Geometric Algebra Transformers (GATr)

NN learns from symmetric data.

- Symmetric data: transform data without changing the context.
- Want NN built to be *equivariant* to transformations.
- Equivariance: exists a transformation for *each* input transformation.
 - Feature mapping $f: X \to Y$ is equivariant to a group of transformations if:
 - Every transformation $\pi \in \Pi$ of the input $x \in X$
 - Is associable with a transformation $\psi \in \Psi$ of the features f(x)

$$\psi[f(x)] = f(\pi[x])$$

- Invariance: exists a transformation for every input transformation
 - The feature transformation isn't different for different input transformation.

E(3) symmetry = Euclidean 3D symmetry.

- Symmetry to rigid transformations.
 - Rigid transformations: rotations, translations, flips.
 - **SE(3) symmetry:** E(3) without flips.
- **N-body experiment:** simulate movements of N point masses moving according to gravitation laws.
 - Law of physics don't depend on global translation and rotation.
 - With E(3) the physics law are invariant with respect to spatial translations.

GATr is an equivariant NN.

- Input: multivectors and additional scalars
 - Multivectors: object from geometric algebra that manages geometric objects at once.
 - Can be seen as array of 16 element.
 - Depending on which element is activated, it represents a different object.
 - Additional scalars: sort of lightweight positional embeddings to avoid additional overhead.
 - Multivectors can be very big.
 - 10 multivectors ≅ 1 traditional transformer model
- Works as a transformer but embedded in geometric algebra context.
 - Linear and Bilinear layers: process individual sequence elements
 - Attention layer: mix between the sequence elements.
 - **Equivariant normalization:** consider norm of induvial vectors.
 - Scale non linearity: generalized non linearity.

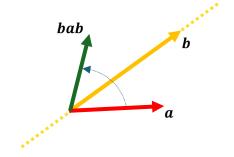
Object / operator	Scalar 1			21.	Bivector e_{0i} e_{ij}		Trivector e_{0ij} e_{123}	
$\overline{\operatorname{Scalar} \lambda \in \mathbb{R}}$	λ	0	0	0	0	0	0	0
Plane w/ normal $n \in \mathbb{R}^3$, origin shift $d \in \mathbb{R}$	0	d	n	0	()	0	0	0
Line w/ direction $n \in \mathbb{R}^3$, orthogonal shift $s \in \mathbb{R}^3$	0	0	0	s	n	0	()	0
Point $p \in \mathbb{R}^3$	0	0	0	()	()	p	1	0
Pseudoscalar $\mu \in \mathbb{R}$	0	0	()	0	0	0	0	μ
Reflection through plane w/ normal $n \in \mathbb{R}^3$, origin shift $d \in \mathbb{R}$	0	\overline{d}	\overline{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	()	p	1	0

Geometric algebra.

- **Basis vector** (e_i) : orthogonal vectors that represent multivector coordinates.
 - Orthogonality: dot product is zero
 - $||e_i^2|| = 1$
- Geometric product: xy
 - Square must be equal to squared norm: $v * v = \langle v, v \rangle = ||v||^2$
 - Special case: $\|e_i * e_j\| = 2$
 - Antisymmetric: $e_i * e_j = -(e_i * e_i)$
 - Proof: $e_i e_j + e_j e_i = (e_i + e_j)^2 e_i^2 e_j^2 = 0$
 - Number of basis (d): how many e_i there are.
 - It doesn't matter what order e_i are multiplied.
 - The output will have the same base vectors with different sign.
 - So, there will be $\sum_{i=0}^d \binom{d}{i} = 2^d$ base combinations (products)
 - \circ Number of basis (d): count of e_i vectors
 - \circ Geometric algebra dimension: $\sum_{i=0}^d {d \choose i} = 2^d$
- Multivector: $x = x_s + x_1e_1 + x_2e_2 + x_3e_3 + x_{12}e_1e_2 + x_{13}e_1e_3 + x_{23}e_2e_3 + x_{123}e_1e_2e_3$
 - This formulation is specifically for 3D Euclidean geometry.
 - **Grade:** number of basis associate to x_i
- Inner product: $\langle x, y \rangle = (xy + yx)/2$
 - Symmetric part of the geometric product
 - Computes the similarity between vectors.
- Outer product: $x \wedge y = (xy yx)/2$
 - Antisymmetric part of the geometric product
 - Represents the weighted and oriented subspace spanned by the vector.
 - \circ $\langle x, y \rangle + x \wedge y = xy$
- **Wedge product:** represent the objects intersection.
- Dual: $x \mapsto x^*$
 - Sends basis vectors to their inverse.
 - As bit flip
 - $e_1 \mapsto e_{23} \equiv e_{001} \mapsto e_{110}$
- Grade involution (\widehat{x}) : flips the sign of the odd-grade elements of xSandwich product: $\rho(x)_u = u[x] = \begin{cases} uxu^{-1} & \text{if } u \text{ is even} \\ u\widehat{x}u^{-1} & \text{if } u \text{ is odd} \end{cases}$
 - Reflect the vector around a point.
 - Any rotation can be represented as two reflections around some vectors.
- Left contraction: $x|y = \langle xy \rangle_{l-k}$
 - o Takes parts geometric product part that corresponds to the difference of vectors grades.
- $Join: x, y = (x^* \land y^*)^*$
 - o Join an object between two elements.
- Blades: $x = x_1 \wedge x_2 \wedge x_3 \wedge ... \wedge x_k$
 - Wedge product of more vectors of grade i from 1 to k.

2D Geometric algebra.

- Two coordinates e_1, e_2
 - Multivector: $x = x_s + x_1e_1 + x_2e_2 + x_{12}e_1e_2$
 - Scalar (x_s): grade 0
 - Vector $(x_i e_i)$: grade 1 = point
 - Bivector $(x_{12}e_1e_2)$: grade 2
 - Number of bases: d = 2
 - Geometric algebra dimension: $2^d = 4$
- Inner product: dot product
- Outer product: gives a bivector.
 - O Bivector area: $||u \wedge v|| = ||u|| * ||v|| * sin(\theta)$
- Sandwich product: reflection of a vector on another one



Projective 2D Geometric algebra.

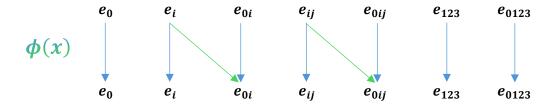
- Three coordinates e_0 , e_1 , e_2
 - $\qquad \text{Multivector: } x = x_s + x_0 e_0 + x_1 e_1 + x_2 e_2 + x_{01} e_0 e_1 + x_{02} e_0 e_2 + x_{12} e_1 e_2 + x_{012} e_0 e_1 e_2$
 - Scalar (x_s): grade 0
 - Vector $(x_i e_i)$: grade 1 = line
 - Bivector $(x_{ij}e_ie_j)$: grade 2
 - **Trivector** $(x_{012}e_0e_1e_2)$: grade 3
 - Describe a line.
 - $\circ \quad e_0^2=0$
- Destroy bivector/trivectors.
- Number of bases: d = 3
- Geometric algebra dimension: $2^d = 8$
- Join: the output of joining two objects
 - Two joined points (scalar) give a line (vector).

Projective 3D Geometric algebra.

- The geometric algebra used by GATr
- Four coordinates e_0, e_1, e_2, e_3
 - Multivector: $x = x_s + \sum_{i=0}^3 x_i e_i + \sum_{i=0}^2 \sum_{j=i+1}^3 x_{ij} e_i e_j + \sum_{i=0}^1 \sum_{j=i+1}^2 \sum_{k=j+1}^3 x_{ijk} e_i e_j e_k + x_{0123} e_0 e_1 e_2 e_3$
 - Scalar (x_s) : grade 0
 - Vector $(x_i e_i)$: grade 1 = plane
 - Bivector $(x_{ij}e_ie_j)$: grade 2
 - Trivector $(x_{012}e_0e_1e_2)$: grade 3 = points
 - Describe a plane.
 - $\circ \quad e_0^2 = 0$
 - Destroy bivector/trivectors.
 - Number of bases: d = 3
 - Geometric algebra dimension: $2^d = 8$
 - **Wedge product:** the output of intersect two objects.
 - Two intersected planes (vectors) give a line (bivector).
 - Is a geometric product for orthogonal planes (vectors).
 - Opposite of joint

Equivariant linear layer

- GATr neurons are multivectors.
- GATr linear layer: linear mapping from a (input) multivector to a (neuron) multivector
 - One mapping for each multivector.
 - n^2 mappings, where n = input multivectors
 - Summed all together at each output neuron.
- An equilinear layer has always the form $\phi(x) = \sum_{k=0}^{d+1} w_k < x >_k + \sum_{k=0}^d v_k e_0 < x >_k$
 - Sum of weighted blade projections
 - Each weight is a learnable scalar.
 - w_k multiplies each multivector ($\langle x \rangle_k$) component.
 - $e_i \rightarrow e_i$ map
 - $lack v_k$ multiplies each multivector (< $x>_k$) that doesn't have e_0 component.
 - Turns $< x >_k$ component into the analogue with e_0 component.
 - $oldsymbol{e}_i
 ightarrow e_{0i}$ map
 - Blade projection ($\langle x \rangle_k$): multivector x with only the components of grade k
 - So, each component of grade ${m k}$ will have same weights.



- The addictive scalars are processed with a classic linear layer.
 - Weight + bias
 - Equilinear layer **CANNOT** have bias.
 - Lost of equivariance

