E(3)-Equivariant Neural Networks

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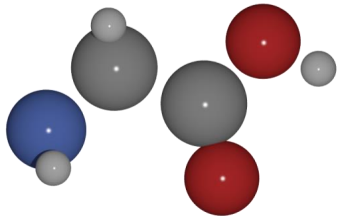
Motivation: Functions of 3D coordinates should rotate in line with the input

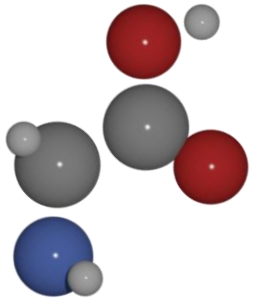
Input

$\boldsymbol{r} \in \mathbb{R}^{n\times 3}$



3D rotation

$R \in \mathbb{R}^{3\times 3}$



Neural Network $f(r)$

Neural Network $f(r)$

Output

Scalar

$s \in \mathbb{R}$

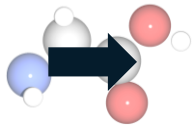
$f_0(\boldsymbol{r}) = s$

$f_0(\boldsymbol{r}R) = s$

Vector

$v \in \mathbb{R}^3$

$f_1(\boldsymbol{r}) = \vec{\boldsymbol{v}}$



$f_1(\boldsymbol{r}R) = \vec{\boldsymbol{v}}R$

Benefits

Model is guaranteed to have correct symmetry

No need for data augmentation

Can generalize much better from little data

Examples of equivariant functions

Equivariance: $f(\boldsymbol{r}R) = D_R f(\boldsymbol{r})$

$f: \mathbb{R}^{n\times 3} \rightarrow \mathbb{R}^d$

$D \in \mathbb{R}^{d\times d}$ orthogonal representation matrix of rotation

Equivariant

Linear combinations of vectors

$f(\boldsymbol{a}, \boldsymbol{b}) = c_1\boldsymbol{a} + c_2\boldsymbol{b}$

Scalar product

$f(\boldsymbol{a}, \boldsymbol{b}) = \sum_i a_i b_i$

Cross product

$h(\boldsymbol{a}, \boldsymbol{b}) = \boldsymbol{a} \times \boldsymbol{b}$

Outer product

$g(\boldsymbol{a}, \boldsymbol{b}) = a_i b_j$

Function of a scalar, e.g.

$h(\boldsymbol{a}, \boldsymbol{b}) = \sigma(\sum_i a_i b_i)$

Not equivariant

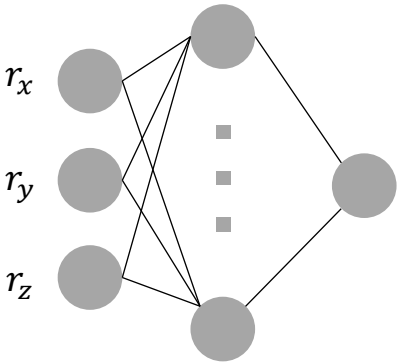
Linear combination of vector coordinates

$f(\boldsymbol{r}) = \sum_i r_i\, c_i$

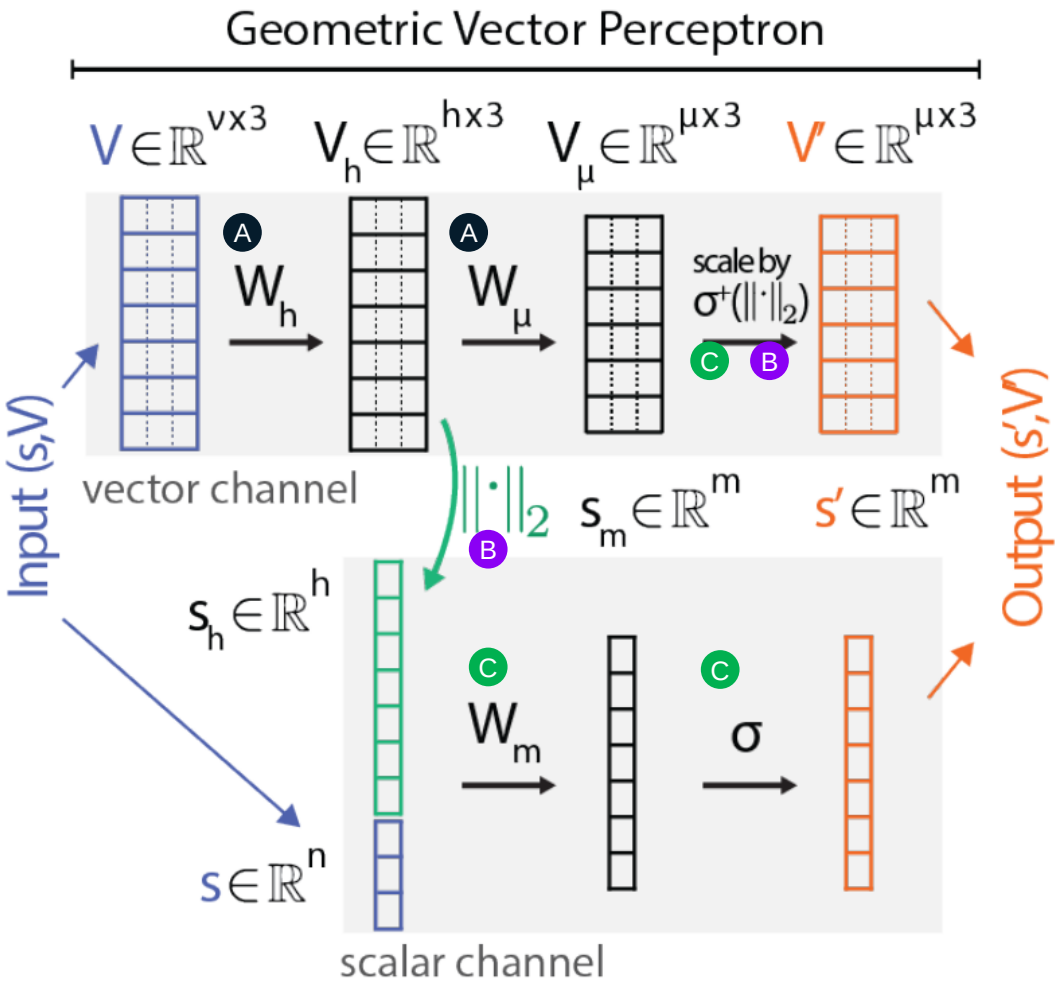
General elementwise operations

$f(\boldsymbol{r}) = \begin{bmatrix}\sigma(r_x) & \sigma(r_y) & \sigma(r_z)\end{bmatrix}$

Naïve MLP



Example of equivariant layer: Geometric vector perceptrons



Used operations

- A Linear combination of vectors
- B Scalar products / norms
- C Functions of scalars

Uses only small subset of possible operations!

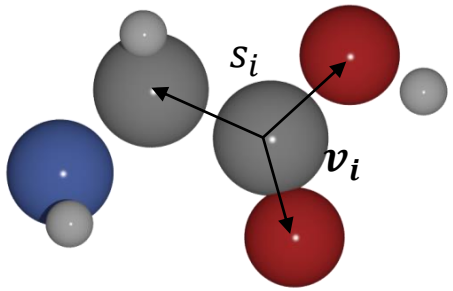
Full architecture: Message passing networks

Input

- 3D coordinates $\boldsymbol{r_i}$ of each particle i
- Properties of each particles (e.g. color)

Compute input features of each particle

- **Scalars** $s_i^{(0)}$**,** e.g. one-hot encoding of color
- **Vectors** $\boldsymbol{v_i^{(0)}}$**,** e.g. directions to k nearest neighbors

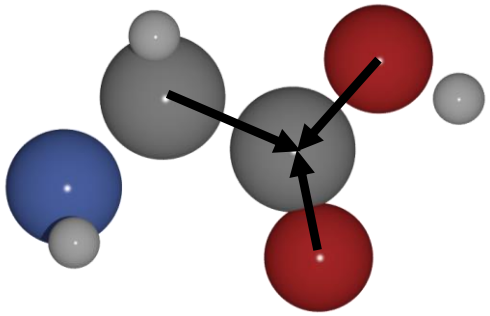


$s_i \in \mathbb{R}^{\#\, scalar\ feat.}$

$\boldsymbol{v_i} \in \mathbb{R}^{\#\, vect.\ feat. \times 3}$

Multiple update rounds

$$s_i^{(t+1)}, \boldsymbol{v_i^{(t+1)}} = \sum_{j \in \boldsymbol{neighbors}} GVP_\theta(s_i^{(t)}, \boldsymbol{v_i^{(t)}}, s_j^{(t)}, \boldsymbol{v_j^{(t)}})$$



Read-out

$$y_{scalar} = \sum_i MLP_\theta(s_i^{(T)})$$

$$y_{vector} = \sum_i \boldsymbol{v_i^{(T)}}$$

Representations of rotations

Representation: Matrix corresponding to a rotation

$D(R): R \rightarrow \mathbb{R}^{d \times d}$

Must form a group

$D(R_1 \circ R_2) = D(R_1)D(R_2)$ $\quad$ $D(Id) = I$ $\quad$ $D(-R) = D(R)^{-1} = D^T$

Reducible: Can be decomposed into lower-dimensional representations

$\exists$ projector $P \in \mathbb{R}^{d \times s}$ $s \leq d$: $\quad$ $P^T DP$ is a representation

Irreducible representations of O(3) rotations

$d = 2l + 1, l \in \mathbb{N}_0$

Fundamental objects have dimensionality 1, 3, 5, …
Typically indexed by $l \in \mathbb{N}_0$ and $m \in [-l, \dots, l]$

Example: Outer product

$$f(\boldsymbol{a},\boldsymbol{b}) = a_i b_j = \begin{bmatrix} a_1b_1 & a_1b_2 & a_1b_3 \\ a_2b_1 & a_2b_2 & a_2b_3 \\ a_3b_1 & a_3b_2 & a_3b_3 \end{bmatrix}$$

$\boldsymbol{l = 0}$**, 1D scalar: Trace**

$$f_0(\boldsymbol{a},\boldsymbol{b}) = tr\big(f(\boldsymbol{a},\boldsymbol{b})\big) = \sum_i a_i b_j$$

$\boldsymbol{l = 1}$**, 3D vector: Antisymmetric part**

$$f_1(\boldsymbol{a},\boldsymbol{b}) = f(\boldsymbol{a},\boldsymbol{b}) - f(\boldsymbol{a},\boldsymbol{b})^{\boldsymbol{T}} = \boldsymbol{a} \times \boldsymbol{b}$$

$\boldsymbol{l = 2}$**, 5D object: Symmetric traceless part**

$$f_2(\boldsymbol{a},\boldsymbol{b}) = f(\boldsymbol{a},\boldsymbol{b}) + f(\boldsymbol{a},\boldsymbol{b})^{\boldsymbol{T}}$$

General decomposition: Clebsch-Gordan

$$y = a \otimes b$$

$$y_{LM} = \sum_{m_1 m_2} C^{LM}_{l_1 l_2 m_1 m_2}\ a_{l_1 m_1}\ b_{l_2 m_2}$$

$C^{LM}_{l_1 l_2 m_1 m_2} \neq 0$ for $|l_1 - l_2| \leq L \leq |l_1 + l_2|$

C is fixed and can be precomputed

1. Take tensorproduct of basic objects a,b
2. Decompose result again into basic objects
3. Truncate?

NequIP: General E(3) equivariant message passing network for molecular properties

Input

- 3D coordinates $\boldsymbol{r_i}$ of each particle i
- Particle type Z_i

Target: Energy E of molecule

Each particle has a feature vector:

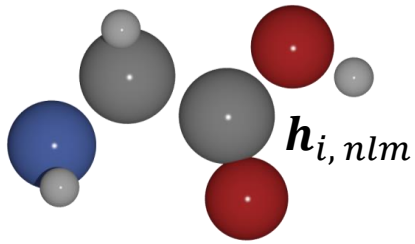
$$\boldsymbol{h}_{i,\,nlm}$$

i … index of particle

n … feature index (e.g. 1-64)

l … type of feature
($l = 0$ scalar, $l = 1$ vector, …)

m… index within this feature



Multiple update rounds

$$\boldsymbol{h}_{i,\,nlm}^{(t+1)} = \sum_k W_{nk} \sum_{m_f m'} C_{l_f l' m_f m'}^{lm} \sum_{\substack{j \in \\ \boldsymbol{neighb.}}} f_\theta(\boldsymbol{r}_{ij})_{k l_f m_f} \otimes \boldsymbol{h}_{j,\,kl'm'}^{(t)}$$

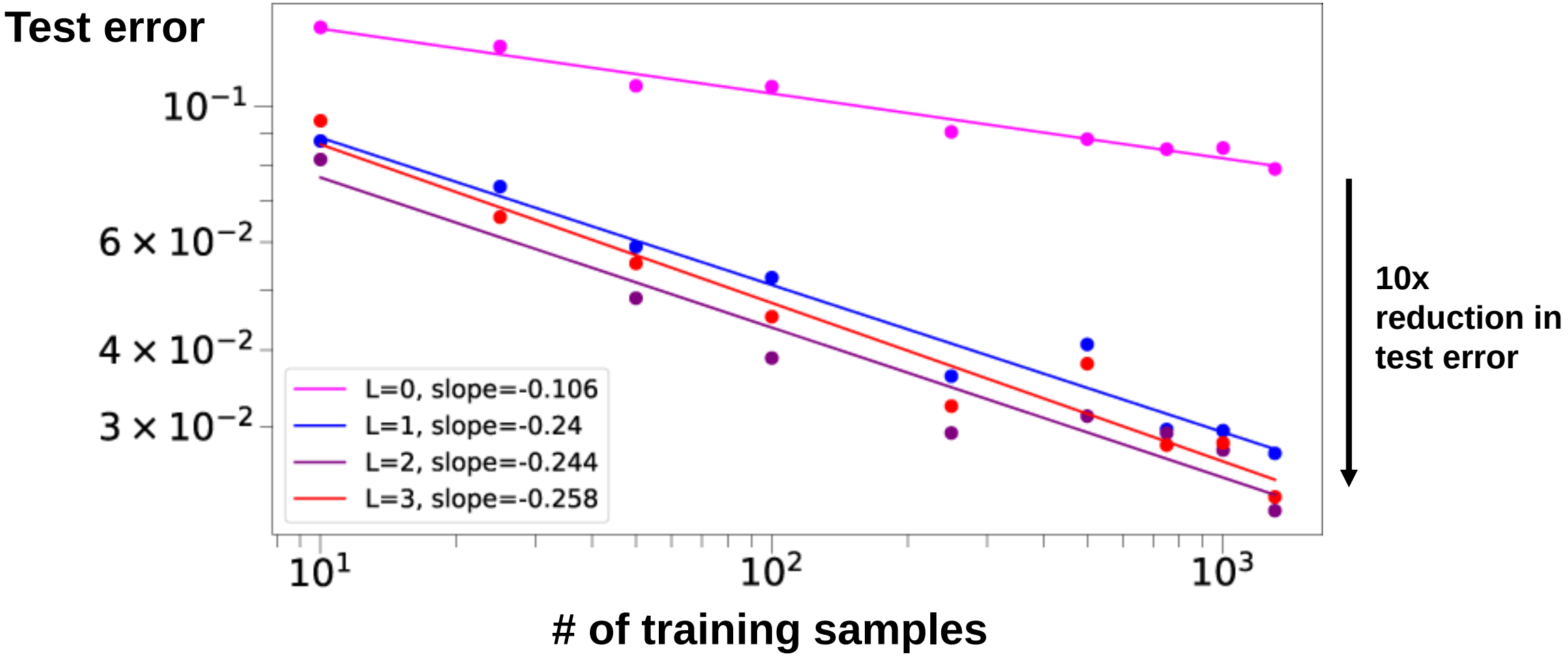
Learnable linear mixing

Reduction to irreducible objects

Convolution with trainable filters f_θ

$$\boldsymbol{E} = \sum_i f_\theta(\boldsymbol{h}_{i,l=0}^{(T)})$$

Including higher-order rotaational features improves data efficiency



NequIP outperformed all other existing surrogate models at the time

Table 1 Energy and Force MAE for molecules on the original MD-17 data set, reported in units of [meV] and [meV/Å], respectively, and a training budget of 1000 reference configurations.

Molecule		SchNet	DimeNet	sGDML	PaiNN	SpookyNet	GemNet-(T/Q)	NewtonNet	UNiTE	NequIP (l = 3)
Aspirin	Energy	16.0	8.8	8.2	6.9	6.5	-	7.3	-	**5.7**
	Forces	58.5	21.6	29.5	14.7	11.2	9.4	15.1	**6.8**	8.0
Ethanol	Energy	3.5	2.8	3.0	2.7	2.3	-	2.6	-	**2.2**
	Forces	16.9	10.0	14.3	9.7	4.1	3.7	9.1	4.0	**3.1**
Malonaldehyde	Energy	5.6	4.5	4.3	3.9	3.4	-	4.2	-	**3.3**
	Forces	28.6	16.6	17.8	13.8	7.2	6.7	14.0	6.9	**5.6**
Naphthalene	Energy	6.9	5.3	5.2	5.0	5.0	-	5.1	-	**4.9**
	Forces	25.2	9.3	4.8	3.3	3.9	2.2	3.6	2.8	**1.7**
Salicylic acid	Energy	8.7	5.8	5.2	4.9	4.9	-	5.0	-	**4.6**
	Forces	36.9	16.2	12.1	8.5	7.8	5.4	8.5	4.2	**3.9**
Toluene	Energy	5.2	4.4	4.3	4.1	4.1	-	4.1	-	**4.0**
	Forces	24.7	9.4	6.1	4.1	3.8	2.6	3.8	3.1	**2.0**
Uracil	Energy	6.1	5.0	4.8	**4.5**	4.6	-	4.6	-	**4.5**
	Forces	24.3	13.1	10.4	6.0	5.2	4.2	6.5	4.2	**3.3**

For GemNet, the best result out of the T/Q versions is presented and for PaiNN the best between force-only and joint force and energy training. For UNiTE, we compare to the "direct-learning" results reported in[26].
Best results are marked in bold.