Irreps. of SO(3)

$SO(3) = \{ \text{3D rotations } Rot_{\vec{a}}(\theta) \}$

Irreps.	ρ_0,	ρ_1,	ρ_2,	$\cdots$,	ρ_k
dim.	1	3	5		

$\rho : SO(3) \longrightarrow GL(\mathbb{R}^n)$

$D^i_j(g) = 3\times 3$ matrix

$\dim(\rho_k) = 2^{k+1}$

$D^j(g_1 g_2) = D^j(g_1)\, D^j(g_2)$

$D^j_{kl}(g_1 g_2) = \sum_i D^j_{ki}(g_1)\, D^i_{il}(g_2)$

Tensor Products of SO(3)-repos

$\rho_0 \otimes \rho_0 \cong \mathbb{R} \cong \rho_0$

$g(1 \otimes 1) = (g\cdot 1) \otimes (g \cdot 1) = 1 \otimes 1$

$\rho_0 \otimes \rho_1 \cong \mathbb{R}^3 = \rho_1$

$c_1 v \longmapsto v$

$\rho_1 \otimes \rho_1 \cong \rho_0 \otimes \rho_1 \otimes \rho_2$

$3\times 3 = 1 + 3 + 5$

$$\rho_k \otimes \rho_k = \rho_0 \otimes \rho_1 \otimes \dots \otimes \rho_{2k}$$

$$k \times k = 1 + 3 + 5 + \dots + 2(2k) + 1$$

— Should hold. Sum of odd numbers formula.

$$\rho_k \otimes \rho_l = \cancel{\rho_{|k-l|} \otimes \dots \otimes \rho_{k+l}}$$

$$= \rho_{|k-l|} \otimes \dots \otimes \rho_{k+l}$$

$$\rho_j$$

$$C^j_{k,l} : \rho_k \otimes \rho_l \longrightarrow \rho_j$$

By definition, this map is equivariant.

$$(\rho_1(g)v_1, \rho_2(g)v_2) \longmapsto \rho_2(g)v$$

Peter-Weyl for $SO(3)$

Recall $L^2(\underset{\underset{S^1}{\parallel}}{SO(2)}) \cong \rho_0 \hat{\oplus} \rho_1 \hat{\oplus} \rho_2 \hat{\oplus} \dots$

— Fourier transform over a circle.

$$L^2(SO(3)) = \rho_0 \hat{\oplus} \underbrace{\rho_1 \hat{\oplus} \rho_1 \hat{\oplus} \rho_1}_{3} \hat{\oplus} \underbrace{\rho_2 \hat{\oplus} \dots \hat{\oplus} \rho_2}_{5}$$

$$\dots \underbrace{\rho_k \hat{\oplus} \rho_k \dots \hat{\oplus} \rho_k}_{\dim(\rho_k)}$$

$SO(3) \circlearrowright S^2 = \{ \vec{u} \in \mathbb{R}^3 \mid \|\vec{u}\| = 1 \}$

$L^2(S^2) = \{ f : S^2 \mapsto \mathbb{R} \mid \text{square-integrable} \}$

$(\rho_{sphere}(g) f) = f \circ g^{-1}$

$L^2(S^2) = \rho_0 \hat{\oplus} \rho_1 \hat{\oplus} \rho_2 \hat{\oplus} \dots \longrightarrow$ spherical harmonics

$$L^2(S^2) = \rho_0 \hat{\oplus} \rho_1 \hat{\oplus} \rho_2 \hat{\oplus} \dots$$

$\hookrightarrow Y_0^0(\vec{u}) = 1$ → not the usual physics normalization

↳ point on a sphere

ρ_1: $Y_{-1}^1 \quad Y_0^1 \quad Y_1^1$ — $\dim(\rho_1) = 3$

$$\left(\rho_{sphere}(g) Y_i^1\right) = Y_i^1 \circ g^{-1} = a Y_{-1}^1 + b Y_0^1 + c Y_1^1$$

$$= D_{-1\,i}^1(g) Y_{-1}^1 + D_0^1(g) Y_0^1 + D_{1\,i}^1(g) Y_1^1$$

→ each g gives 3×3 coefficients

3×3 coeffs. are $D^1(g) = \rho_1(g)$

Group together

$$Y^1(\vec{u}) = \begin{pmatrix} Y_{-1}(\vec{u}) \\ Y_0(\vec{u}) \\ Y_1(\vec{u}) \end{pmatrix} : S^3 \mapsto \mathbb{R}^3$$

$$\boxed{Y^1(g^{-1}\vec{u}) = \rho_1(g) Y^1(\vec{u})}$$

→ equivariant mapping

$$Y^\ell(g^{-1}\vec{u}) = \rho_\ell(g)\, Y^\ell(\vec{u})$$

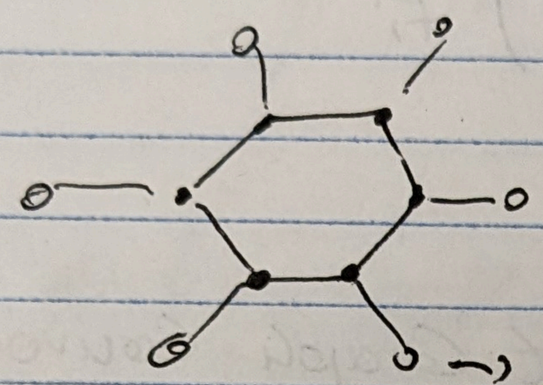
irreps

$$Y^\ell : S^2 \longmapsto \mathbb{R}^{2\ell+1}$$

We bundle up $Y^\ell_{-\ell}, \dots, Y^\ell_\ell$.

Lecture 11: Tensor Field Networks

Input data: 3D molecular graph



$\vec{f}_i \in (\mathbb{R}^n, \rho)$

$\longmapsto t$

$\vec{x}_i \in (\mathbb{R}^3, \rho_i)$

$\{\vec{x}_i\} \longrightarrow$ node positions

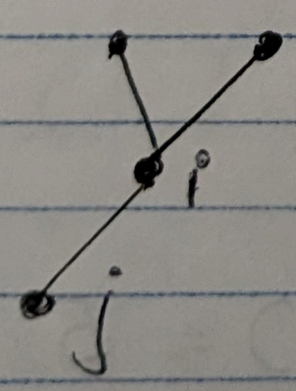
$\{\vec{f}_i\} \longrightarrow$ node features

$\{\vec{f}_i\} \longmapsto \{h_i\}$

$(\mathbb{R}^n, \rho_{in}) \longmapsto (\mathbb{R}^n, \rho_{hid})$

Generalize graph convolutions to be 3D equivariant

same W for all i, j



$$h_i = \sum_{j \in N(i)} W \vec{f}_j$$

Conv 2D depends on relative pixel positions

$$f_{\vec{v}} = \sum_{\vec{w}} W(\vec{w} - \vec{v})\, f_{\vec{w}}$$

Geometric Embedded Graph Convolution

$$h_i = \sum_{j \in N(i)} W(\vec{x}_j - \vec{x}_i) f_i$$

3D Rotationally Equivariant Graph Convolution

Need

$$f_j \mapsto \rho_{in}$$

$$h_i \mapsto \rho_{out}$$

$$\boxed{W(g\vec{r}) = \rho_{out}(g)\, W(\vec{r})\, \rho_{in}(g)^{-1}}$$

↳ Constraint on the weights.

Example:

$$\rho_{in} = \rho_1$$

$$\rho_{out} = \rho_1$$

Choose $Y^2 : S^2 \mapsto \mathbb{R}^5$

$$\dim(\rho_2) = 5$$

$$\hat{Y}^2(g\vec{x}) = \rho_2(g)\, \hat{Y}^2(\vec{x})$$

$$\cancel{h_i = \sum_{j \in N(i)} C^2_{1,1}}$$

$$\rho_1 \oplus \rho_1 \mapsto \rho_2$$

$$h_i = \sum_{j \in N(\vec{r})} \overset{\rho_2 \oplus \rho_1 \mapsto \rho_1}{C^{1}_{2,1}} \overbrace{\left[\underbrace{\hat{Y}^2\left(\frac{\vec{x}_j - \vec{x}_i}{\|x_j - x_i\|}\right)}_{\rho_2} \underbrace{R(\|x_j - x_i\|)}_{\text{MLP}: \mathbb{R}^+ \to \mathbb{R}} \otimes \underbrace{f_j}_{\rho_1} \right]}^{W(\vec{r})}$$

ρ_2

<u>Claim</u>: this solves the equivariance constraint.

<u>Proof</u>: $g \in SO(3)$

$$\left(\rho_1(g)\vec{x}_i,\ \rho_{in}(g)\vec{f}_j\right) \longmapsto \rho_{out}(g)\vec{h}$$

$$\sum_j C\left[\hat{Y}^k\left(\frac{g\vec{r}}{\|g\vec{r}\|}\right) R(\|g\vec{r}\|) \otimes (\rho_{in}(g) f_j)\right] =$$

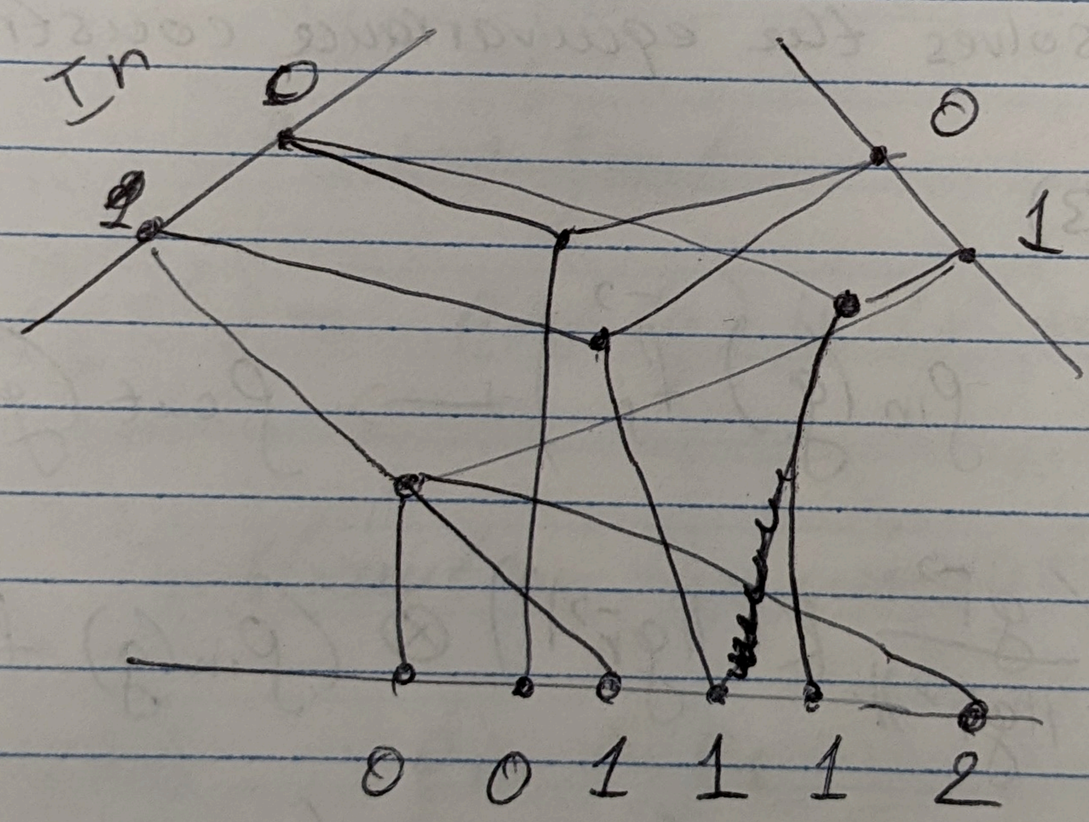
$$= \sum_j C\left[\hat{Y}^k\left(g\frac{\vec{r}}{\|\vec{r}\|}\right) R(\|\vec{r}\|) \otimes (\rho_{in}(g) f_j)\right] =$$

$$= \sum_j C\left[\rho_k(g)\hat{Y}^k\left(\frac{\vec{r}}{\|\vec{r}\|}\right) R(\|\vec{r}\|) \otimes (\rho_{in}(g) f_j)\right] =$$

$$= \sum_j C\left[(\rho_k \otimes \rho_{in})(g)\left(\hat{Y}^k\left(\frac{\vec{r}}{\|\vec{r}\|}\right) R(\|\vec{r}\|) \otimes f_j\right)\right] =$$

$$= \sum_j \rho_{in}(g)\, C\left[Y^k\left(\frac{\vec{r}}{\|\vec{r}\|}\right) R(\|\vec{r}\|) \otimes f_j\right] =$$

$$= \rho_{out}(g)\left[\sum_j C\left[\hat{Y}^k\left(\frac{\vec{r}}{\|\vec{r}\|}\right) R(\|\vec{r}\|) \otimes f_j\right]\right] =$$

$$= \rho_{out}(g)\,\vec{h} \qquad \square$$

<u>Multiplicity</u> Input $\rho_0 \otimes \rho_1$, kernel $\rho_0 \otimes \rho_1$ $\quad Y^0 \quad Y^1$