Irreducible Representations of SO(3)

EX: H_2O molecule with configuration

$$C = \{x_O, x_{H_1}, x_{H_2}\}$$ list of atomic positions

⇓ apply rotation $R \in SO(3)$

$$R \cdot C = \{R x_O, R x_{H_1}, R x_{H_2}\}$$

⇒ { Energy E (scalar): doesn't change
Force F_i (vector, per atom): rotated by R

? Is there a systematic way to label these transformation rules?

Math Recap

The irrep V^{ℓ}

$m = -\ell, -\ell+1, \dots, +\ell$

$V^{(\ell)}$ = abstract vector space of dimension $\boxed{2\ell+1}$ on which SO(3) acts irreducibly

For a represention $D: G \to GL(V)$,
V has no proper subspace invariant under all $D(g)$

(a) Label ℓ: which irrep? how many components?

$\ell = 0 \to 1$ component ⇒ scalar (e.g. energy)

$\ell = 1 \to 3$ components ⇒ vector (e.g. vector)

$\ell = 2 \to 5$ components ⇒ traceless symm. tensor

(b) Spherical harmonics Y^l_m

① $SO(3)$ acts on S^2 & on functions on S^2

② space $L^2(S^2) = \oplus_l V^l$ decomposes irreducibly

$\Rightarrow Y^l_m$, $m = -l, \ldots, +l$ is the natural basis used to write irreps down concretely as functions on the sphere

(c) Wigner D-matrix

A rotation R becomes a matrix on V^l:

$$Y^l(R\hat{x}) = D^l(R)\, Y^l(\hat{x}),$$

$$D^l(R) \in \mathbb{R}^{(2l+1)\times(2l+1)} \longrightarrow$$ matrix of a linear map

$\Rightarrow \begin{cases} D^0(R) = 1 \Rightarrow \text{scalar unchanged} \\ D^1(R) = R \Rightarrow \text{vector rotated} \end{cases}$

Application 1 Classify Physical Observables

1. Energy is $l=0$ irrep

$$E(R\cdot C) = E(C)$$

2. Energy is $l=1$ irrep

$$F_i(R\cdot C) = R\cdot F_i(C)$$

$\Rightarrow$ Same physical configuration carries observables of different irrep types

What about $\ell = 2$?

Many tensorial observables in physics are rank-2 Cartesian tensors (9 components), and they're reducible under $SO(3)$:

$$\overset{9}{T^{ij}} = \overset{\substack{\ell=0 \\ \text{(scalar)} \\ 1}}{\mathrm{Tr}(T)} + \overset{\substack{\ell=2 \\ \text{(traceless sym)} \\ 5}}{\tilde{S}^{ij}} + \overset{\substack{\ell=1 \\ \text{(anti-sym)} \\ 3}}{A^{ij}}$$

irreducible

$$\mathbb{R}^{9\times 9} \xrightarrow{\text{reducible}} \begin{pmatrix} \boxed{}^{\,1\times1} & & \\ & \boxed{}^{\,3\times3} & \\ & & \boxed{\text{new}}^{\,5\times5} \end{pmatrix}$$

$3 \otimes 3 = 1 \oplus 3 \oplus 5$

Coupling Rule $\ell_1 \otimes \ell_2$

$$\ell_1 \otimes \ell_2 = |\ell_1 - \ell_2| \oplus |\ell_1 - \ell_2| + 1 \oplus \cdots \oplus (\ell_1 + \ell_2)$$

$$\Uparrow \; |\ell_1 - \ell_2| \le \ell_3 \le \ell_1 + \ell_2 \;\; \& \;\; m_1 + m_2 = m_3$$

$$\left(u^{\ell_1} \otimes v^{\ell_2}\right)^{\ell_3}_{m_3} = \sum_{m_1 m_2} \langle \ell_1 m_1 ; \ell_2 m_2 | \ell_3 m_3 \rangle \, u^{\ell_1}_{m_1} v^{\ell_2}_{m_2}$$

Clebsh-Gordan coeff.

(same numerical values as QM)

Application 2 Equivariant Graph Neural Networks

1. Features

- Node (atom-type embedding)

$$H_i = \bigoplus_{l=0}^{l_{max}} H_i^{l}, \quad \dim H_i^{l} = 2l+1$$

$H_O^0 = E_{Z=8}$, $H_{H_1}^0 = H_{H_2}^0 = E_{Z=1}$

embedding table $E \in \mathbb{R}^{K \times d_0}$ ($H_i^0 = E_{Z_i}$)

- Edge (encode geometry)

↳ relative vector $r_{ij} = x_j - x_i$

distance $r_{ij} = |r_{ij}|$ → radial basis expansion
(invariant scalars) $RBF(r_{ij}) \in \mathbb{R}^n$

direction $\hat{r}_{ij} = \dfrac{r_{ij}}{r_{ij}}$ → spherical harmonic $Y^{l}_{\hat{r}_{ij}}$
(equivariant as the l-irrep)

2. Coupling (1 layer) (combine each neighbor's features)

↳ message passing ×1

$$H_i'^{\,l_3, m_3} = \sum_{j \sim i} \sum_{l_1, l_2} W_{l_1 l_2 l_3}(r_{ij}) \sum_{m_1, m_2} \langle l_1 m_1 ; l_2 m_2 | l_3 m_3 \rangle H_j^{l_1, m_1} Y^{l_2}_{m_2}(\hat{r}_{ij})$$

$W_{l_1 l_2 l_3}(r_{ij})$ → $MLP(RBF(r_{ij}))$ (a distance-dep. learnable scalar)

H_i': atom i's updated feature (after this layer)

* $l_1 / l_2 / l_3$ = input / edge / output irrep labels

EX : Simplest non-trivial path is

$l_1 = 0,\ l_2 = 1 \rightarrow l_3 = 1$ at atom O (for H_2O)

$$H_O^{1,1} = \sum_{j \in \{H_1, H_2\}} \underbrace{w_{0,1,1}(r_{0,j})\, H_j^{0}}_{\text{scalars}}\ \underbrace{Y^1(\hat{r}_{0,j})}_{D^1(R) = R}$$

$\therefore\ H_O^{1,1} \rightarrow R H_O^{1,1}$ is equivariant on an edge

3. Read-out (decode + pool)

- Total energy $E = \sum_i \text{MLP}(H_i^{0,L})$

  sum of final scalar channels

- Force on atom i : $F_i = H_i^{1,L}$

  final vector channel