Equivariant Neural Networks for chemistry.

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September 13, 2023

In this document we define the main mathematical concepts, and equations behind all the models that are described in the repo.

1 MLPs

2 Invariance and Equivariance

For simplicity we will consider the n-dimensional euclidean group $\mathrm{E}(n)$. Given a group element $\epsilon \in \mathrm{E}(n)$ we define its representation as the map $\rho : \mathrm{E}(n) \to \mathbb{R}^{n\times n}$, where $\rho(\epsilon)$ is a matrix.

Definition 1. We say a function $f : \mathbb{R}^n \to \mathbb{R}^n$ is $\mathrm{E}(n)$ invariant if for all $x \in \mathbb{R}^n$ and all $\epsilon \in \mathrm{E}(n)$ we have that $f(\rho(\epsilon)x) = f(x)$.

Or in other words, The fuction maps all euclidean transformations of a given input to the same value.

Definition 2. We say a function $f : \mathbb{R}^n \to \mathbb{R}^n$ is $\mathrm{E}(n)$ equivariant if for all $x \in \mathbb{R}^n$ and all $\epsilon \in \mathrm{E}(n)$ we have that $f(\rho(\epsilon)x) = \rho(\epsilon)f(x)$.

Which means the function maps a transformed value to another value transformed in the same way.

3 GNNs

4 Equivariant GNNs