

Symmetry, Geometry, Machine Learning and all that.

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1 Unstructured Notes

1.1 Symmetric Preserving MLP

Paper

Link: End to End Symmetry - Zhang

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

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.

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.

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}

As a rule $D_{init} = L(r, y)$ gives an initial guess for the descriptor. Realizing R_s involves the orthogonality of Rotation matrices.

Let $U \in SO(n)$, then

$$\begin{aligned} UU^\dagger &= \mathbb{I} \\ R_s &:= UU^\dagger \end{aligned}$$

Assume that an arbitrary function $\eta(r)$ is capable of preserving permutation symmetry. Then by the Universal Approximation Theorem.

$$\eta(r) = \mu(\Sigma_i \phi(r_i))$$

This function is parametrized using a Deep Neural Network ergo $P_s := \eta_{NN}$ When one makes use of relative coordinates of the particles, then Translational Symmetry is already preserved. Consequently, $D = \eta_{NN_1}^\dagger U U^\dagger \eta_{NN_2}$. With this formulation symmetry is preserved.

Potential Flaws

1. Defining Full Matrices for the Rotation Matrices is computationally expensive.
2. A Better Network architecture preserving permutation needs to be suggested improving on DeepSets.