Optimizing the Reduction of Tensors to Irreducible Representations

March 30, 2022

Abstract

In mathematics, a group representation D describes the action of a group G on a vector space V:

$$D : G \to \text{linear operation on } V$$

The “smallest” representations for a group are called *irreducible representations*, or “irreps”.

Within the orthogonal group, $O(3)$, irreps satisfy the following properties:

1. Any representation can be decomposed via a change of basis into a direct sum of irreps.

2. Any physical quantity, under the action of $O(3)$, transforms with a representation of $O(3)$.

These concepts have been used to develop E(3) (3-dimensional Euclidean group) equivariant neural networks[1], which are designed to be used to 3-dimensional constructs that can be rotated, translated, and inverted.

One current algorithm used to reduce tensors into direct sums of irreps takes a “formula” indicating the tensor's indices (and symmetries if they exist) as input, e.g. `ijk = -jik = ikj`, and returns a change of basis Q from the tensor to irreps, along with the irreps themselves. The overall structure of this algorithm is as follows.

1. Germinate formula: create a full group of indices from the input. For example, if the input formula is `ijk = jki`, then `kij` should be added to the group by symmetry. This process is fast and memory-cheap.

2. Create a basis P (represented by a $p \times d$ matrix) from permutation symmetry. P should be of the same size as the output.

[1] https://e3nn.org/

3. Create a basis Q ($q \times d$ matrix) from the Clebsch-Gordan coefficients. This process is memory-expensive.

4. Find projectors into the intersection of P and Q. This process is memory-expensive and slow; in particular, it involves finding the eigenvalue decomposition of a large ($p \times q$) matrix.

5. Choose a basis by orthonormalizing the projector found in step 4.

6. Create the final change of basis Q.

The aim of this project is to speed up this process, likely focusing on improving the third and fourth steps of the algorithm listed above.