Point Group Equivariant Convolutional Graph Neural Networks

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Overview

- Point Group Irreps
  - Scalar Harmonics
  - Transformation Matrices
  - State Labelling
- PGEqnn
  - Graphs
  - Models
- Band Representations
  - What is a band representation?
  - What basis do they act on?

Scalar Harmonics

The scalar-valued point group harmonics $H : \mathbb{R}^3 \to \mathbb{R}$ are analogous to the scalar-valued spherical harmonics $Y : \mathbb{R}^3 \to \mathbb{R}$ in $SO(3)$:

$$H^{\ell}_{\mu ds} = (U^{\ell})^{m}_{\mu ds} Y^{\ell}_{m}$$

Where H is indexed by ℓ as usual, as well as the irreducible representation μ of the point group, dimension d and, (sometimes) multiplicity s.

Example: Cubic Harmonics

The cubic harmonics are the point group harmonics of the cubic point group O_h. See `https://winter.group.shef.ac.uk/orbitron/atomic_orbitals/5f/index.html` for the $5f$ cubic orbitals.

Subgroup Chains

$SO(3)$ only partitions spaces into $2\ell + 1$-dimensional subspaces, with *rotational index* ℓ , labeling the $SO(3)$ irrep as which it transforms.

$$\{Y^\ell\}$$

The additional m of Y^ℓ_m is the *azimuthal index* resulting from a labeling according to $SO(2)$ irreps, conventionally chosen to align with the x, y plane in Cartesian space.

$$SO(3) \subset SO(2)$$

$$\ell \qquad m$$

This compound labeling is thus according to some *subgroup chain*.

Subgroup Chains (cont.)

Example: $O(3)$ Harmonics
Consider the subgroup chain

$$O(3) \subset O(2) \subset C_i$$

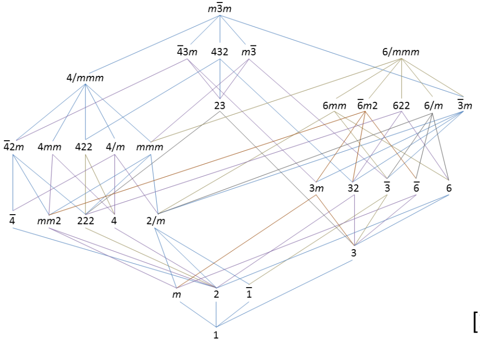
where C_i is the group of order two containing the inversion operation. In this case, we can label harmonics along an additional index p for parity,

$$Y_\ell^{mp}$$

This denotes the irrep of C_i which the harmonic transforms as.

Point Group Labels

This compound labeling can be applied to point groups, which are always subgroups of $O(3)$.



[1]

These provide a convenient labeling scheme for states and properties of physical systems with such symmetries.

[1] https://commons.wikimedia.org/wiki/File:Group-subgroup_relationship_%283D%29.png

Wigner-D Matrices

The different irrep-labeled subspaces of some vector space transform independent of one another under the representation of such group elements.

$$H(Rx) = \sum_{\ell} \mathcal{D}^{\ell}(R) H^{\ell}(x)$$

For the point groups, these are the Wigner-D matrices $\mathcal{D}^{\ell}$, which are block-diagonal in PG bases for their group operations.

$$\mathcal{D}^{\ell}(g)_{\mu_i \nu_j} \propto \delta_{\mu\nu} \quad \text{for } g \in PG$$

These can be gotten from the usual m-component instantiations with U.

$$D^{(\ell)}_{\mu_i \nu_j} = U_{m\nu_j} D^{(\ell)}_{mn} U^{*}_{n\mu_i}$$

Wigner-Eckhart Theorem

The Wigner Eckhart Theorem states that the resultant state of an operator of some irrep label depends on the irrep label of the state of the vector on which it acts.

$$\langle j\ m | T_q^{(k)} | j'\ m' \rangle = \langle j'\ m'\ k\ q | j\ m \rangle \langle j \| T^{(k)} \| j' \rangle$$

These relations allow us to reduce the number of free components of operators into a minimal set of *irreducible tensor components*.

Example: Tight-Binding Hamiltonians In symmetric systems, the Hamiltonian must transform as the trivial irrep A_1:

$$\langle \ell \Gamma d | H_{A_1}^{(k)} | \ell' \Gamma' d' \rangle = \delta_{\Gamma,\Gamma'} \delta_{d,d'} \langle \ell \Gamma d, k A_1 | \ell' \Gamma' d' \rangle \langle \ell \| H^{(k)} \| \ell' \rangle$$

Equivariant Network Components

- Self-interaction:

$$V^{\ell}_{acm} \rightarrow \sum_{c} W^{\ell}_{c'c} V^{\ell}_{acm}$$

- Convolution:

$$V^{\ell_i}_{acm_i} \rightarrow \sum_{m_f, m_i} c^{\ell_o m_o}_{\ell_i m_i \ell_f m_f} \sum_{b} F^{\ell_f \ell_i}_{cm_f}(r_{ab}) V^{\ell_i}_{bcm_i} Y^{\ell_f}_{m_f}(\hat{r}_{ab})$$

- Non-linearities:

$$V^{\ell=0}_{acA_1} \rightarrow \sigma(V^{\ell=0}_{acA_1})$$

- Steering:

$$V^{\ell_i}_{acm_i} \rightarrow \mathcal{D}^{\ell}_{m_i' m_i} V^{\ell_i}_{acm_i}$$

- Pooling:

$$\mathrm{AGG}_a(\{V^{\ell}_{acm}\})$$

PGEqNN

Code implementing the above can be found at:
`https://github.com/qmatyanlab/PGEqNN/`

```
pg_eqnn
├── core
│   ├── transformation
│   ├── vector
│   ├── wigner
│   └── scalar_harmonic
└── torch
    ├── model
    └── graph
```

Note this package require manual installation of MultiPie [1] for the transformation matrices U.

[1] `https://github.com/CMT-MU/MultiPie/`.

Scalar Harmonics

Handled with core/harmonic.py

- Class ScalarPGH can be used to evaluate scalar harmonics

- Calling ScalarPGH returns a set of all scalar harmonics for some $\mathbb{R}^3$ vector

- Used to evaluate edge harmonics through convolution

Transformation Matrices

Handled with core/tranformation.py

- Class generate_U returns transformation matrices from $SO(2)$ bases

- Class generate_C returns complex-to-real transformation matrices in $SO(2)$ bases and openmx reordering matrices for

- Class generate_R returns reordering matrix for OpenMX real harmonics from conventional

Vectors

Handled with core/vector.py

- Class PGHVectorSet track irrep and channel dimensions of features
- Class CGSet returns PG Clebsch-Gordan coefficients
- Can transform vectors with PG Wigner-D's (imported from core/wigner.py)
- Perform CG expansions between PGHVectorSets

Crystal Graphs

Handled with torch/graph.py

- Generates graphs from material structures
- Can create minimal symmetrized graphs for materials, associates node features with Wyckoff positions
- Expands radii with RBFs

Equivariant Model

Handled with torch/model.py

- Self-interaction
- Radial functions
- Convolution

Band Representation

Band representations are induced representations of space groups, formed from it's corresponding point group representation.

$$\text{Band Representation} = \rho_{PG \uparrow SG}$$

Since a point group can be used to generate a coset decomposition of it's space group.

Induced Representations

An induced representation is conceptually the opposite of a 'reduced representation'

Use subgroup G representation $\tilde{\rho}$ to form representation ρ of parent H:

$$\rho_{\alpha i,\beta j}(h) = \begin{cases} \tilde{\rho}(g)_{ij} & \text{if } h_\alpha^{-1} h h_\beta = g \in G \\ 0 & \text{else} \end{cases}$$

where α indexes a coset decomposition of H into $G \subset H$.

Example: Induced Representation of S_2

Take trivial group E with representation $\tilde{\rho}(E) = 1$. Induced rep. of S_2 then is:

$$\rho_{S_2}(\mathbb{I}) = \begin{bmatrix} \tilde{\rho}(\mathbb{I}) & \tilde{\rho}([12]) \\ \tilde{\rho}([12]) & \tilde{\rho}([12][12]) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\rho_{S_2}([12]) = \begin{bmatrix} \tilde{\rho}([12]) & \tilde{\rho}([12][12]) \\ \tilde{\rho}([12][12]) & \tilde{\rho}([12][12][12]) \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Band Rep. Bases

What's really interesting is the basis on which these band representations act.

$$\rho_{PG\uparrow SG}(Tg)W_{i\alpha}(r-t) = \sum_{j}^{d_\rho}[\rho(g)]_{ji}W_{j\beta}(r - Rt - t_{\beta\alpha})$$

This basis represents exponentially-localized Wannier functions [1].

However, not all bands admit a band representation! Those that do not are considered topological bands.

[1] `https://arxiv.org/pdf/2006.04890`

Conclusion

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Computational Resource Repo

A latex document detailing the set up of new cluster nodes is available at:

```
https://github.com/qmatyanlab/ComputationalResources/
├── tex
├── slurm
│   └── sbatch-example
└── ansible-playbooks
    └── openmx-setup
```

This contains ansible-playbooks for the automated setup and an example sbatch file.

TQC Tables

The label of a state along with it's Wyckoff position allow us to determine the high-symmetry k-points which it will have some influence over.

These effects are tabulated for instance, on bilbao or in certain Julia packages (SymmetricTB.jl).