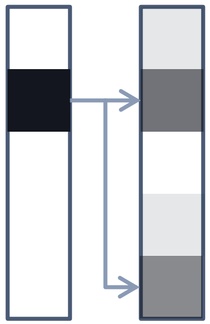
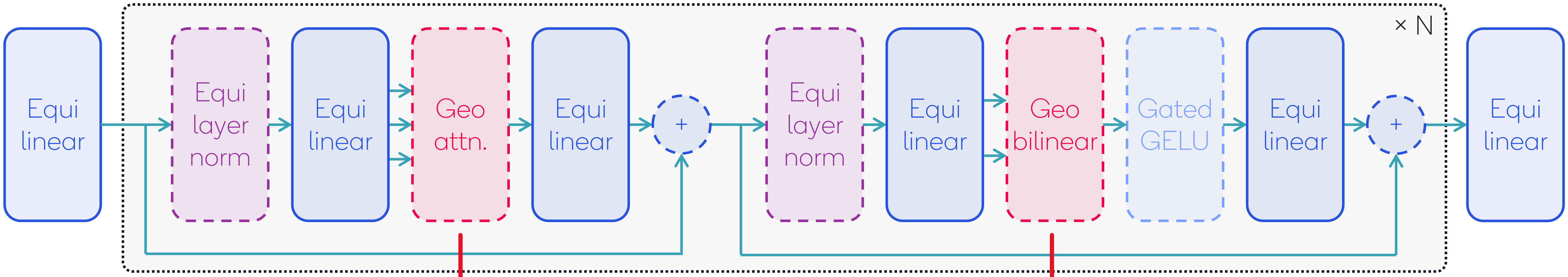


Transformer architecture

Input and output data
can have one or multiple token dimensions

Attention blocks
can be stacked to large depth, gradients are propagated efficiently



Geometric attention
generalizes scaled dot-product attention

Geometric bilinears
allow for construction of new geometric types

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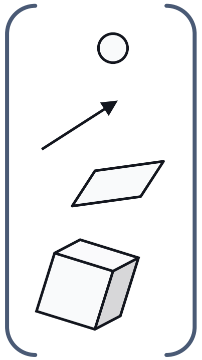

Geometric algebra
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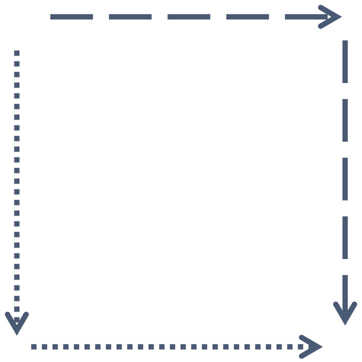

Equivariant
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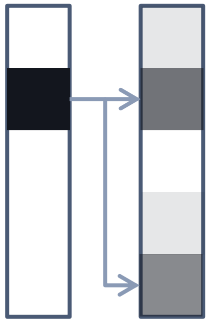

Transformer
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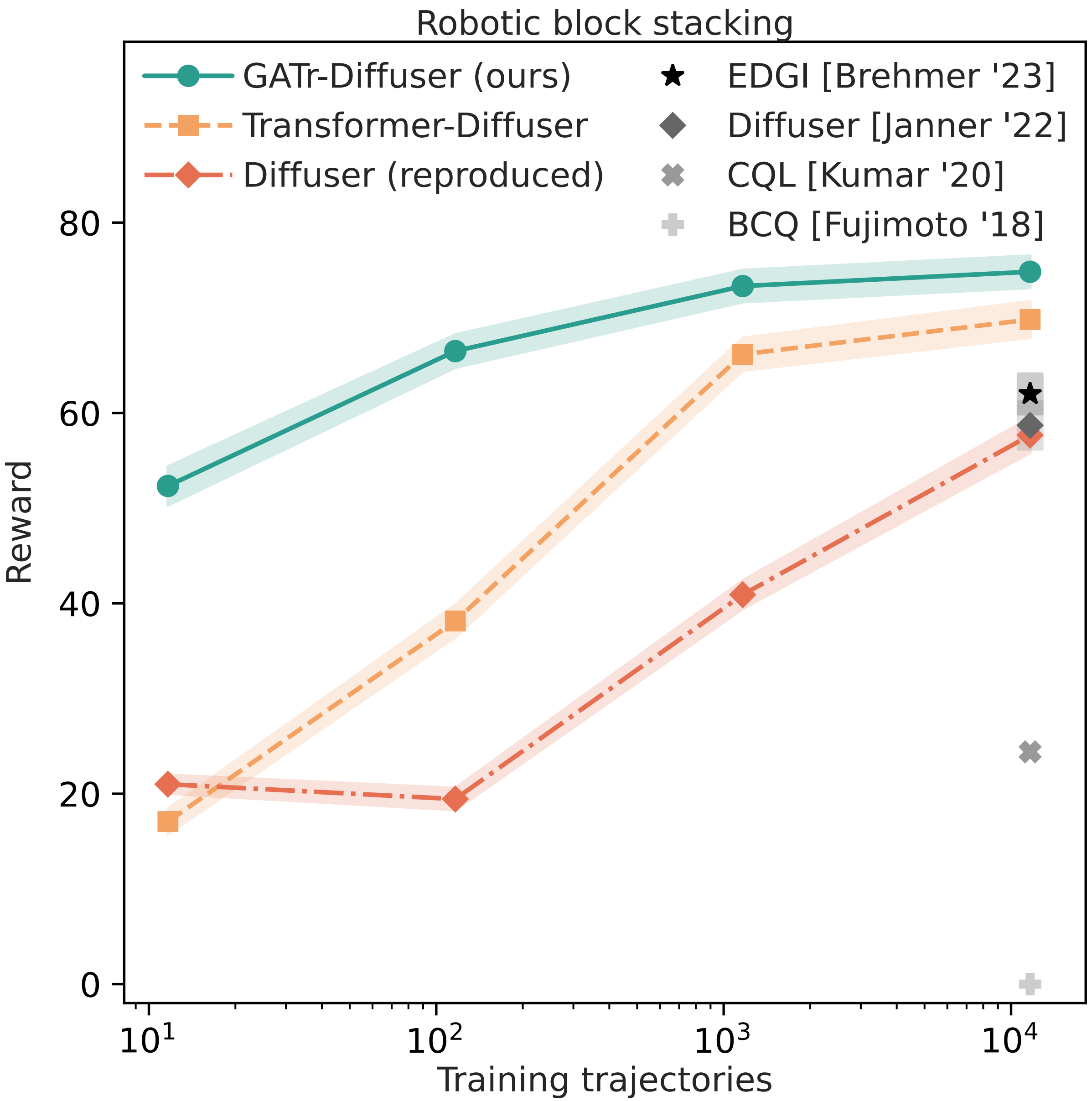

Robotic block stacking task
[Janner et al, ICML 2022]:

GATr outperforms all baselines
with 1% of the training data

Related and concurrent:

arXiv:2305.11141

Clifford Group Equivariant Neural Networks

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Abstract

We introduce Clifford Group Equivariant Neural Networks: a novel approach for constructing $\mathrm{E}(n)$-equivariant networks. We identify and study the *Clifford group*, a subgroup inside the Clifford algebra, whose definition we slightly adjust to achieve several favorable properties. Primarily, the group's action forms an orthogonal automorphism that extends beyond the typical vector space to the entire Clifford algebra while respecting the multivector grading. This leads to several non-equivalent subrepresentations corresponding to the multivector decomposition. Furthermore, we prove that the action respects not just the vector space structure of

Geometric Algebra Transformer

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arXiv:2305.18415

2305.18415v1 [cs.LG] 28 May 2023

Geometric Algebra Transformers

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Abstract

Problems involving geometric data arise in a variety of fields, including computer vision, robotics, chemistry, and physics. Such data can take numerous forms, such as points, direction vectors, planes, or transformations, but to date there is no single architecture that can be applied to such a wide variety of geometric types while respecting their symmetries. In this paper we introduce the Geometric Algebra Transformer (GATr), a general-purpose architecture for geometric data. GATr represents inputs, outputs, and hidden states in the projective geometric algebra, which offers an efficient 16-dimensional vector space representation of common geometric objects as well as operators acting on them. GATr is equivariant with respect to $\mathrm{E}(3)$, the symmetry group of 3D Euclidean space. As a transformer, GATr is scalable, expressive, and versatile. In experiments with n-body modeling and robotic planning, GATr shows strong improvements over non-geometric baselines.

1 Introduction

From molecular dynamics to astrophysics, from material design to robotics, fields across science and engineering deal with geometric data: points, directions, surfaces, orientations, and so on. The geometric nature of data provides a rich structure: a notion of common operations between geometric types (computing distances between points, applying rotations to orientations, etc.), a well-defined behaviour of data under transformations of a system, and the independence of certain properties of coordinate system choices.

When learning relations from geometric data, incorporating this rich structure into the architecture has the potential to improve the performance, especially in the low-data regime. To implement such

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