Demystifying E(3)-equivariant Neural Networks

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6.S898 Deep Learning Class project

DMSE DEPARTMENT OF MATERIALS SCIENCE & ENGINEERING

TTA: Tensor product ≈ learnable equivariant operation is the building block of equivariant NN.

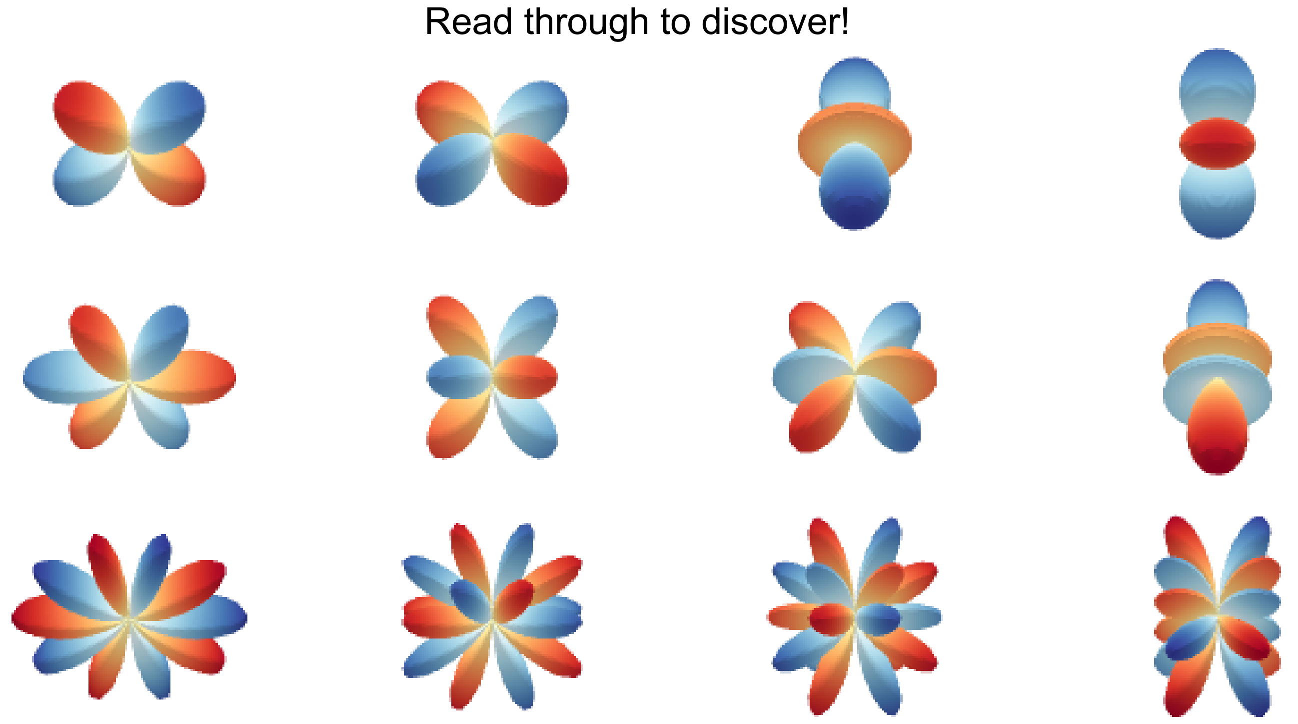
Check out our interactive visualizations!

Poster

Interactive blog post

What are those?

Read through to discover!



Background & motivation

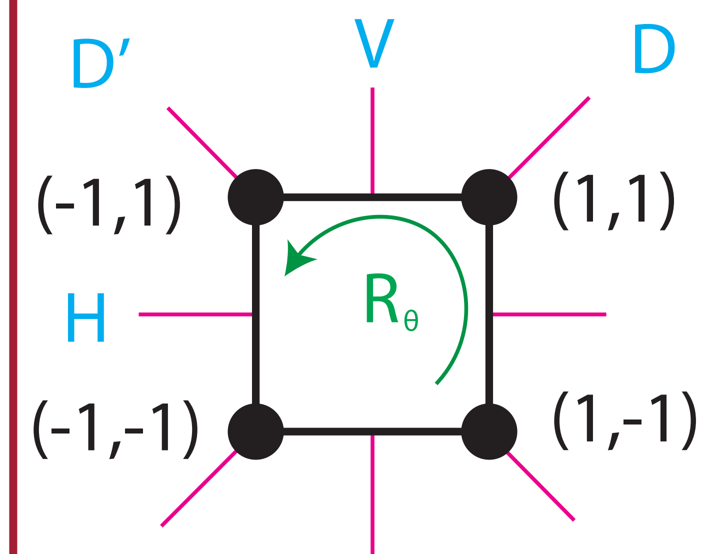
1. Due to the **structural complexity** and **spatial variability** of **atomic systems**, **traditional Neural Networks (NN) rely** on techniques such as **data augmentation** or **feature engineering** to make **physically meaningful predictions** of the materials properties.
2. This comes to the **expense of significant computational time** and **reduced information retention capabilities.**
3. **Geometrical tensors** that **respect Euclidean symmetry** (3D rotations, 3D translations, and inversion) have been found to be **an efficient data type for atomic systems**.
4. **Equivariant 3D Euclidean symmetry-aware NN (e3nn)** can be **orders of magnitude more data-efficient** than traditional NN due to their **natural ability to operate on geometry and understand the given coordinate system.**

References

[1] M. Geiger and T. Smidt. "e3nn: Euclidean Neural Networks". **[2]** S. Batzner, A. Musaelian, L. Sun, M. Geiger, et al. E(3)-equivariant graph neural networks for data-efficient and accurate interatomic potentials.
[2] I. S. Novikov, K. Gubaev, E. V. Podryabinkin, and A. V. Shapeev. "The MLIP package: moment tensor potentials with MPI and active learning".
[3] A. Thompson, L. Swiler, C. Trott, S. Foiles, et al. "Spectral neighbor analysis method for automated generation of quantum-accurate interatomic potentials
[4] K. T. Sch¨utt, P.-J. Kindermans, H. E. Sauceda, S. Chmiela, et al. "SchNet: A continuous-filter convolutional neural network for modeling quantum interactions".

Concepts

Group Representation



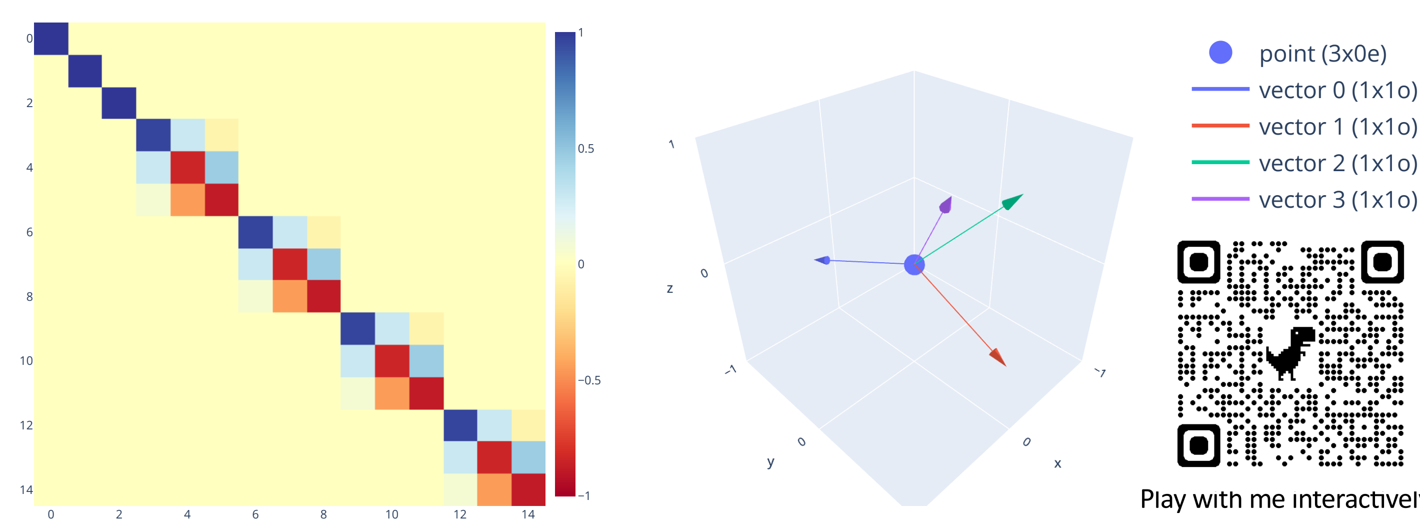
- Each **symmetry element** $\hat{s}$ can be **represented by a matrix**:

$$R_{90} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad V = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

- **Its acts on the square coordinates** $\vec{x}$ **by matrix multiplication**, and displace it to new coordinates $\hat{\vec{x}}$:

$$\hat{\vec{x}} = \hat{s}\vec{x}$$

Transformation under Euclidean Symmetries

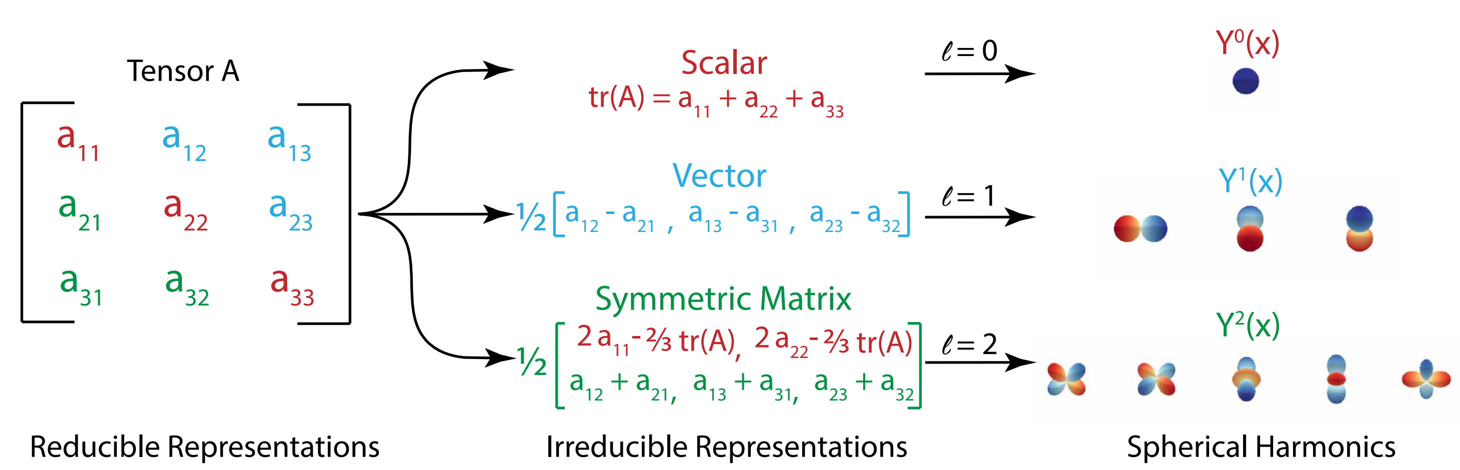


$D^l(R)$ $\qquad$ $x \in \mathcal{R}^{15}$

Play with me interactively!

- **Informing the network of the data types** of its input **tells him how things should transform under symmetry**: under 3D rotation, a vector should rotate, a scalar feature should not, it is an invariant quantity.

Irreducible Representations

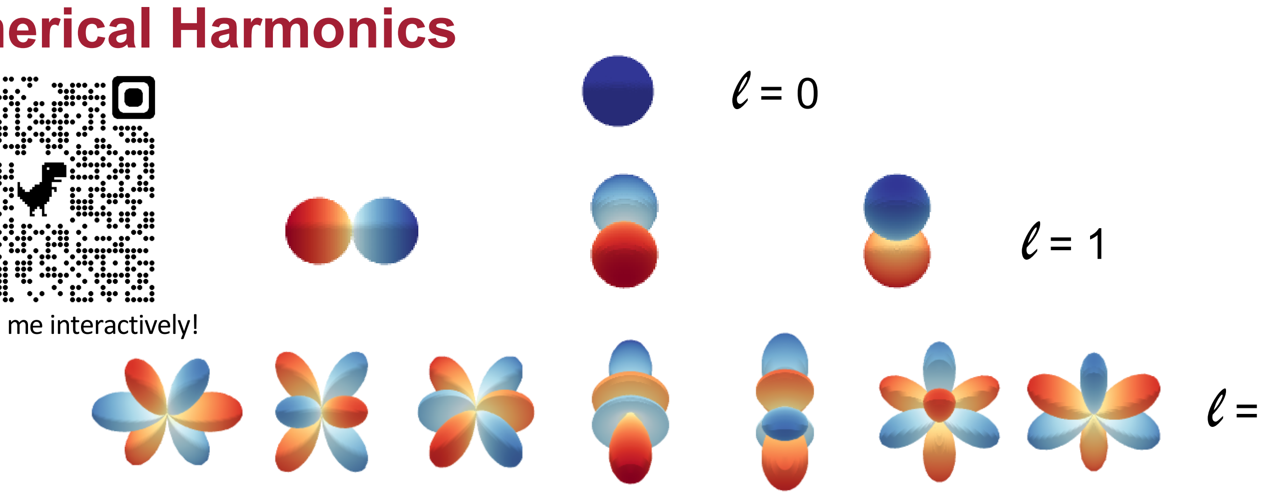


- In E(3)-equivariant NN, **mathematical objects are further decomposed** into **irreps**, **approximated** by **spherical harmonics**, which **are equivariant** objects.

Concepts

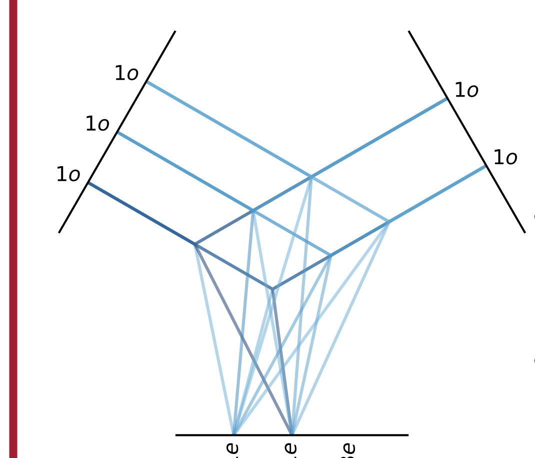
Spherical Harmonics

Play with me interactively!



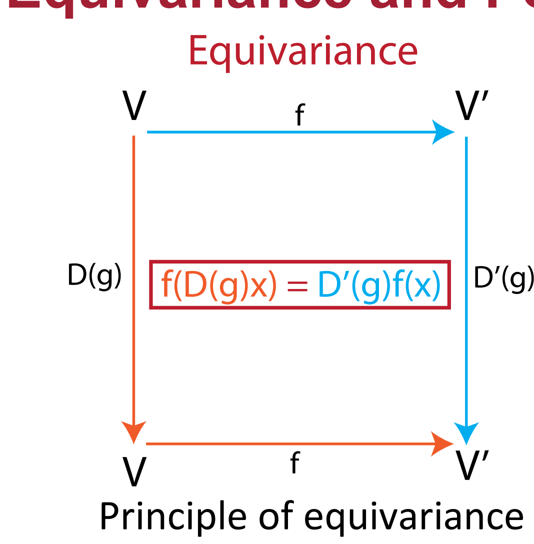
- Spherical harmonics ($Y^l(x)$) are **basis** for all equivariant polynomials on the sphere.
- Extending from unit sphere to R^3, $Y^l(x)$ can be chosen to be **polynomials of x.**

Tensor Product with Learnable parameters



- **Tensor product**: the equivariant multiplication operation of two representations: $x \otimes y$
- The **Irrep** forms of x, y decides the number of **pathways** for tensor products to take place.
- Each pathway of tensor product can be **parametrized** independently, serving as the building block for **equivariant NN.**

Equivariance and Polynomials

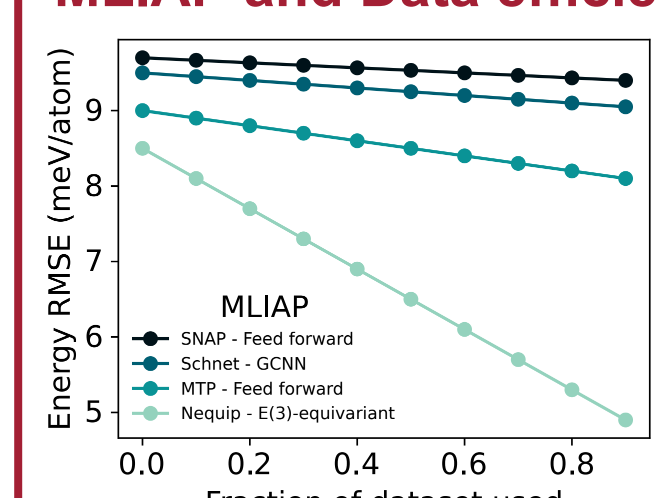


Let f, g be equivariant polynomials, then:

$$f + g \text{ is equivariant}$$
$$f \circ g \text{ is equivariant}$$
$$f \otimes g \text{ is equivariant}$$

What's next…

MLIAP and Data efficiency



- We will showcase the **data efficiency of equivariant-NN** by comparing its prediction performance with several non-equivariant interatomic potentials fitted with **different-sized** training dataset.

The figure shown on the left is just an illustration