Point Group Equivariant Convolutional Graph Neural Networks

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Overview

Vector Space Definition

A vector space V over a field K

Example: $\mathbb{R}^3$, Real 3 Dimensional Space
Locations in physical space may be modeled with a three dimensional vector space $\mathbb{R}^3$ over the real numbers $\mathbb{R}$ with basis functions $\hat{x}, \hat{y}, \hat{z}$.

Often, we may construct new vector spaces from sets of known vector spaces.

Example: Functions on Real 3 Dimensional Space
Scalar functions on physical space also form a vector space over the real numbers, albeit infinite-dimensional. In this case, the group operation between vectors (functions) is point-wise addition.

Group Definition

A group G is a set of elements $\{g_1, ..., g_n\}$ with a binary operation $* : G \times G \to G$ between elements that satisfies the conditions of identity, associativity, invertability, and closure.

Example: General Linear Group

The general linear group $GL(V)$ formed over some vector space V is the set of non-singular $d_v \times d_v$ matrices acting on V. The general linear group is itself a vector space, and we may also form tensor products and direct sums of general linear group vectors.

Cartesian Products

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Direct Sums

We may form direct sums $V \oplus W$ of vector spaces V, W by stipulating that the operation further enforces scalar distributivity to respective subspaces with a set of scalars $K_V \oplus K_W$.

Example: Direct Sum of Matrices

$$\begin{bmatrix} a_1 & b \\ c & a_2 \end{bmatrix} \oplus \begin{bmatrix} d_1 & 0 \\ 0 & d_2 \end{bmatrix} = \begin{bmatrix} a_1 & b & 0 & 0 \\ c & a_2 & 0 & 0 \\ 0 & 0 & d_1 & 0 \\ 0 & 0 & 0 & d_2 \end{bmatrix}$$

Direct sums of vector spaces are themselves vector spaces.

Tensor Products

We may construct tensor products $V \otimes W$ of vector spaces V, W.

Example: Tensor Product of Matrices Also known as "Kronecker Product".

$$\begin{bmatrix} a_1 & b \\ c & a_2 \end{bmatrix} \otimes \begin{bmatrix} d_1 & 0 \\ 0 & d_2 \end{bmatrix} = \begin{bmatrix} a_1 d_1 & 0 & bd_1 & 0 \\ 0 & a_1 d_2 & 0 & bd_2 \\ cd_1 & 0 & a_2 d_1 & 0 \\ 0 & cd_2 & 0 & a_2 d_2 \end{bmatrix}$$

Tensor products of vector spaces are themselves vector spaces.

Group Representations

A representation ρ_G of a group G is a homomorphism from elements g to a set of linear operators (square matrices).

Example: 3D Representation of C_3

Consider three identical points:
These clearly are symmetrical under three-fold rotations about the origin in the xy plane. These C_3 group actions act on this Cartesian basis with the representation ρ defined:

$$\rho(\mathbb{I}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \rho(C_3) = \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \rho(C_3^2) = \begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Irreducible Representations (IRs)

For atomic arrangements, 3D group representations ρ are often reducible in terms of a direct sum of 'smaller' group representations $\rho^{(\alpha)}$:

$$\rho = \bigoplus_{\alpha} c_\alpha \rho^{(\alpha)}$$

Maschke's theorem guarantees that any given representation is always decomposable as a direct sum of irreducible representations.

This set may always be taken to satisfy:

- Unitarity
- Orthogonality
- $\sum_\alpha d_\alpha^2 = N$ where d_α is the dimension of IR α and N is the order

IRs (cont.)

Example: IRs of C_3 The previously shown representation of C_3 elements is reducible into a two-dimensional subspace and a one-dimensional subspace.

$$\rho(\mathbb{I}) = \rho^{(2)}(\mathbb{I}) \oplus \rho^{(1)}(\mathbb{I}) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \oplus [1]$$

$$\rho(C_3) = \rho^{(2)}(C_3) \oplus \rho^{(1)}(C_3) = \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix} \oplus [1]$$

$$\rho(C_3^2) = \rho^{(2)}(C_3^2) \oplus \rho^{(1)}(C_3^2) = \begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix} \oplus [1]$$

Equivalence Classes

Equivalence classes are subsets of group elements that mutually exchange under conjugation, where element g conjugated by element h means:

$$g \to hgh^{-1}$$

In the space of a representation, this is referred to as a similarity transformation, which is essentially a change of basis.

Note that the number of equivalence classes N_c is equal to the number of irreducible representations.

$$N_{\text{IR}} = N_c$$

Character Tables

Irreducible representations are only unique up to change of basis, but their traces are invariant.

$$\chi^{(\alpha)}(g) = \mathrm{Tr}\big(\rho^{(\alpha)}(g)\big)$$

The trace of a representation is known as it's character χ, which is unique for equivalence classes $\langle g \rangle$.

Example: C_4 Character Table

C_4	$\langle \mathbb{I} \rangle$	$\langle C_4 \rangle$	$\langle C_4^2 \rangle$	$\langle C_4^3 \rangle$
a_1	1	1	1	1
a_2	1	-1	1	-1
a_3	1	i	-1	$-i$
a_4	1	$-i$	-1	i

Characters are often displayed in 'character tables', with IRs on one axis and equivalence classes along the other.

Orthogonality Theorems

IRs are orthogonal in the following ways:

$$\frac{1}{N}\sum_{g}\chi^{(\alpha)*}(g)\chi^{(\beta)}(g) = \delta_{\alpha\beta}$$

$$\sum_{\alpha}\chi^{(\alpha)*}(c_k)\chi^{(\alpha)}(c_h) = \frac{N}{N_k}\delta_{kh}$$

where N is the number of elements in G and N_k is the number of elements in equivalence class k.

This allows us to decompose reducible representations by determining the coeffecients of expansion c_α as:

$$c_\alpha = \frac{1}{N}\sum_{g}\chi^{(\alpha)*}(g)\chi(g)$$

Orthogonality Theorems (cont.)

Example: d-shell Splitting in Octohedral Coordinations
Take the Hydrogen-like orbitals $\psi_{\ell m}$ as a basis for spherically symmetric states. The d-shell orbitals are the basis functions of the $\ell = 2$ representations.

The octohedral complex's symmetry group is O, with it's character table and the $\Gamma^{\ell=2}$ representation:

O	$1\langle \mathbb{I} \rangle$	$8\langle C_3 \rangle$	$3\langle C_2 \rangle$	$6\langle C_2' \rangle$	$6\langle C_4^3 \rangle$
$(d)\ \Gamma^{\ell=2}$	5	-1	1	1	-1
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	-1	1
T_2	3	0	-1	1	-1

Orthogonality then gives $\gamma^{\ell=2} = E \oplus T_2$. In practice, this results in a 5-fold degeneracy being lifted into a two- and three-fold degeneracy.

Basis Functions

Suppose we have some Hamiltonian group, so that the group operators $\hat{O}(g)$ commute with $\hat{H}$.

$$[\hat{H}, \hat{O}(g)] = 0 \qquad \forall g \in G$$

In such a case, the operators must have a simultaneous set of eigenvectors ψ_α^k that span the space of functions:

$$f(\vec{r}) = \sum_{k,\alpha} c_k^\alpha \psi_\alpha^k = \sum_{k,\alpha} f_\alpha^k(\vec{r})$$

We have some freedom in choice of this set of basis functions on which the linear operators of the representations act.

Basis Functions (cont.)

Example: Tight Binding
The tight binding approximation often uses localized Hydrogen-like orbitals ψ_{ellm} as a basis for many-body systems

Example: Group of a Hamiltonian
Consider a general Hamiltonian $\hat{H}(\vec{r})$ that depends only on the spatial coordinate $\vec{r}$ of some particle. We then define the operator $\hat{O}_G$ to be a representation of a group G that acts on H's input space $\vec{r}$ as:

$$\hat{O}_G(g)\hat{H}(\vec{r}) = \hat{H}(g^{-1}\vec{r})$$

The "group of the Hamiltonian" is the largest group of the form above that commutes with the Hamiltonian.

Projection Operators

If we have an explicit form for IR α, we may project an arbitrary function onto the k-th basis function f_k^α of IR α with $\hat{P}_\alpha^{kk}$:

$$\hat{P}_\alpha^{kk} = \frac{d_\alpha}{N} \sum_g \left[\Gamma_\alpha^{kk}(g)\right]^* O(g)$$

where d_α is the dimensional of IR α, and then we have:

$$f_\alpha^k(\vec{r}) = \hat{P}_\alpha^{kk} f(\vec{r})$$

From the characters alone, we may project a function onto it's total α subspace with $\hat{P}_\alpha$:

$$\hat{P}_\alpha = \sum_k \hat{P}_\alpha^{kk} = \frac{d_\alpha}{N} \sum_g \chi^{(\alpha)*}(g) \hat{O}(g)$$

Coupling Coefficients

Consider a direct product decomposition of the irreps Γ:

$$\Gamma^\alpha \Gamma^\beta = \bigoplus_\gamma c_{\alpha\beta\gamma} \Gamma^\gamma$$

Products of basis functions $u_i^\alpha v_j^\beta$ then decompose similarly into a direct sum of irreps with basis functions ψ_n^γ via the coupling coefficients $U_{\alpha i \beta j}^{\gamma n}$ as:

$$\psi_n^\gamma = \sum_{i,j} U_{\alpha i \beta j}^{\gamma n} u_i^\alpha v_j^\beta$$

Example: Clebsch-Gordan Coefficients

The Clebsch-Gordan coefficients are the coupling coefficients of $SO(3)$, which relate tensor product spaces of spherical harmonics to direct sums of spherical harmonics.

Equivariant Functions

An equivariant function $f : X \to Y$, where X, Y are vector spaces, is one that 'commutes' with a group's actions, satisfying:

$$f\left(\mathcal{D}^X(g)x\right) = \mathcal{D}^Y(g)f(x)$$

SO(3) Equivariant *Tensor Field Networks*

$$\left(v_{nc}^{L+1}\right)_m^{\ell} = v_{nc}^{L} + \sum_{b \in \mathcal{N}(n)} \sum_{\ell_f, m_f, \ell_i, m_i} c_{\ell_f m_f \ell_i m_i}^{\ell m} \left(F_c^L(r_{nb})\right)_{m_f}^{\ell_f} \left(v_{bc}^{L}\right)_{m_i}^{\ell_i}$$

DeepH

- Take hydrogen-like orbitals and treat them as $SO(3)$ features in e3nn.
- Allows for the learning of all rotational symmetries but doesn't enforce them from physical considerations.

• Incorporate point group symmetry of crystal and molecular sites by directly learning features associated with basis functions that transform as irreducible representations.