Point Group Equivariant Networks for Material Systems

Thesis Proposal

Alex Heilman

July 23, 2025

Overview

Graph Neural Networks for Materials Science

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- Hypergraph representations

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- Importance of Equivariance

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- $O(3)$ Equivariance & Tensor Predictions

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- Hypergraph representations
- Importance of Equivariance
- $O(3)$ Equivariance & Tensor Predictions
- Why we should use material symmetry groups!

Why Neural Networks?

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Physics assumes there exists a map between configurations and properties of physical systems:

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But how do we apply this to material systems?

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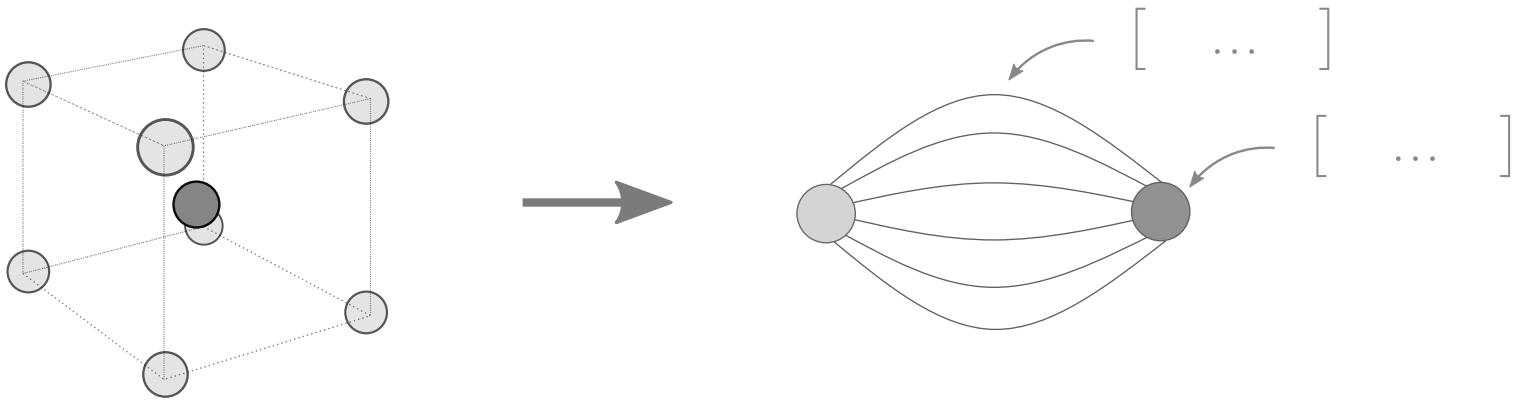
2. A trainable model that acts on this representation

Usual Crystal Graph Construction (a la CGCNN)

- Common techniques represent crystalline systems as graphs (nodes and edges) [2, 3, 4]



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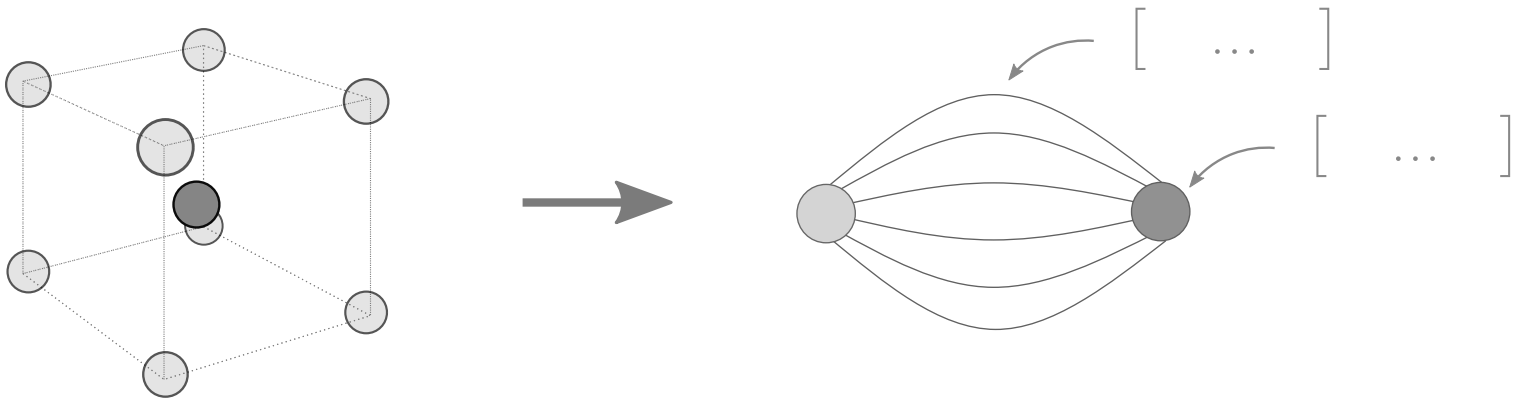

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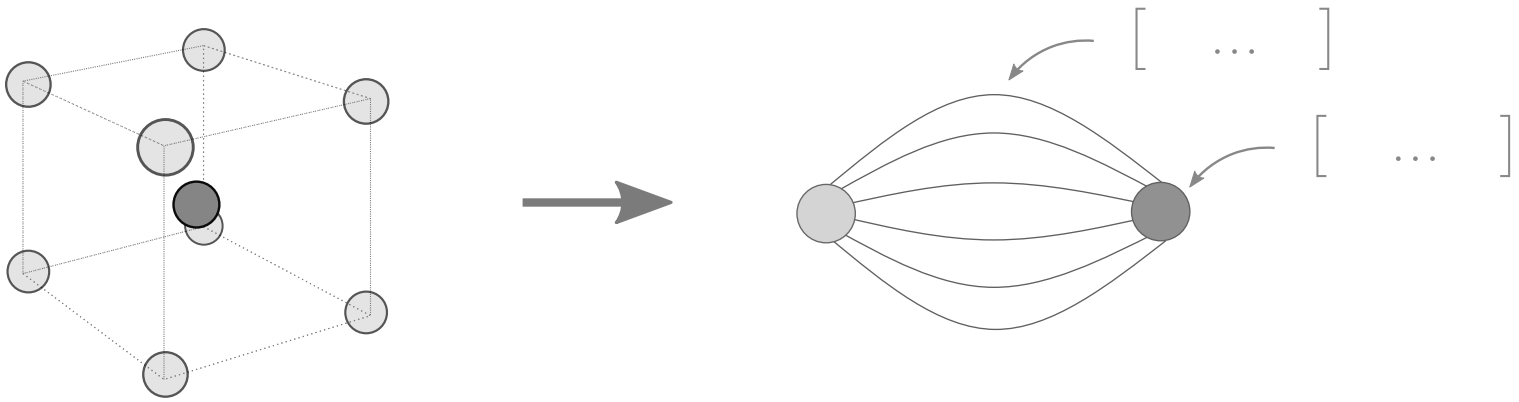

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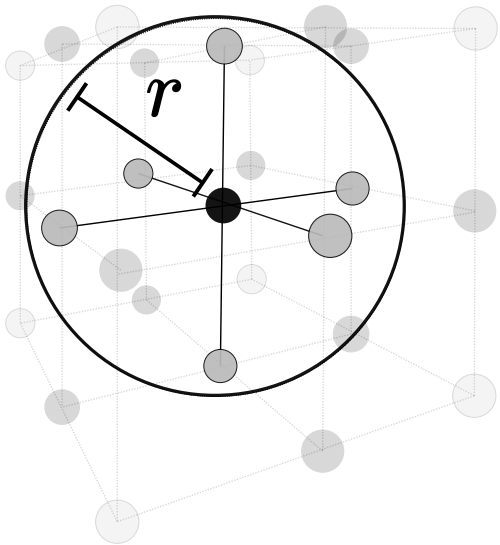
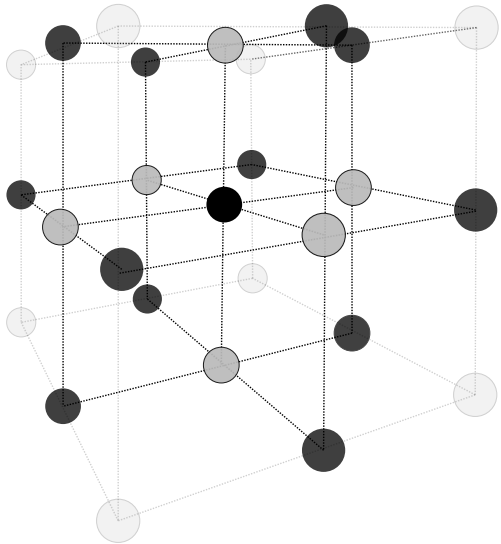
How do we construct these?

Crystal Graphs cont. I

- Edges are determined by distance cutoff (8 Ang.) and maximum number of neighbors (12)



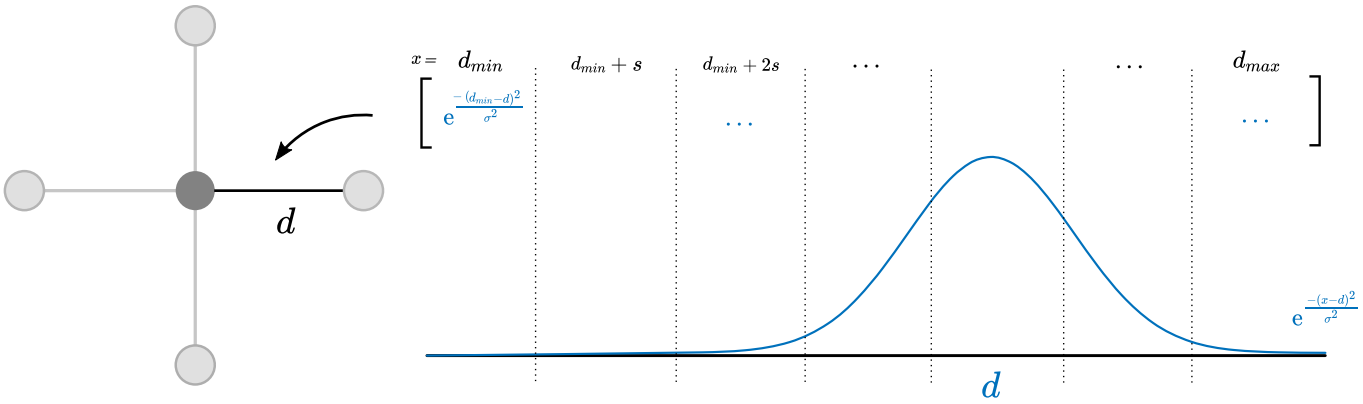
(within) Max radius r



N nearest neighbors

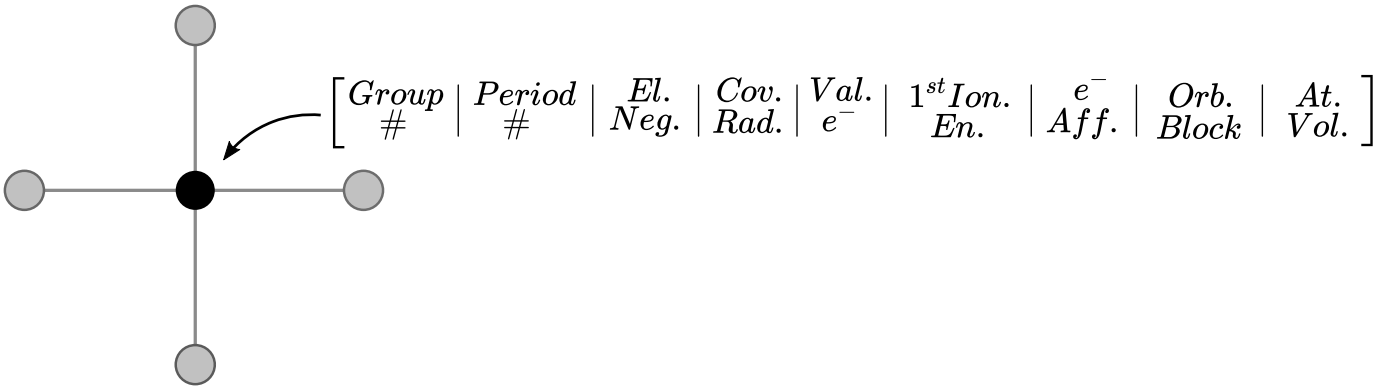
Crystal Graphs cont. II

- Edge attributes e then are a Gaussian distance expansion



Crystal Graphs cont. III

- Node features n are encoded physical properties



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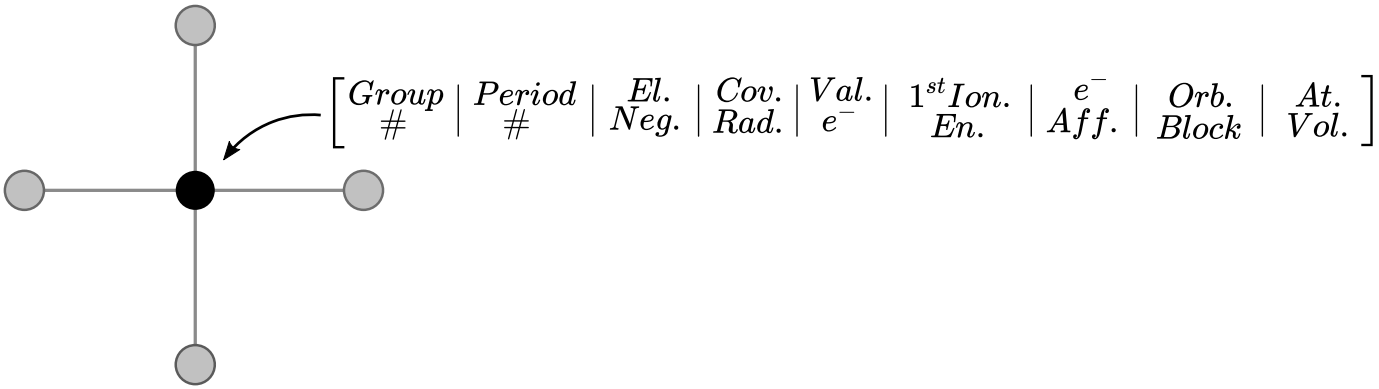

What do we do with these things?

Message Passing on Graphs

Update with GNN or message passing network [5]:

$$m_i^{t+1} = \sum_{n_j \in \mathcal{N}(i)} M_t(n_i^t, e_{ij}, n_j^t)$$

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Then, read out prediction from updated node features.

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- CGConv [2]:

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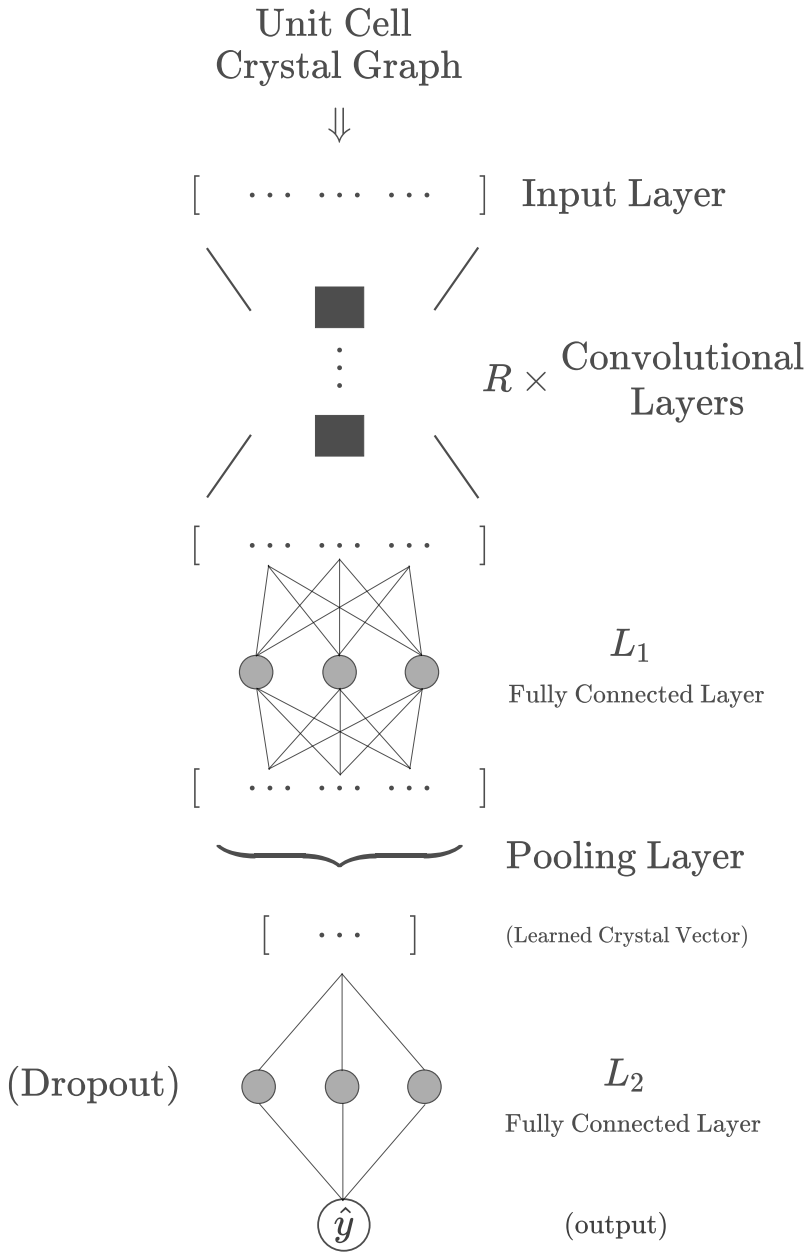
Graph Neural Network



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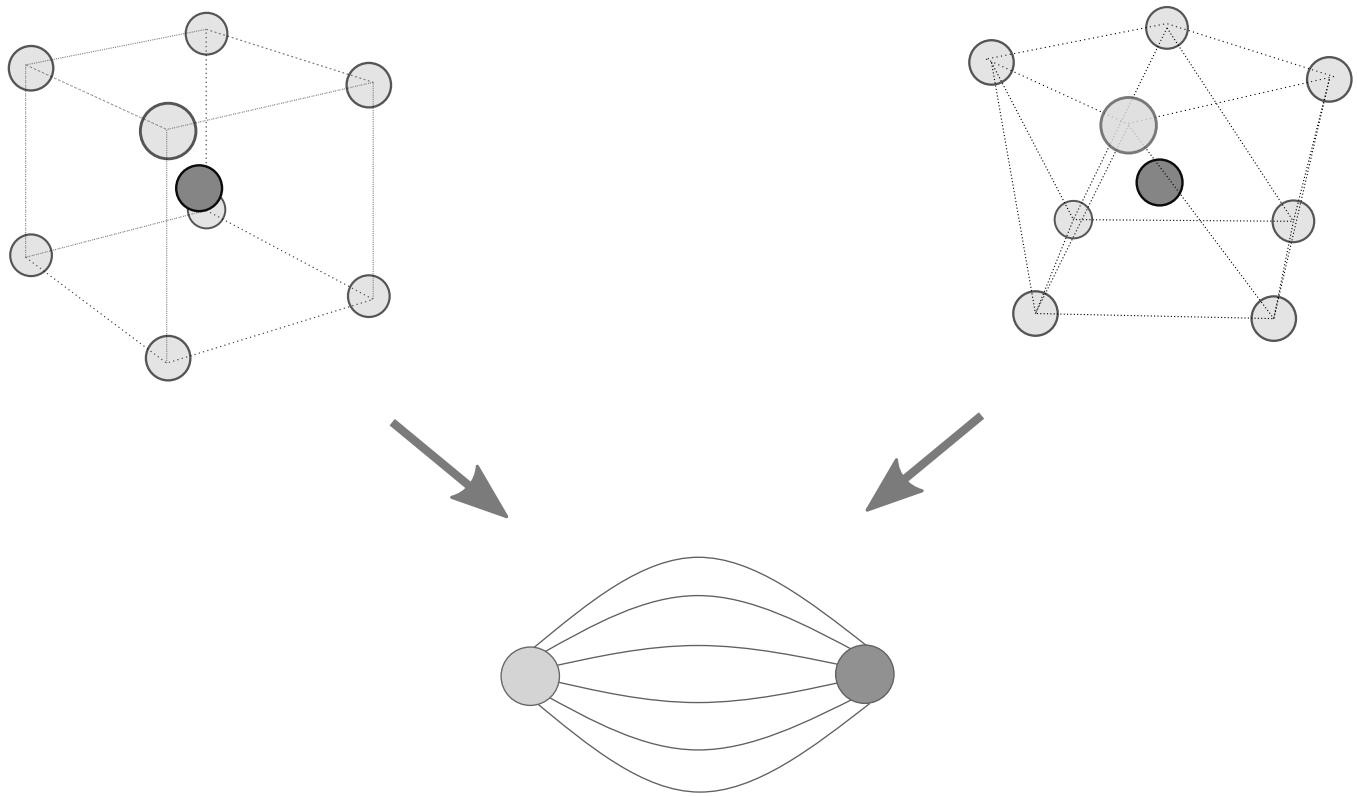
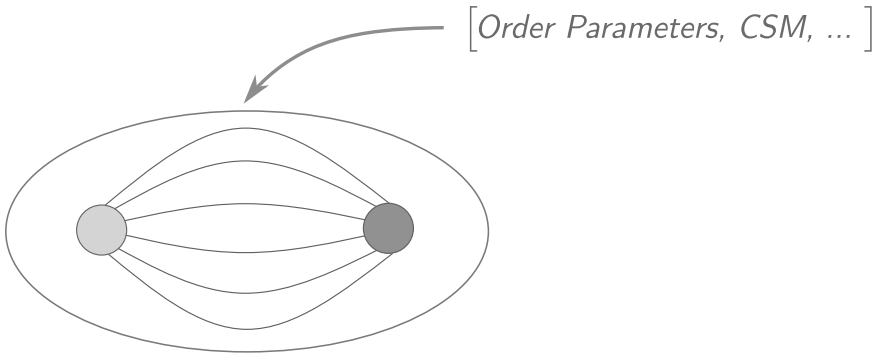


These two have the same representations!

(One) Solution: Hypergraphs!

Hypergraphs allow us to have edges containing more than (or less than) two nodes.



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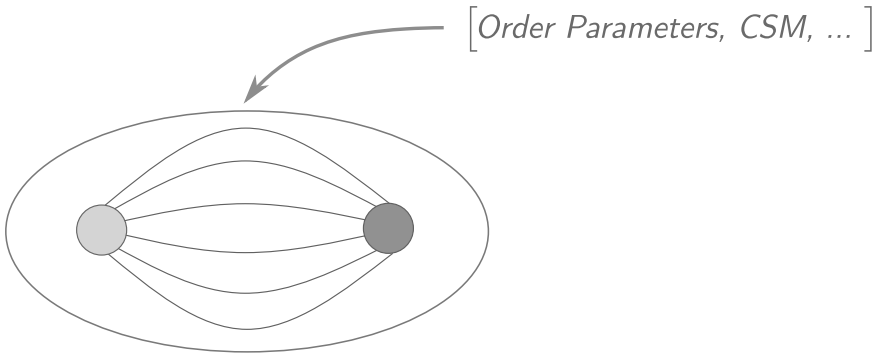

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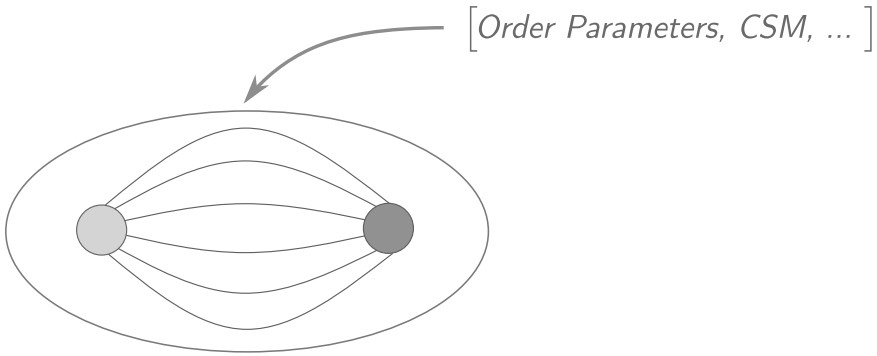

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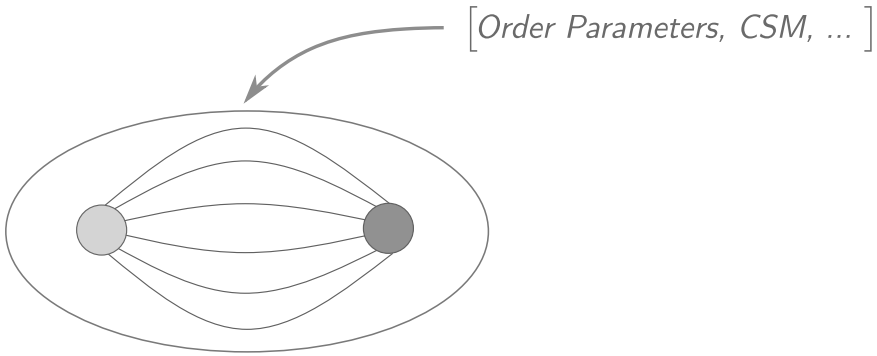

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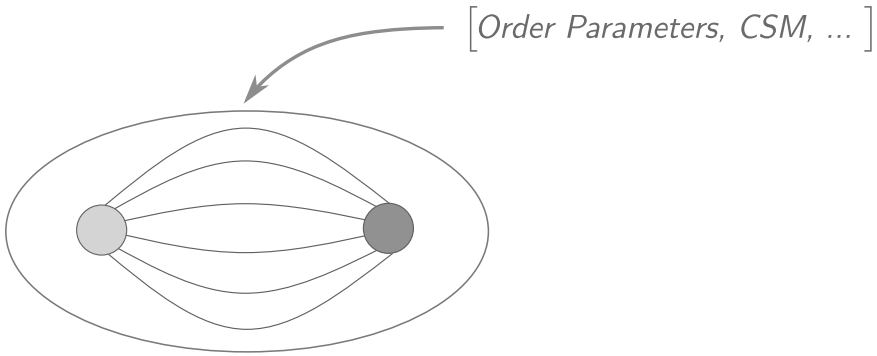

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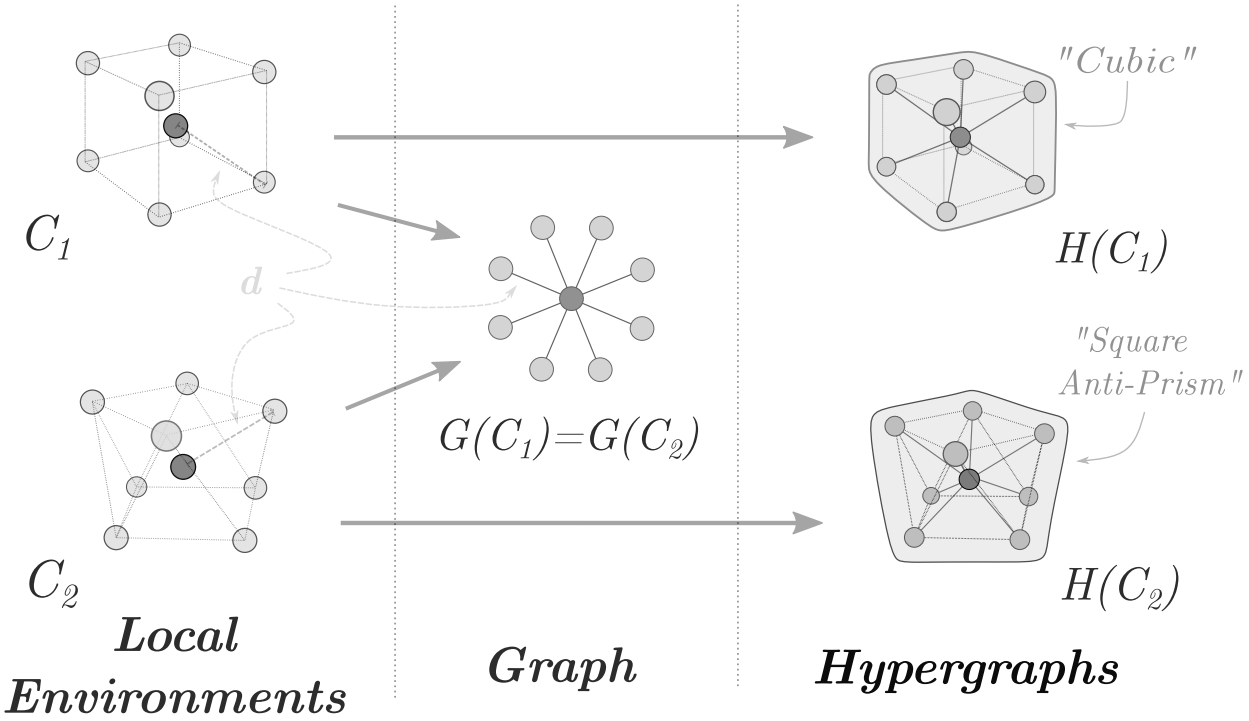

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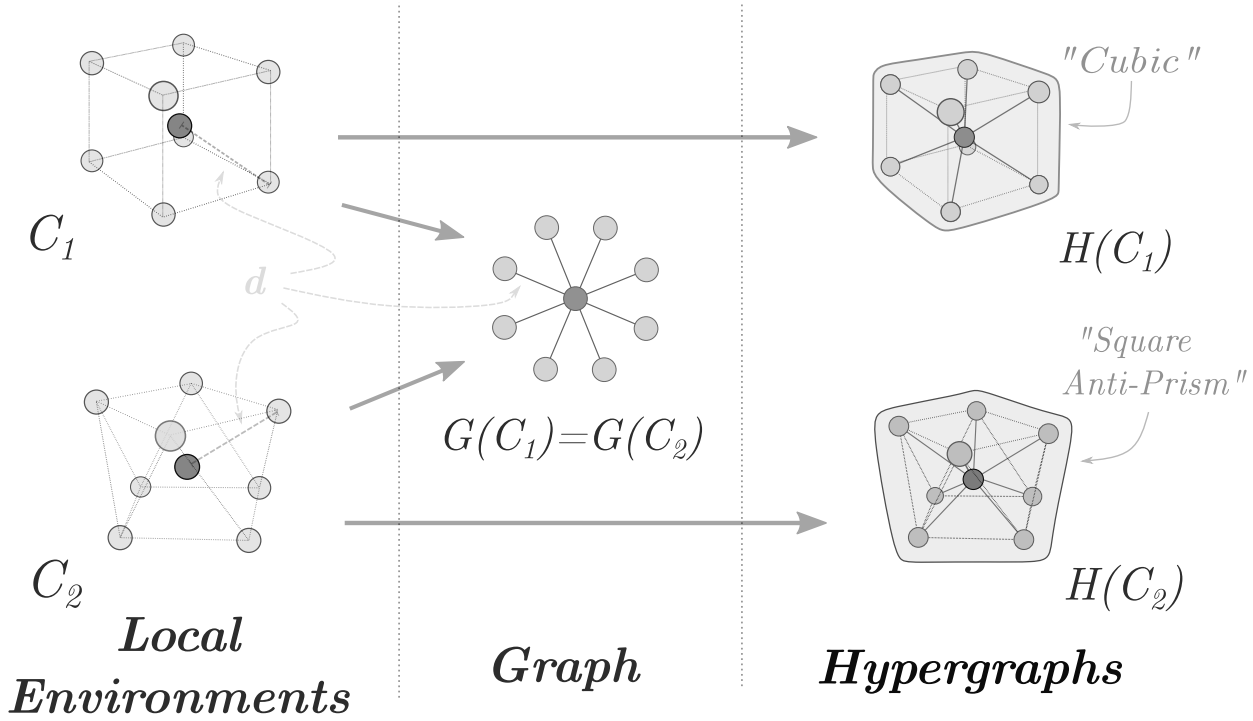

• Geometrical information can be encoded quantitatively with continuous symmetry measures, local structure order parameters, etc.

Extending Message Passing to Hypergraphs

Now, we need a suitable convolutional structure that applies to hypergraphs...

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Hypergraph Convolution

Aggregate the node features!

$$n_i \rightarrow n_i + \sum_{e_{ij}} M_b(n_i \oplus e_{ij} \oplus n_j)$$
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- Can also be learnable mix of above with attention

CHGConv

A generalization of CGConv with hyperedge aggregation:

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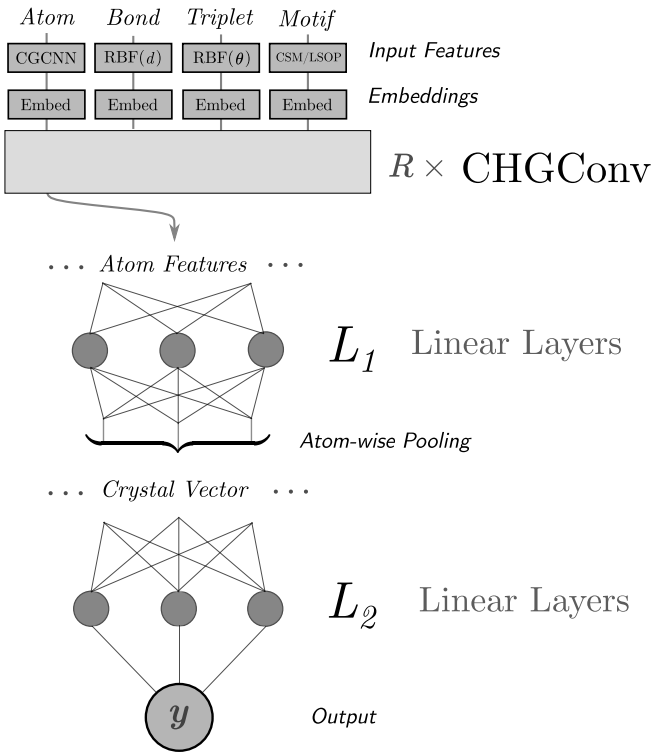
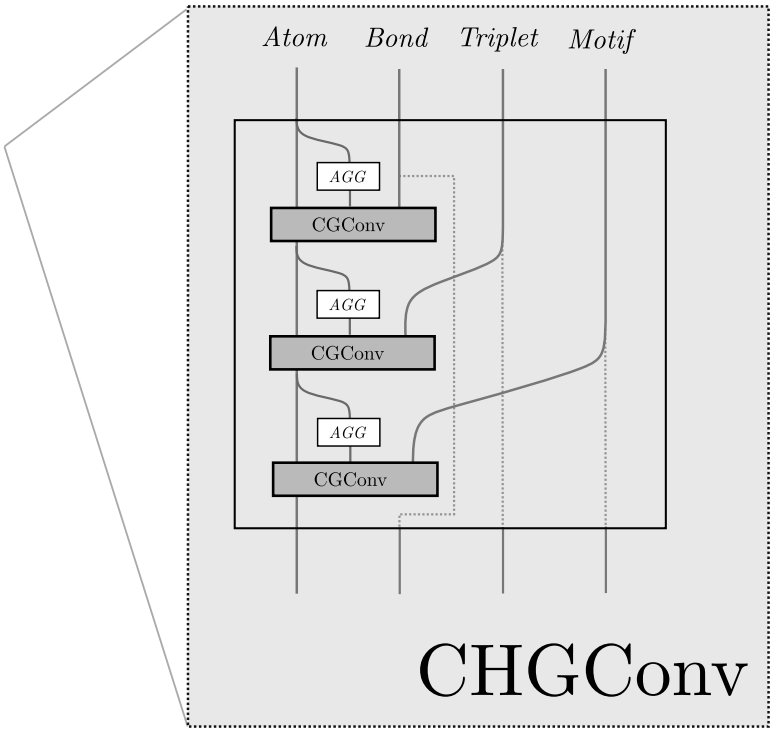
CHGCNN Schematic





CHGCNN Results

Hyperedge Types	E_g MAE (eV)	G_{vrh} MAE (Log_{10}GPa)	K_{vrh} MAE (Log_{10}GPa)
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But what if we care about about coordinate-system dependent quantities?

Equivariant Functions

A function $f : X \to Y$ is *equivariant* if it 'commutes' with a group:

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

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Note: Equivariance is always with respect to some group!

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Index α denotes irrep, and i the dimension of irrep space α.

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- Pooling over nodes or channels:

$$v_c = \sum_{n} v_{nc}$$

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Many models are further referred to as $E(3)$-equivariant [8] for the Euclidean group (add parity and translation invariance).

Tensor Field Networks

Tensor field networks [9] use SO(3) equivariant convolution:

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- F_c^L: Filter function (trainable)

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

- v_{nc}^{L}: Node feature of node n, channel c, layer L
- $c_{\ell_f m_f \ell_i m_i}^{\ell_o m_o}$: Clebsch-Gordan coefficients
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F is generally a neural network; r is often expanded with some radial basis function (RBF): Gaussian, Bessel, etc.

$SO(3)$-Equivariant Features

Remember that node (and edge) features now have additional indices ℓ and m!

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But what can we do with this?

J_z Basis

Recall $\ell = 1$ spherical harmonics (with Racah normalization):

$$Y_1^{+1} = -\frac{1}{\sqrt{2}}(x + iy) = \frac{1}{\sqrt{2}} \sin\phi e^{i\theta}$$
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Define J_z basis [10, 11]:

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\begin{bmatrix} a_+ \\ a_0 \\ a_- \end{bmatrix} = \begin{bmatrix} -\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ -\frac{1}{\sqrt{2}} & +\frac{i}{\sqrt{2}} & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}
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so that $\vec{n} = a_+ \hat{Y}_1^1 + a_0 \hat{Y}_1^0 + a_- \hat{Y}_1^{-1}$

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Build larger spherical harmonic tensors with CG expansion:

$$Y_{\ell_1}^{m_1} \otimes Y_{\ell_2}^{m_2} = \sum_{L=|\ell_1-\ell_2|}^{\ell_1+\ell_2} \sum_{M=-L}^{L} C_{\ell_1 0 \ell_2 0}^{L0} C_{\ell_1 m_1 \ell_2 m_2}^{LM} Y_L^M$$

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But, what about asymmetric tensors?

$SO(3)$ Invariant Tensor Subspaces

- An arbitrary tensor T transforms as:

$$T_{x_1 x_2 \ldots x_n} \rightarrow T_{x_1' x_2' \ldots x_n'} = R^{x_1}_{x_1'} R^{x_2}_{x_2'} R^{x_3}_{x_3'} T_{x_1 x_2 \ldots x_n},$$

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- This decomposition can be constructed by consecutive decomposition with respect to GL and then O and SL

$$SO = (SL \cap O) \subset GL$$

Decomposition Example: Rank 2

Consider a rank-two tensor T_{ij}:

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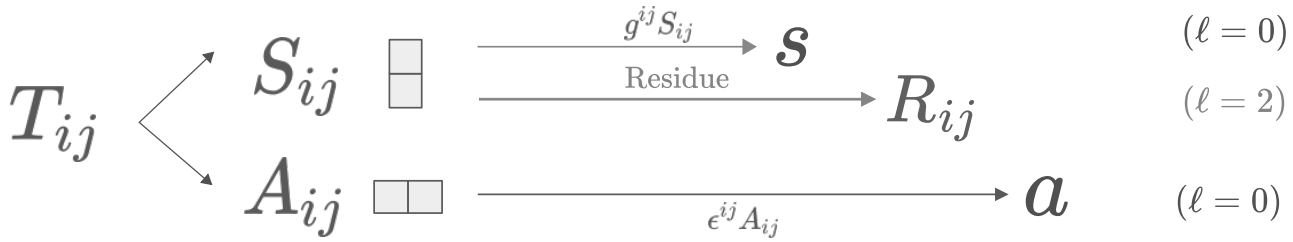
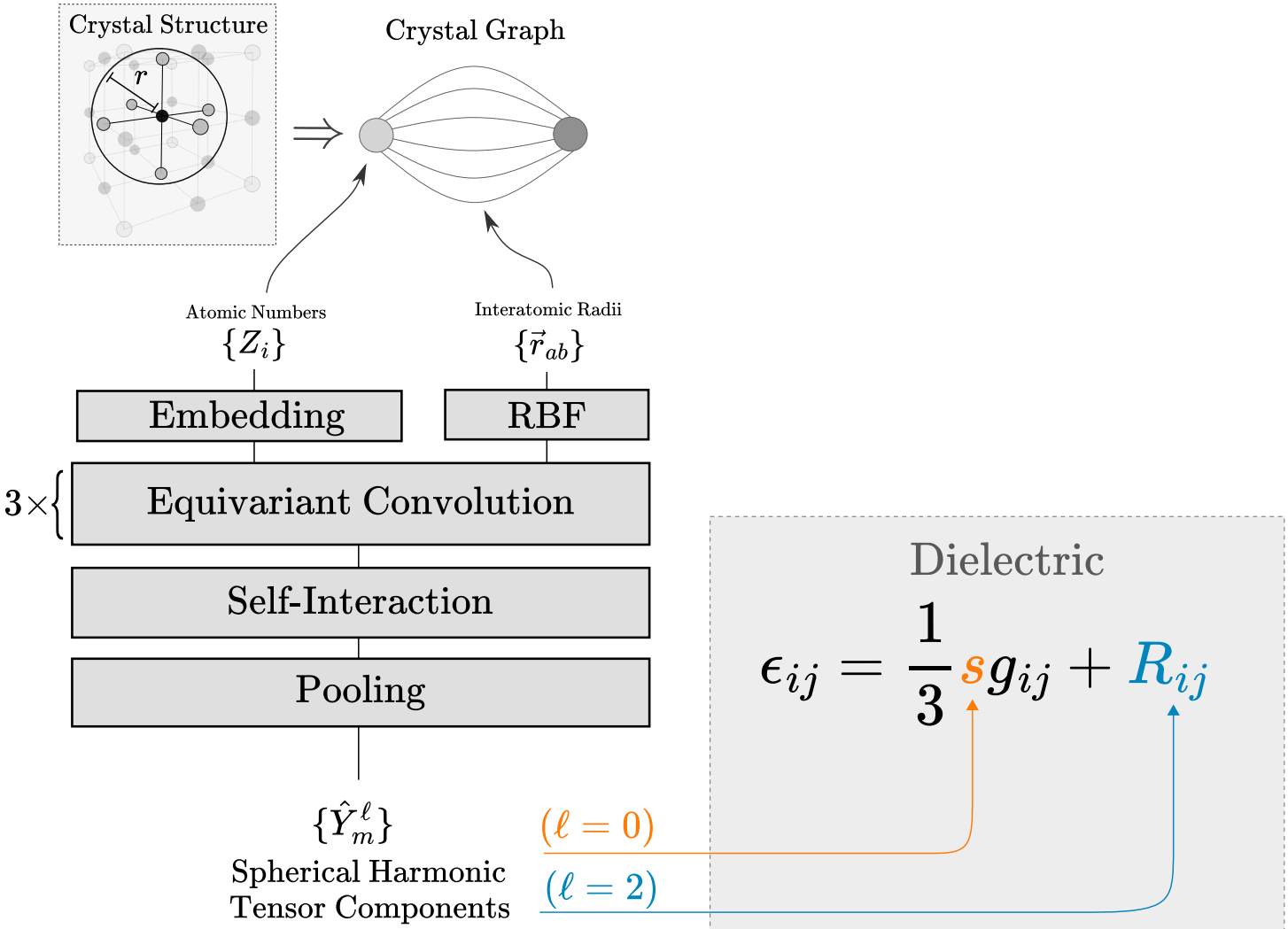
Then, contract with g and ε:



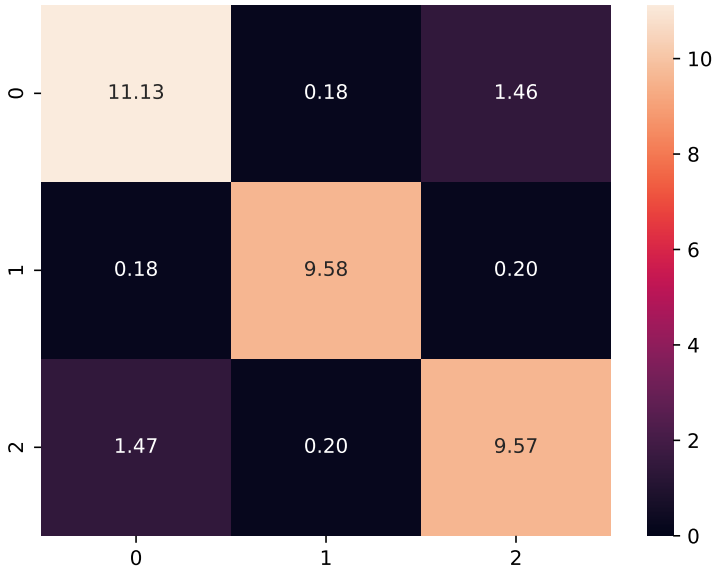
Model Architecture



Tensor Prediction: Examples

Applications to materials:

- Dielectric Tensor ϵ_{ij}



Tensor Prediction: Examples

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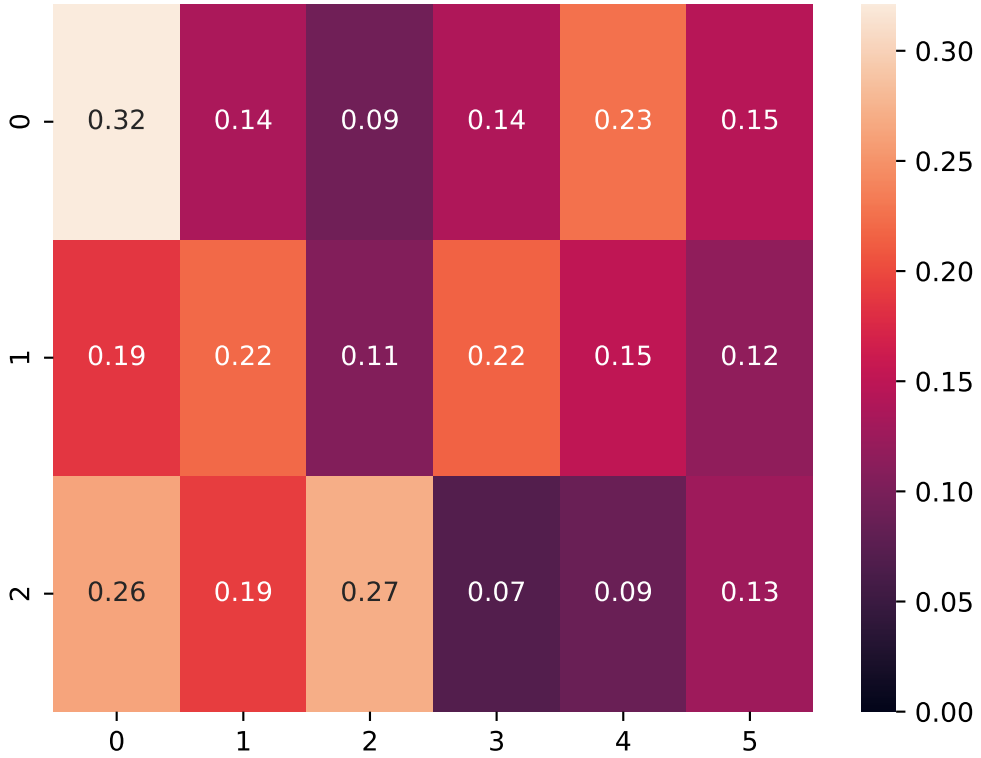
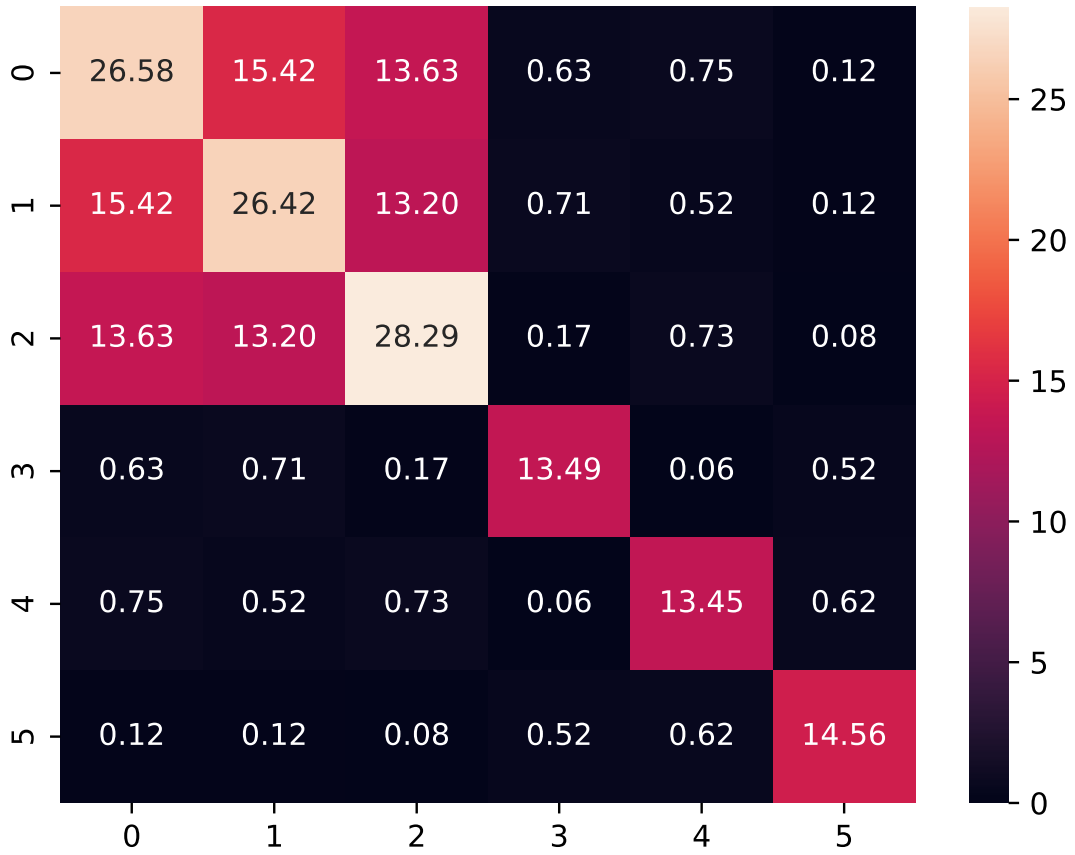


Tensor Prediction: Examples

- Elasticity Tensor C_{ijkl}



Tensor Prediction with $SO(3)$-Networks

Target Components	MAE (Averaged Over Components) SEGNN	SEConv	SETransformer
Elastic *[GPa]*	8.139	7.689	7.941
Dielectric	4.82	4.702	4.718
Piezoelectric $[C/m^2]$	0.170	0.170	0.1714

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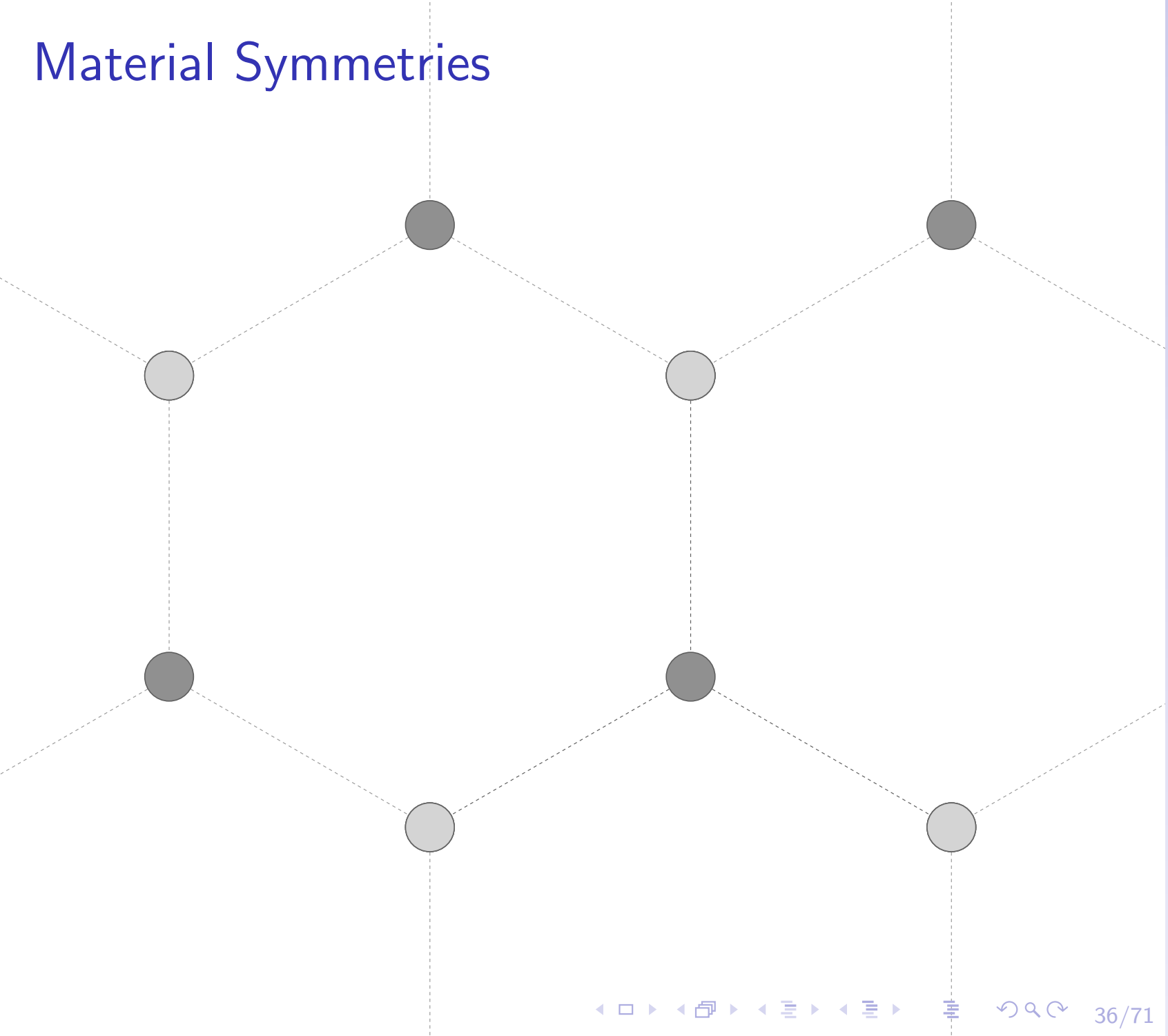
Can we get more out of symmetry considerations?

Material Symmetries



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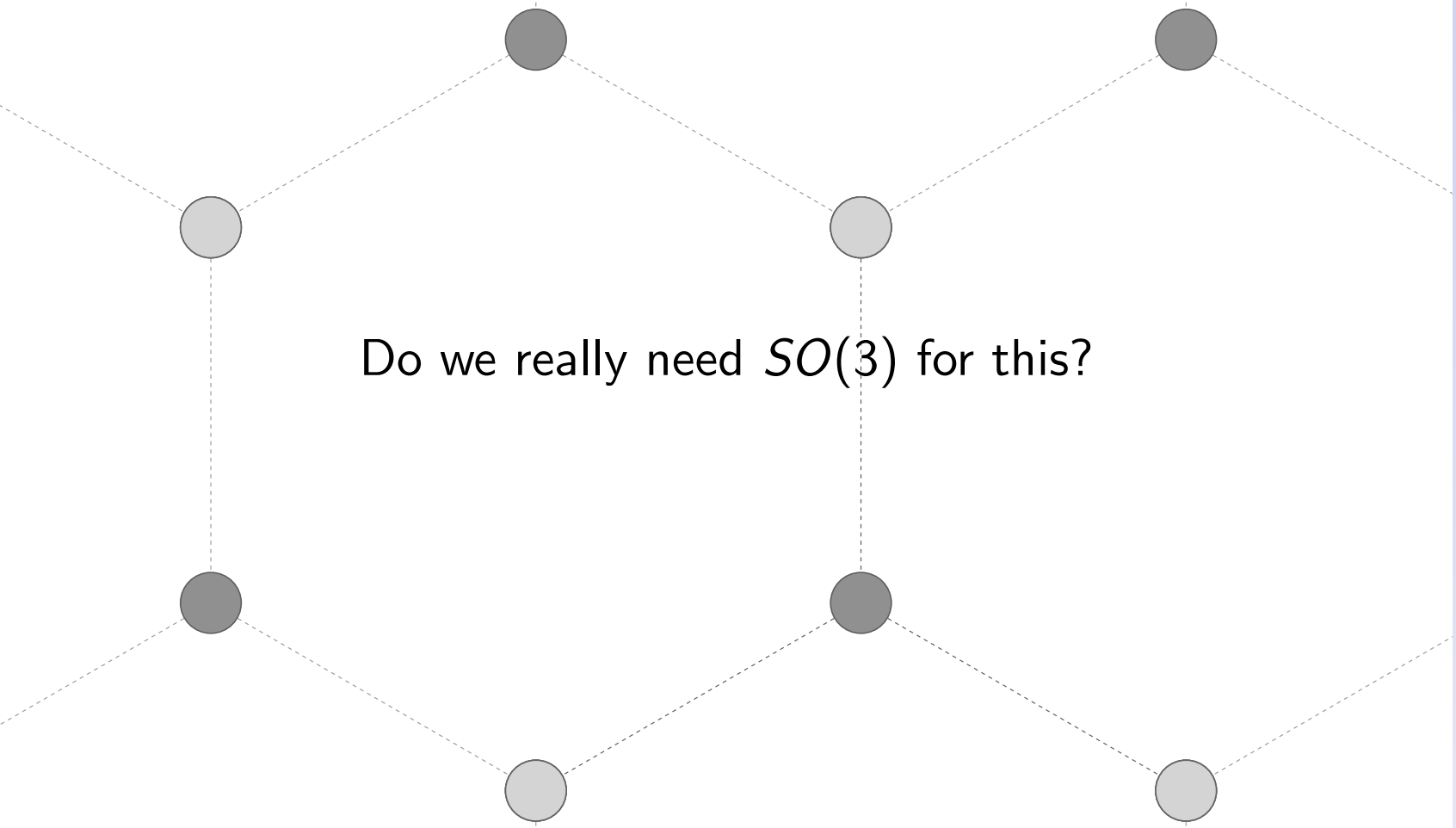

Do we really need $SO(3)$ for this?

Point Group Properties

Groups of operations that leave at least one point fixed and are compatible with a Bravais lattice.

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(Point group representations may be used to generate induced representations of space groups)

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Index vectors by α, i from site-symmetry group instead!

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- Accounts for all physical symmetry but not more

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- Symmetry-adapted Hamiltonian elements [14, 15]

Coupling Coefficients

Coupling coefficients for point groups can be computed from irreps with Dirl's Formula [16]:

$$(U^{\gamma n}_{\alpha i \beta j})^m = \sqrt{\frac{d_\gamma}{N_G}} \Big[\sum_{g \in G} \Gamma^{\alpha}_{qq}(g) \Gamma^{\beta}_{ss}(g) \Gamma^{\gamma\dagger}_{aa}(g) \Big]^{-\frac{1}{2}} \cdot \sum_{g \in G} \Gamma^{\alpha}_{iq}(g) \Gamma^{\beta}_{js}(g) \Gamma^{\gamma\dagger}_{na}(g)$$

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T **70**.11 Clebsch–Gordan coefficients *(cont.)*

^2e	t	T		
		1	2	3
1	1	1	0	0
1	2	0	ω^*	0
1	3	0	0	ω

^2e	$e_{1/2}$	$^2F_{3/2}$	
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^2e	$^1f_{3/2}$	$E_{1/2}$	
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Projection Operators

- We may project onto the k-th basis function f_k^α of IR α with $\hat{P}_\alpha^{kk}$[19]:

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- This may also be applied to tensors [13]

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The Hydrogen Hamiltonian $\hat{H}_H(\vec{r})$ for a non-relativistic electron has separable eigenfunctions [12]:

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Furthermore, $\hat{H}_H$ commutes with $SO(3)$ so these must be simultaneous with $SO(3)$:

$$[\hat{H}, \hat{O}(g)] = 0 \quad \forall g \in SO(3) \quad \Rightarrow \quad \psi^{\ell}_{nm}(\vec{r}) = R^{\ell}_n(r)\, Y^{\ell}_m(\theta, \phi)$$

(where R is also indexed by ℓ due to an 'accidental' symmetry)

- θ, ϕ dependence determined by group theory
- r dependence determined by specific form of $\hat{H}_H$

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Simplest form: H-like orbitals $|\psi^{\ell}_{nmp}\rangle$

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Now, in point group symmetry adapted basis $|\phi^{\alpha}_{ndp}\rangle$ that transform as irreducible representations [14, 15]

- $\hat{H}$ components in symmetry-adapted basis:

$$\hat{H}_{ndp\alpha,jqh\beta} = \langle \psi^{\beta}_{jqh} | \hat{H} | \psi^{\alpha}_{ndp} \rangle$$

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- We should use material symmetry groups!

References I

[1] Kurt Hornik, Maxwell Stinchcombe, and Halbert White. "Multilayer feedforward networks are universal approximators". In: *Neural networks* 2.5 (1989), pp. 359–366.

[2] Tian Xie and Jeffrey C Grossman. "Crystal graph convolutional neural networks for an accurate and interpretable prediction of material properties". In: *PRL* 120.14 (2018), p. 145301.

[3] K. T. Schütt et al. "SchNet – A deep learning architecture for molecules and materials". In: *J. Chem. Phys.* 148.24 (Mar. 2018), p. 241722. ISSN: 0021-9606. DOI: 10.1063/1.5019779. eprint: https://pubs.aip.org/aip/jcp/article-pdf/doi/10.1063/1.5019779/16655678/241722_1_online.pdf. URL: https://doi.org/10.1063/1.5019779.

References II

[4] Chi Chen et al. "Graph networks as a universal machine learning framework for molecules and crystals". In: *Chem. Mater.* 31.9 (2019), pp. 3564–3572.

[5] Justin Gilmer et al. "Neural message passing for quantum chemistry". In: *34th Int. Conf. Mach. Learn.* 70 (2017), pp. 1263–1272.

[6] Taco Cohen and Max Welling. "Group Equivariant Convolutional Networks". In: *Proceedings of The 33rd International Conference on Machine Learning*. Ed. by Maria Florina Balcan and Kilian Q. Weinberger. Vol. 48. Proceedings of Machine Learning Research. New York, New York, USA: PMLR, June 2016, pp. 2990–2999. URL: https://proceedings.mlr.press/v48/cohenc16.html.

References III

[7] Nathaniel Thomas et al. "Tensor field networks: Rotation- and translation-equivariant neural networks for 3D point clouds". In: (2018). arXiv: 1802.08219 [cs.LG].

[8] Mario Geiger and Tess Smidt. "e3nn: Euclidean neural networks". In: *arXiv:2207.09453* (2022).

[9] Nathaniel Thomas et al. "Tensor field networks: Rotation- and translation-equivariant neural networks for 3D point clouds". In: *arXiv:1802.08219* (2018). arXiv: 1802.08219 [cs.LG]. URL: https://arxiv.org/abs/1802.08219.

[10] Eiji Mochizuki. "Spherical harmonic decomposition of an elastic tensor". In: *Geophysical Journal International* 93.3 (1988), pp. 521–526. URL: https://academic.oup.com/gji/article/93/3/521/662002.

References IV

[11] Eiji Mochizuki. "Spherical Harmonic Decomposition of an Elastic Tensor II". In: *Journal of Physics of the Earth* 44.1 (1996), pp. 79–84. URL: https://www.jstage.jst.go.jp/article/jpe1952/44/1/44_1_79/_article/-char/ja/.

[12] Jun John Sakurai and Jim Napolitano. *Modern quantum mechanics*. Cambridge University Press, 2020.

[13] Hiroaki Kusunose, Rikuto Oiwa, and Satoru Hayami. "Symmetry-adapted modeling for molecules and crystals". In: *Phys. Rev. B* 107 (19 2023), p. 195118. DOI: 10.1103/PhysRevB.107.195118. URL: https://link.aps.org/doi/10.1103/PhysRevB.107.195118.

References V

[14] R. Sakuma. "Symmetry-adapted Wannier functions in the maximal localization procedure". In: *Physical Review B* 87.23 (June 2013). ISSN: 1550-235X. DOI: 10.1103/physrevb.87.235109. URL: http://dx.doi.org/10.1103/PhysRevB.87.235109.

[15] Rikuto Oiwa et al. "Symmetry-adapted closest Wannier modeling based on complete multipole basis set". In: *Physical Review B* 112.3 (July 2025). ISSN: 2469-9969. DOI: 10.1103/2s5q-p42x. URL: http://dx.doi.org/10.1103/2s5q-p42x.

[16] R Dirl. "Clebsch–Gordan coefficients: General theory". In: *Journal of Mathematical Physics* 20.4 (1979), pp. 659–663.

[17] George F. Koster et al. *Properties of The Thirty-Two Point Groups*.

References VI

[18] Simon L. Altmann and Peter Herzig. *Point-group Theory Tables*.

[19] Artur F Izmaylov. "On construction of projection operators". In: *The Journal of Physical Chemistry A* 123.15 (2019), pp. 3429–3433.

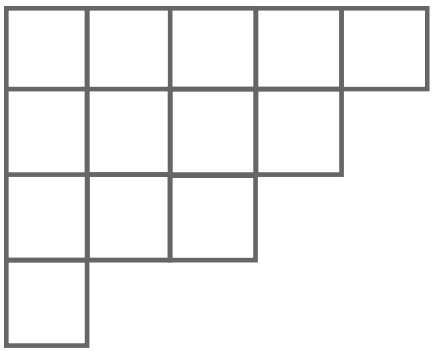
[20] Xiaoxun Gong et al. "General framework for E (3)-equivariant neural network representation of density functional theory Hamiltonian". In: *Nature Communications* 14.1 (2023), p. 2848.

References VII

[21] Anubhav Jain et al. “Commentary: The Materials Project: A materials genome approach to accelerating materials innovation”. In: *APL Mater.* 1.1 (July 2013), p. 011002. ISSN: 2166-532X. DOI: 10.1063/1.4812323. eprint: https://pubs.aip.org/aip/apm/article-pdf/doi/10.1063/1.4812323/13163869/011002_1_online.pdf. URL: https://doi.org/10.1063/1.4812323.

GL Decomposition

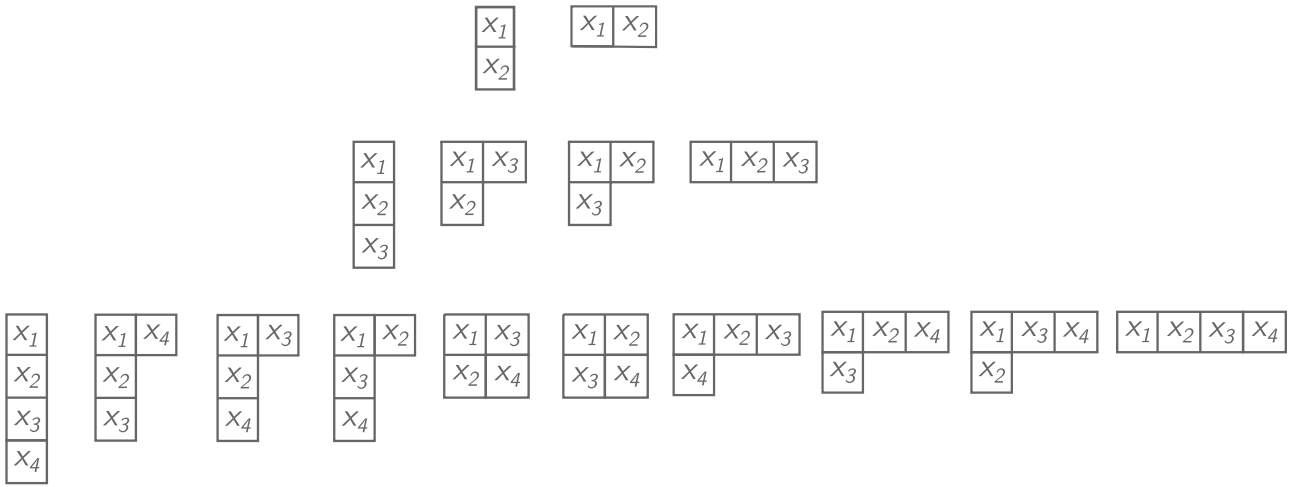
- Decompositions under general linear group *GL* are simultaneous with decompositions under symmetric group *S* (*Schur-Weyl Duality*)
- Irreducible representations of symmetric group are diagramatically described by Young diagrams.



Young diagrams are said to be of some shape $\lambda : (\lambda_1, \lambda_2, ..., \lambda_k)$, where λ_i refers to the depth of row i and $\lambda_{i+1} \leq \lambda_i \leq \lambda_{i-1}$. Above: $(5, 4, 3, 1)$

GL Decomposition cont.

We can then form a set of Young tableaux from diagrams by filling in the boxes from a set of ordered indices $\{x_1, x_2, ..., x_k\}$ corresponding to tensor components $T^{x_1 x_2 \dots x_k}$.



A standard tableu is one filled with indices x_i (without repeats) with entries increasing in index i down each column and across (to the right) rows.

GL Decomposition cont.

Each of these standard tableaux correspond to an invariant subspace under S_k.

These invariant subspaces may be constructed by correspond products of symmetrizers s and antisymmetrizers a:

$$s_\lambda = \prod_{\mathcal{I} \in \text{Cols}(\lambda)} \mathcal{S}(\mathcal{I})$$

$$a_\lambda = \prod_{\mathcal{I} \in \text{Rows}(\lambda)} \mathcal{A}(\mathcal{I})$$

where $\mathcal{S}$ and $\mathcal{A}$ act component-wise as:

$$\left[\mathcal{S}(\mathcal{I})\, T\right]_{ijk\ldots} = \sum_{\sigma_\mathcal{I}} T_{\sigma_\mathcal{I}(ijk\ldots)}$$

$$\left[\mathcal{A}(\mathcal{I})\, T\right]_{ijk\ldots} = \sum_{\sigma_\mathcal{I}} \text{sgn}(\sigma_\mathcal{I})\, T_{\sigma_\mathcal{I}(ijk\ldots)}$$

O Decomposition

Orthogonal group O, preserves inner product between vectors $< \cdot, \cdot >$. defined by means of a metric tensor g_{ij} , which transforms as a second rank tensor under some transformation R as:

$$g_{x_1 x_2} \rightarrow g_{x_1' x_2'} = R^{x_1}_{x_1'} R^{x_2}_{x_2'} g_{x_1 x_2}$$

Contractions of arbitrary tensors T with g_{ij} are invariant under O.

For example, consider the rank-3 covariant T^{ijk}:

$$g_{i'j'} T^{i'j'k'} = S^{k'} = R^i_{i'} R^j_{j'} g_{ij} R^{i'}_i R^{j'}_j R^{k'}_k T^{ijk} = R^{k'}_k S^k$$

so that S acts like an invariant vector subspace under O.

SL Decomposition

Special linear group SL of transformations is defined as invertible linear transformations with determinant equal to positive one.

Under SL, orientation and volume are preserved, where volume is defined as the contraction of a tensor with the fully antisymmetric tensor ϵ_{ijk}, which transforms under $R \in GL(3)$ as:

$$\epsilon_{x_1 x_2 x_3} \rightarrow \epsilon_{x_1' x_2' x_3'} = \det(R) R^{x_1}_{x_1'} R^{x_2}_{x_2'} R^{x_3}_{x_3'} \epsilon_{x_1 x_2 x_3}$$

Similar to the case of g_{ij} in O, contractions with ϵ_{ijk} of arbitrary tensors yield SL invariant subspaces.

$SO(3)$ Decompositions

In $SO(3)$, we may use all of the above (Young, g_{ij}, ϵ_{ijk}):

- Young symmetrizers return a set of tensors of known symmetries (under index permutation).
- Contractions with g_{ij} along antisymmetric pairs of indices vanish.
- Contractions with ϵ_{ij} along symmetric sets of indices vanish.

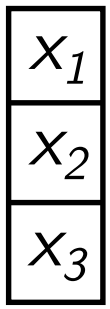
These may all be used together to decompose an arbitrary tensor into a set of symmetric, $SO(3)$ invariant, symmetric tensor subspaces. These then may be related to harmonic coefficients by way of the CG expansion from the J_z basis given before.

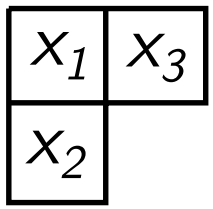
Example: Piezoelectric Tensors

The piezoelectric strain components d_{ijk} are symmetric under i, j so that:

$$d_{ijk} = d_{jik}$$

according to this symmetry, we see all Young tableaux but the following must disappear:





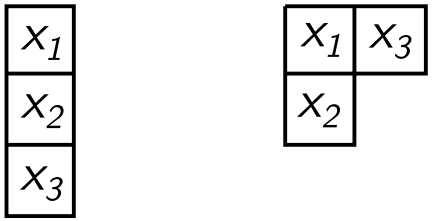
defined component-wise (using the defining symmetry):

$$S_{ijk} = \frac{1}{3}\left(d_{ijk} + d_{jki} + d_{ikj}\right)$$

$$A_{ijk} = \frac{1}{3}\left(2d_{ijk} - d_{jki} - d_{ikj}\right)$$

Example: Piezoelectric Tensors

This may be derived as (adopting the convention of symmetrization before antisymmetrization):



$$\mathcal{S}(ijk) \qquad \mathcal{A}(ij)\mathcal{S}(ik)$$

$$\begin{aligned}\mathcal{S}(ijk)d_{ijk} &= d_{ijk} + d_{ikj} + d_{kji} + d_{jki} + d_{kij} + d_{kji} \\ &= 2(d_{ijk} + d_{ikj} + d_{kji})\end{aligned}$$

$$\begin{aligned}\mathcal{A}(ik)\mathcal{S}(ij)d_{ijk} &= \mathcal{A}(ij)(d_{ijk} + d_{jik}) \\ &= d_{ijk} - d_{kji} + d_{jik} - d_{jki} \\ &= 2d_{ijk} - d_{kji} - d_{jki}\end{aligned}$$

Where the respective normalization coefficients (neglected here) may be derived from the diagram's shape via the hook-length formula.

Example: Piezoelectric Tensors

Further decompose A into the trace vector v_i:

$$v^i = g_{jk} A^{ijk}$$

and the traceless, symmetric tensor b_{ij}:

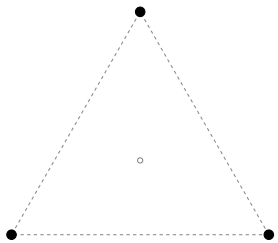
$$b_{ij} = \frac{1}{2}\left(\epsilon_i^{mk} A_{mkj} + \epsilon_j^{mk} A_{mki}\right)$$

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 in 3D space forming an equilateral triangle.



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 D_3 The previously shown representation of C_3 elements is reducible into a two-dimensional subspace and a one-dimensional subspace of D_3.

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

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

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

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

Every representation of a group inherits a vector space on which it has a natural action. This vector space is spanned by a chosen set of basis functions $|\psi_i^\alpha\rangle$.

- An irrep Γ^α's components are determined by basis:

$$\left(\Gamma^\alpha(g)\right)_i^j = \langle\psi_j^\alpha|\Gamma^\alpha(g)|\psi_i^\alpha\rangle$$

- Basis functions are said to "transform as an irrep α" if:

$$\Gamma^\alpha(g)|\psi_i^\alpha\rangle = \sum_j \left(\Gamma^\alpha(g)\right)_i^j |\psi_j^\alpha\rangle$$

Basis Functions (cont.)

Example: $3D$ Basis Functions of D_3
Consider previous $3D$ representation of C_3 rotations in D_3, which act on vectors $\vec{r}_\rho$:

$$\vec{r}_\rho = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \vec{r}_{\rho^{(2)}} \oplus \vec{r}_{\rho^{(1)}} = \begin{bmatrix} x \\ y \end{bmatrix} \oplus \begin{bmatrix} z \end{bmatrix}$$

Clearly, x, y is a basis transforming as Γ^2 and z is a basis for Γ^1.

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

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 some irreps Γ:

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

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 $U^{\gamma n}_{\alpha i \beta j}$ as:

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

Example: Clebsch-Gordan Coefficients

The Clebsch-Gordan coefficients $C^{\ell_f m_f}_{\ell_1 m_1 \ell_2 m_2}$ are the coupling coefficients of $SO(3)$, which relate tensor product spaces of spherical harmonics Y^ℓ_m to direct sums of spherical harmonics.

$$Y^{m_1}_{\ell_1}(\Omega) Y^{m_2}_{\ell_2}(\Omega) = \sum_{\ell_3, m_3} \sqrt{\frac{(2\ell_1+1)(2\ell_2+1)}{4\pi(2\ell_3+1)}} C^{\ell_3 m_3}_{\ell_1 m_1 \ell_2 m_2} C^{\ell_3 0}_{\ell_1 0 \ell_2 0} Y_{\ell_3 m_3}(\Omega)$$