

Symmetry, Geometry, Machine Learning and all that.

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1 Unstructured Notes

1.1 Geometric Symmetry Preserving Structures.

1.1.1 Paper

Link: End to End Symmetry - Zhang

The ideas from the paper are summarized, fallbacks in the model identified and suggestions provided.

1.1.2 Problem Statement

The paper seeks a "descriptor" - aka feature representation to the configuration of a molecule that preserves Isometric (Translation and Rotation) and Permutation invariant properties.

1.1.3 Idea

Machine Learning Potentials modelled using Neural Networks are commonplace today. A descriptor that could be represented using a Neural Network is sought after. Ideas from Spherical CNNs and DeepSets are borrowed for realizing this.

1.1.4 Math (not really)

Let $r \in \mathbb{R}^p$ and $y \in \mathbb{B}$ be the position and label of an atom in the molecule.

$$F(r, y) := U_f U_p P_s T_s R_s L(r, y)$$

where

- U_f : Operator computing the forces from Potential $U(r)$
- U_p : Operator computing Potential $U(r)$ from the descriptor $D := P_s T_s R_s$.
- P_s : Symmetry under permutation Operator
- T_s : Symmetry under Translation Operator
- R_s : Symmetry under Rotation Operator
- L : Is the Lookup map from (r, y) to the initial state of the descriptor D_{init}