1 Introduction

2 Graph Neural Networks

Neural networks are a class of universal function approximators, composed layer-wise by functions $\mathcal{L}^1 \circ \mathcal{L}^2 \circ ... \circ \mathcal{L}^n$, where each layer-to-layer transition map $\mathcal{L}^i$ is a trainable function from some feature space associated with layer L to a feature space associated with layer $L+1$.

Many modern approaches use a specific type of neural network, referred to as a Graph Neural Network (GNN), which act on data encoded in features associated with some representative graph (i.e. a collection of nodes and connections between them).

A group G is a set with a binary, associative product defined between it's elements under which it is closed, and for which every element, there exists an inverse element (and which also contains an identity element).

A matrix representation $\mathcal{D}_V$ of a group G is a map from elements of G to square matrices such that for all elements $g, h \in G$, there are representations satisfying:

$$\mathcal{D}(g)\mathcal{D}(h) = \mathcal{D}(gh)$$

Note that we often discard the 'matrix' from 'matrix representation' and often refer only to representations of groups, though these are synonymous for our purposes here.

A function $f : X \to Y$ is equivariant with respect to a group G if, for representations $\mathcal{D}_X$ and $\mathcal{D}_Y$ of G (over spaces X and Y, respectively), it satisfies:

$$f(D_X(g)x) = D_Y(g)f(x) \qquad \forall g \in G$$

Essentially, a function is equivariant with respect to some group if it 'commutes' with the representations of groups on it's input and output space.

A special case of equivariance then is *invariance*, where the representations of all group elements in the output space are identity (i.e. D_Y is the trivial representation). That is, a function $f : X \to Y$ is invariant under a group G if it satisfies:

$$f \circ \mathcal{D}_X(g) = f \quad \forall g \in G.$$

In the case of $SO(3)$, representations over a vector space of dimension $2\ell+1$ are Wigner-$\mathcal{D}^\ell$ matrices. Thus, we define an $SO(3)$ equivariant network to be a neural network $f : H_1 \to H_2$, with domain $H_1 : \{h_{(\ell_1)}\}$ and codomain $H_2 : \{h'_{(\ell_2)}\}$ (both being direct products of harmonic tensor spaces), that satisfies:

$$f(\{\mathcal{D}^{\ell_1}(R)h_{(\ell_1)}\}) = \{\mathcal{D}^{\ell_2}(R)h'_{(\ell_2)}\} \qquad \forall R \in SO(3)$$

The harmonic components h_ℓ^m (where h_ℓ generally refers to a $2\ell+1$ dimensional vector) correspond most naturally to the coefficients of spherical harmonic tensors, and in the context of machine learning, act as a feature space for data.

2.1 Representation/Feature Space

In an $SO(3)$-network, features are generally associated with irreducible representations of groups. In the case of $SO(3)$, these irreducible representations are spherical harmonics Y_ℓ^m, indexed by two sets, the rotational order $\ell \geq 0$, and the azimuthal order $-\ell \leq m \leq \ell$.

Thus, a traditional feature set $V^{(n)a}$ of channel a and associated with object n, has an additional two indices ℓ and m in an $SO(3)$ network, corresponding to the aformentioned indices of a harmonic expansion.

2.2 Layers

Compositions of equivariant functions are themselves equivariant functions. As such, we may form an equivariant network by composing it layer-wise from a set of common equivariant functions.

Here, we consider three types of $SO(3)$-equivariant functions from which we may compose our equivariant networks: namely, $SO(3)$-feature convolutions, ℓ-wise self-interactions and non-linearities, and pooling. An overview of each is given below.

2.2.1 $SO(3)$ Convolution

To maintain equivariance, for an input feature set of the type described above, through convolution with some filter F, the filter also must be associated with a set of spherical harmonics, and thus also has an additional two indices ℓ_f and m_f.

Note here that the tensor product of two representation spaces is equivariant under transformation of the two subspaces, i.e.:

$$\mathcal{D}^V \otimes \mathcal{D}^W = \mathcal{D}^{V\otimes W}$$

Tensors products of $SO(3)$ representations are cleanly related to a third set of $SO(3)$ representations by way of Clebsch-Gordan coefficients $c^{\ell_3 m_3}_{\ell_1 m_1 \ell_2 m_2}$ as:

$$(u \otimes v)^{m_o}_{\ell_o} = c^{\ell_o m_o}_{\ell_1 m_1 \ell_2 m_2} u^{m_1}_{\ell_1} v^{m_2}_{\ell_2}$$

where u and v are harmonic vectors of order ℓ_1 and ℓ_2, respectively.

Thus, we maintain equivariance by defining convolution to be the scaled tensor product of the two representation spaces (i.e. that of the input feature space, and the filter space), so that layer to layer convolutional maps $\mathcal{L}$ may be defined component-wise as:

$$\mathcal{L}^{\ell_o}_{acm_o}(\vec{r}_a, V^{\ell_i}_{acm_i}) = \sum_{m_f, m_i} c^{\ell_o m_o}_{\ell_i m_i \ell_f m_f} \sum_b F^{\ell_f \ell_i}_{cm_f}(r_{ab}) V^{\ell_i}_{bcm_i}$$

where the filter function $F^{\ell_f \ell_i}_{cm_f}(r_{ab})$ depends only on the distance between point a and b (as opposed to directional dependence, to maintain equivariance), but has independent, trainable parameters for different rotational orders ℓ_f, ℓ_i, azimuthal orders m, and channels c.

2.2.2 Self-Interaction

Feature sets for individual objects may also update according to themselves as long as they act across m for every ℓ and only update accordign to the different channels c. That is, functions of the form:

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

are also equivariant.

2.2.3 Non-Linearities

We can also apply point-wise non linearities and maintain equivariance, as long as they also respect the across m indices for every order feature ℓ.

2.2.4 Pooling

Pooling, or aggregation, across all elements or objects (index a) while preserving the m and ℓ indices is itself equivariant. Thus, functions of the form:

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

where AGG is an arbitrary aggregation function performed only over the object index a, are also available in the construction of $SO(3)$ networks.

2.3 Predicting Tensorial Data with SO(3) Networks

Such $SO(3)$ equivariant networks are naturally well suited for the prediction of tensorial properties. Tensors may generally be decomposed into a set of $SO(3)$ invariant subspaces which can then each be associated with a set of spherical harmonics (see spherical harmonic decomposition of a tensor).

2.3.1 Feature Pathways

It should be clear that, from our definition of $SO(3)$ equivariant convolution, different order ℓ representations in the output space $V_{acm}^{(L),\ell}$ of final layer L, will be the result of interactions with potentially different ℓ_f order filters and the input layer features of order ℓ_i. We here term the set of filter orders through the layers that result in a final output feature of order ℓ_o to be the *feature pathway* of feature order ℓ_o.

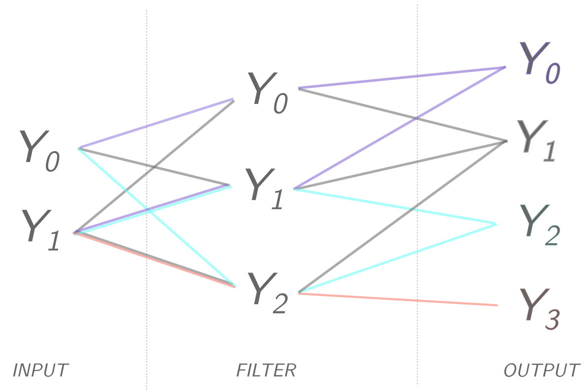
This feature pathway depends most generally on the chosen input feature orders ℓ_i, as well as the order of the filters ℓ_f for each layer, and the total number of layers. The pathway then may be determined by the selection rules of Clebsch-Gordon coefficients. That is, CG coefficients $c_{\ell_1 m_2 \ell_2 m_2}^{LM}$ can only be non-zero when the following hold for some set of inputs ℓ_1, m_1 and ℓ_2, m_2:

- $M = m_1 + m_2$
- $|\ell_1 - \ell_2| \leq L \leq \ell_1 + \ell_2$

Thus, we may determine what filter orders ℓ_f contribute to some output of order ℓ_o of some network, for an input of order ℓ_i.

Feature pathways are particularly relevant in the case of tensorial multi-target training sets, or transfer-learning applications, where different targets have different rotational order decompositions. In such cases, the filters learned for different datasets may not overlap at all, and thus would have disjoint feature pathways.

For example, consider one layer of $SO(3)$ convolution, with input features of order $\ell_i = 0, 1$ and filters of order $\ell_f = 0, 1, 2$. The outputs of order $\ell_o = 1$ would depend only on the trained parameters in filters of orders $\ell_i, \ell_f = (0, 1), (1, 0)$, whereas the outputs of order $\ell_o = 2$ would depend only on filters of $\ell_i, \ell_f = (0, 2), (1, 1)$.



So, if a network was trained on a tensorial target set with a decomposition of order $\ell_o = 2$ (i.e. a rank-two symmetric, traceless tensor), and then transfered and trained on a tensorial target of order $\ell_o = 3$ (i.e. a symmetric, traceless rank-3 tensor), there would only be overlap in the training of the $\ell_f = 1$ filter weights.

3 Spherical Harmonic Decomposition of a Tensor

A spherical harmonic decomposition of a tensor is a partitioning of a tensor space into a set of disjoint harmonic subspaces $\mathcal{H}^{(\ell)}$ that are invariant under the special orthogonal group $SO(3)$. That is, for a tensor T of rank n (over the vector space), a spherical harmonic decomposition of T refers to a set $\{h^\ell\}$ of harmonic components where $0 \leq \ell \leq n$; such that for transformations of T under $R \in SO(3)$ (taking $\hat{e}_i \to R^i_{i'} \hat{e}_i$) with contravariant components transforming as:

$$T_{x_1 x_2 \ldots x_n} \to T_{x'_1 x'_2 \ldots x'_n} = R^{x_1}_{x'_1} R^{x_2}_{x'_2} R^{x_3}_{x'_3} T_{x_1 x_2 \ldots x_n},$$

the harmonic subspaces remain invariant and transform as:

$$\{h^{(\ell)}\} \to \{h'^{(\ell)}\} = \{\mathcal{D}^\ell(R) h^{(\ell)}\}$$

where $\mathcal{D}^\ell(R)$ is the ℓ-th order Wigner-$\mathcal{D}$ matrix representation of the transformation R, and $h^{(\ell)}$ represents a $(2\ell+1)$-dimensional vector $[h_\ell^{-\ell}, h_\ell^{-\ell+1}, ...h_\ell^\ell]$, with h_ℓ^m as coefficients of tensor spherical harmonics Y_ℓ^m.

3.1 Constructing $SO(3)$ Invariant Subspaces

An invariant subspace of a tensor is a subspace which is closed under the action of some group of transformations. That is, invariant and disjoint subspaces of a tensor shouldn't 'mix' at all under the corresponding group transformations.

Invariants under $SO(3)$ of an arbitrary tensor T may be constructed by way of Young symmetrizers, and subsequent contractions with the metric tensor g_{ij} or the fully antisymmetric tensor ϵ_{ijk}. Note that these three methods correspond to the decomposition of a tensor with respect to the general linear group (by way of Young symmetrizers), the orthongonal group (contractions with g_{ij}), and the special linear group (contractions with ϵ_{ijk}), respectively.

Since $SO(3) = SL(3) \bigcap O(3) \subset GL(3)$, to construct invariants of SO, we generally form invariant subspaces under GL by way of Young symmetrizers first, and then construct invariants under O and/or SL of these GL invariant subspaces. This often results in several different harmonic subspaces of the same order ℓ in the harmonic decomposition of a tensor. Also, note that the GL decompositions for tensors of rank greater than two are not, in general, unique.

Below, we introduce the tools used in the construction of such invariant subspaces and demonstrate their invariance. These tools are then applied in three cases of tensor spaces with importance in the field of materials science: corresponding to the space of dielectric tensors, piezoelectric response tensors, and elasticity tensors.

3.1.1 GL Decompositions

By way of the Schur-Weyl duality, the invariant subspaces of a tensor under the general linear group GL determine the invariant subspaces of the tensor under the symmetric group S_n, where symmetric group elements act as permutations on tensor indices.

Under the symmetric group, the invariant subspaces of a tensor are described by way of standard Young tableaux, and then constructed from an arbitrary tensor by means of the corresponding Young symmetrizers. Below, these concepts are briefly introduced for the purpose of GL decompositions of tensors over $\mathbb{C}^n$. Note that these decompositions are in general not unique for tensors of rank > 2, so some conventions must be adopted.

Schur-Weyl Duality:

Under the joint action of the symmetric group S_k and GL_n acting on a tensor of rank-k over $(\mathbb{C}^n)^{\otimes k}$, the tensor space may be decomposed into a direct sum of tensor products of representations of S_k, π_k and representations of GL_n, here ρ_n, simultaneously indexed by the set of Young diagrams λ of order k. That is,

$$\underbrace{\mathbb{C}^n \otimes ... \otimes \mathbb{C}^n}_{k} = \bigoplus_{\lambda} \pi_k^{(\lambda)} \otimes \rho_n^{(\lambda)}.$$

This is a statement of the Schur-Weyl duality without proof. The point here though is that the representations under GL of a complex tensor product space, are indexed by the same set (that is, they both are described by the same underlying structure) as the representations under S. Thus, we consider the GL decomposition to be synonymous here with the symmetric group S decomposition.

Young Diagrams, Tableaux, and Symmetrizers

Young diagrams of order n are left-justified arrangements of boxes into k rows stacked vertically in non-increasing order. A Young diagram is said to be of some shape $\lambda : (\lambda_1, \lambda_2, ..., \lambda_k)$, where λ_i refers to the depth of row i and $\lambda_{i+1} \leq \lambda_i \leq \lambda_{i-1}$.

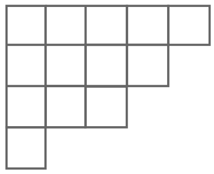


Figure 1: Example Young diagram of shape $(5, 4, 3, 1)$.

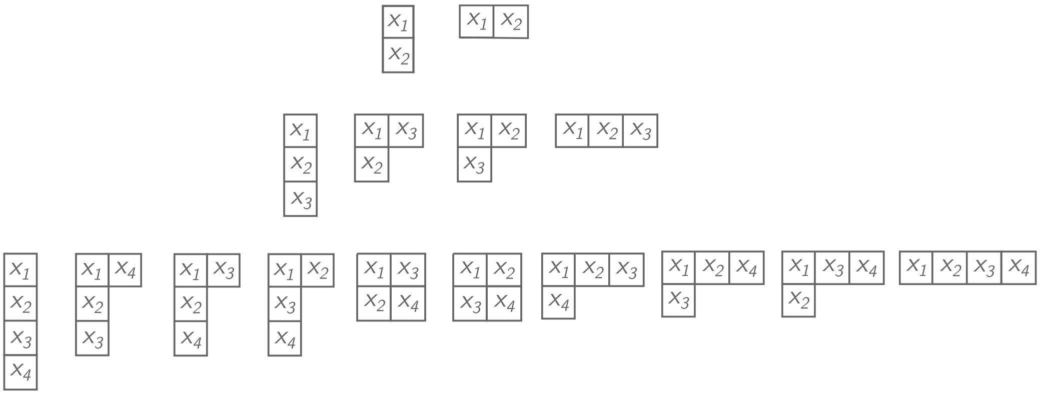


Figure 2: Standard Young tableaux for diagrams of at most 4 boxes.

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.

Each of these standard tableaux correspond to an invariant subspace under S_k. From these tableau, we may construct so-called *Young Symmetrizers*, which project tensors onto their corresponding S_k-invariant subspace.

A Young symmetrizer P_λ corresponding to tableau λ is composed of a compound set of symmetrizing operations s_λ and antisymmetrizing operations a_λ, scaled by an overall normalization constant C_λ:

$$P_\lambda = \mathcal{C}_\lambda s_\lambda a_\lambda$$

Where here, we adopt the convention of anti-symmetrization before symmetrization, following that in Itin [IR22].

The symmetrizing operator s_λ for a diagram λ is composed of a product of symmetrizers $\mathcal{S}(\mathcal{I})$, where $\mathcal{I}$ ranges over all subsets of indices corresponding to some vertically stacked set of indices in tableau λ, i.e.:

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

where $\mathrm{Cols}(\lambda)$ represents the set of disjoint subsets of indices down each column, and symmetrizers $\mathcal{S}$ are defined to act on tensors T component-wise as:

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

where $\sigma_\mathcal{I}$ are permutations of index subset $\mathcal{I}$.

Similarly, the antisymmetrizing operator a_λ can be constructed as a product of antisymmetrizers:

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

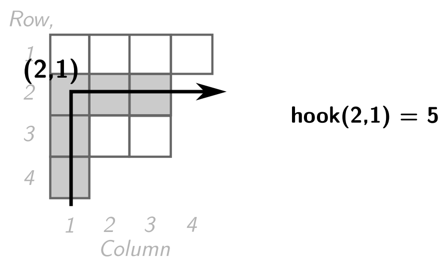


Figure 3: Example value of hook(2, 1) for a diagram of shape $\lambda : (4, 3, 3, 1)$. Note that it's corresponding normalization constant is $C_\lambda = 1/33600$.

where Rows(λ) represents the set of disjoint subsets of indices across each entire row, and antisymmetrizers $\mathcal{A}$ are defined as:

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

where, again, $\sigma_\mathcal{I}$ range over all permutations of index subset $\mathcal{I}$.

The normalization constant C_λ may be derived from the shape of the underlying Young diagram according to the *hook-length formula*, given below, where hook(α, β) returns the number of boxes crossed by a hook coming up (from below) column β and out of the diagram to the right in row α.

$$C_\lambda = \prod_{(\alpha,\beta)\in\lambda} \frac{1}{\mathrm{hook}(\alpha, \beta)}$$

Furthermore, the number of independent components N_λ of a tensor subspace corresponding to some Young tableau with shape λ may also be derived from the diagram by a related hook-length formula:

$$N_\lambda = \prod_{(\alpha,\beta)\in\lambda} \frac{n - \alpha + \beta}{\mathrm{hook}(\alpha, \beta)}$$

where n is the dimension of the vector space forming the tensor space.

Thus, the standard Young tableaux of k boxes can be used to decompose an arbitrary tensor space into a set of GL invariant subspaces with known symmetries (under permutation of indices) by way of corresponding Young symmetrizers. These known symmetries will be relevant in the further decomposition of these subspaces by way of contractions with the metric tensor, and the fully antisymmetric tensor, discussed below.

3.1.2 SL Decompositions

The special linear group SL of transformations is defined as the subset of 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:

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

For $R \in SL$ then, we have $\det(R) = 1$, allowing us to form various invariants of tensors by way of contraction (or partial contraction) with ϵ.

For example, for a rank-three tensor T, the volume may be defined component-wise as:

$$V = \epsilon_{ijk} T^{ijk}$$

This V is then clearly invariant under SO since for any transformation $R \in SO(3)$, we have:

$$V \to \epsilon_{i'j'k'} T^{i'j'k'} = R^i_{i'} R^j_{j'} R^k_{k'} \epsilon_{ijk} R^{i'}_i R^{j'}_j R^{k'}_k T^{ijk} = \epsilon_{ijk} T^{ijk}$$

Note that contractions with ϵ along fully symmetric sets of indices will always vanish; a fact useful when considering particular GL invariant subspaces. Explicitly,

$$\epsilon_{ijk} T_{..(ijk)..} = 0$$

3.1.3 O Decompositions

The orthogonal group O of transformations is defined as the subset of invertible linear transformations satisfying $R^T R = 1$. Under O, we may define an inner product between vectors $< \cdot, \cdot >$ by means of a metric tensor g_{ij} (δ_{ij} in Euclidean space) , which transforms as a second rank tensor under some transformation R as:

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

The inner product of vectors u, v is defined component-wise as:

$$< u, v >= u^i g_{ij} v^j$$

which is then clearly invariant under a transformation $R \in O(3)$ as:

$$< u', v' >= R^{i'}_i u^i R^j_{j'} R^j_{j'} g_{ij} R^{j'}_j v^j = u^i g_{ij} v^j =< u, v >$$

Furthermore, we may construct different invariants for different rank tensor spaces. For example, we may define O invariant scalar-valued traces $Tr(\cdot)$ of second rank tensors M by means of the metric tensor, defined component wise as

$$Tr(M) = g_{ij} M^{ij}$$

and we may form three O invariant trace vectors for third rank tensors T, defined component wise as:

$$\nu^k = g_{ij} T^{ijk}, \quad \mu^j = g_{ki} T^{ijk}, \quad u^i = g_{jk} T^{ijk}$$

That is, with the metric tensor g_{ij} available, as is the case in $SO(3) \subset O(3)$, we may decompose a rank-n tensor into a sets of rank-$(n-2), (n-4), ..., (0 \text{ or } 1)$ tensors by taking sequential traces.

The trace-part of a tensor may then be reconstructed by taking tensor products of metric tensors and trace vectors.

A point which is relevant to GL invariant subspaces is that contractions with respect to g under fully antisymmetric pairs of indices will always vanish. That is,

$$g_{ij} T_{..[ij]..} = 0$$

3.1.4 SO(3) Decompositions

In $SO(3)$, we have all of the above tools (Young diagrams, g_{ij}, and ϵ_{ijk}) available. As such, we may decompose a tensor into a set of $SO(3)$ invariant subspaces by their use, and all will be valid. Unfortunately, for tensors of rank> 2, there is not, in general, a unique and irreducible set of invariant $SO(3)$ spaces. However, we may always decompose an arbitrary tensor into a set of symmetric $SO(3)$-invariant tensor subspaces using the tools given above.

3.2 Spherical Harmonic Tensors and $SO(3)$ Invariant Subspaces

Of course, in the above decompositions, we've mentioned nothing of spherical harmonics. Here it should be stated clearly however: an invariant, symmetric subspace of some rank-n under $SO(3)$ should correspond exactly to a harmonic space $\mathcal{H}^{(n)}$. A rank-n, symmetric, $SO(3)$-invariant subspace of some tensor has dimensionality d^n (where d is the dimension of the underlying vector space) in terms of tensor components, but really only has $(2n+1)$ free and independent components. These $(2n+1)$ free components correspond to the coefficients of the $(2n+1)$ spherical harmonic tensors of rank n; where the rank n spherical harmonic tensors are essentially a basis for symmetric and traceless rank n tensors.

Consequently, we may give explicit definitions for the spherical harmonic tensors and then determine their coefficients by projection. For an approach of this manner, see [LM20].

Alternatively, we may use Clebsch-Gordon coefficients in an expansion of products of spherical harmonics to arrive at a map between a tensor's components in the spherical basis and it's harmonic components, as in [Moc88], and is the approach taken in this paper.

3.2.1 Mochizuki's Trick (Clebsch-Gordan Expansion

Suppose we define the coordinate system, which we term the *spherical* or J_z basis, below:

$$\begin{bmatrix} a_+ \\ a_0 \\ a_- \end{bmatrix} = \begin{bmatrix} -\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ -\frac{1}{\sqrt{2}} & +\frac{i}{\sqrt{2}} & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

where x, y, z are Cartesian components of the same vector. In this basis, the unit vectors associated with these components correspond to unit vector spherical harmonics $\hat{Y}^m_{\ell=1}$ (where we will assume Racah normalization for all definitions).

This correspondence is seen most clearly in the Cartesian basis form of the scalar spherical harmonics of rotational order $\ell = 1$, and noticing the similarity to the above transformation.

$$\begin{aligned} Y_1^{+1} &= -\frac{1}{\sqrt{2}}(x + iy) = \frac{1}{\sqrt{2}} \sin\phi e^{i\theta} \\ Y_1^0 &= z = \cos\phi \\ Y_1^{-1} &= -\frac{1}{\sqrt{2}}(x - iy) = \frac{1}{\sqrt{2}} \sin\phi e^{-i\theta} \end{aligned}$$

Note that we here assume Racah normalization (which guarantees tensor product unity) as opposed to the typical normalization of spherical harmonics (which guarantees unity over surface integrals of products).

Mochizuki's trick then is to draw a correspondence between the spherical basis components (associated with products of rank-1 spherical harmonic tensors) of a tensor and the higher rank spherical tensors by way of Clebsch-Gordon coefficients, by applying the following relation:

$$Y^{m_1}_{\ell_1} \otimes Y^{m_2}_{\ell_2} = \sum_{L=-|\ell_1-\ell_2|}^{\ell_1+\ell_2} \sum_{M=-L}^{L} c^{L0}_{\ell_1 0 \ell_2 0} c^{LM}_{\ell_1 m_1 \ell_2 m_2} Y^M_L$$

Since the components a of a rank-n tensor in this basis transform as the tensor product of rank-1 spherical harmonic tensors, i.e.:

$$T^{(n)} = a_{\underbrace{\alpha\beta...}_{n}} \left(Y_1^\alpha \otimes Y_1^\beta \otimes ... \right) \quad \Rightarrow \quad y^m_\ell Y^M_L$$

This approach gives a clean relation between a symmetric tensor's components in the J_z basis, and it's spherical harmonic components. It even allows for a decomposition into all allowed L and M values for a rank $\ell_1 + \ell_2$ tensor. For example, one need not subtract the trace for a rank-two symmetric tensor (formed by the product $\ell_1, \ell_2 = 1$) and decompose the traceless result, the above approach would simply return the trace from the $L = 0$ case in the expansion.

However, since this correspondence can only be drawn for symmetric tensors, a GL-decomposition and some contractions with ϵ_{ijk} may sometimes be required first to decompose an arbitrary tensor into a set of symmetric tensors. The above approach can then be applied to this set of symmetric components.

Below, we give the coefficients of such a transformation for the case of rank-1,2 and 3 symmetric tensors.

3.3 Real Spherical Harmonics

The spherical harmonics Y^m_ℓ canonically refer to a complex basis, as should be clear from our definition of the J_z basis. Many tensors describing macroscopic responses of materials are strictly real-valued however. Hence, we may desire to then transform into a set of real-valued spherical harmonics.

The (complex) spherical harmonics Y^m_ℓ can be transformed into a set of real spherical harmonics $Y_{\ell m}$ according the following relations:

$$Y_{\ell m} = \begin{cases} \frac{i}{\sqrt{2}} \left(Y_\ell^{-|m|} - (-1)^m Y_\ell^{|m|} \right) : & m < 0 \\ Y_\ell^0 : & m = 0 \\ \frac{1}{\sqrt{2}} \left(Y_\ell^{-|m|} + (-1)^m Y_\ell^{|m|} \right) : & m > 0 \end{cases}$$

Rank 2				
	a_{00}	a_{+-}	$a_{0\pm}$	$a_{\pm\pm}$
y_0^0	1	-2		
y_2^0	1	1		
$y_2^{\pm1}$			$\sqrt{3}$	
$y_2^{\pm2}$				$\sqrt{\frac{3}{2}}$

Rank 3						
	a_{000}	a_{0+-}	$a_{00\pm}$	$a_{+-\pm}$	$a_{0\pm\pm}$	$a_{\pm\pm\pm}$
y_1^0	3	-6				
y_3^0	$\frac{15}{7}$	$-\frac{5}{7}$				
$y_1^{\pm1}$			$\sqrt{\frac{3}{2}}$	$-2\sqrt{\frac{3}{2}}$		
$y_3^{\pm1}$			$2\sqrt{\frac{3}{2}}$	$\sqrt{\frac{3}{2}}$		
$y_3^{\pm2}$					$\sqrt{\frac{15}{2}}$	
$y_3^{\pm3}$						$\sqrt{\frac{5}{2}}$

Elastic (Rank 4)						
$(m=0)$	a_{0000}	a_{00+-}	a_{0+0-}	a_{+-+-}	a_{++--}	
y_0^0	1	2	-6	1	3	
y_2^0	1	2	-3	1	-3	
y_4^0	1	2	4	1	$\frac{1}{2}$	
$(m=1,2)$	$a_{000\pm}$	$a_{+-0\pm}$	$a_{\mp0\pm\pm}$	$a_{00\pm\pm}$	$a_{+-\pm\pm}$	$a_{\mp\pm\mp\pm}$
$y_2^{\pm1}$	$\sqrt{3}$	$\sqrt{3}$	$-3\sqrt{3}$			
$y_4^{\pm1}$	$2\sqrt{\frac{5}{2}}$	$2\sqrt{\frac{5}{2}}$	$\sqrt{\frac{5}{2}}$			
$y_2^{\pm2}$				$-2\sqrt{\frac{3}{2}}$	$-2\sqrt{\frac{3}{2}}$	$3\sqrt{\frac{3}{2}}$
$y_4^{\pm2}$				$\sqrt{\frac{5}{2}}$	$\sqrt{\frac{5}{2}}$	$2\sqrt{\frac{5}{2}}$
$(m=3,4)$	$a_{\pm\pm\pm0}$	$a_{\pm\pm\pm\pm}$				
$y_4^{\pm3}$	$\sqrt{\frac{35}{2}}$					
$y_4^{\pm4}$		$\frac{1}{2}\sqrt{\frac{35}{2}}$				

Figure 4: Coefficients for transformation between spherical basis components $a_{\alpha\beta\gamma\delta}$ and harmonic components y_l^m for a rank-2,3,4 symmetric tensor. Note that the rank-4 is only relevant for symmetric components of elastic tensors and correspond to Mochizuki's transformation [Moc88] between the J_z basis and their symmetric tensor s.

(of course, this choice is not entirely unique, with the choice made here assuming a Condon-Shortley phase included in the definition of Y_ℓ^m).

Thus, we may decompose an arbitrary tensor of rank-n into a set of symmetric tensors of rank-ℓ with $0 \leq \ell \leq n$, and then use the relations between the J_z basis components and the spherical harmonic components y_ℓ^m. We then may arrive at a set of real spherical harmonic components $y_{\ell m}$ using the above relations. Below, we provide sets of symmetric tensors for some types of tensors relevant to materials science.

4 Dielectric Tensors

The dielectric permittivity tensor ϵ of some material is a linear model of it's electric displacement $\vec{D}$ in response to an external electric field $\vec{E}$:

$$\vec{D} = \epsilon \vec{E}$$

Note that here we focus only on static responses, that is, $(\partial/\partial t)\vec{E} = 0$, due to the restriction of data to this case.

The dielectric tensor ϵ then is a rank-two tensor formed from vector spaces over the field $\mathbb{R}^3$, where we ignore the distinction between co- and contravariant components due to the Euclidean structure $g_{ij} = \delta_{ij}$.

The dielectric tensor is also symmetric in it's two indices, apparent from it's nature in the component-wise expansion of the polarization $D(E)$ about some external field E:

$$D_i = D_0 + \epsilon_{ij} E_j + \rho_{ijk} E_j E_k ...$$

so that we may draw the conclusion that:

$$\epsilon_{ij} = \frac{\partial D_i}{\partial E_j}$$

implying that ϵ is symmetric under permutation of it's indices, such that:

$$\epsilon_{ij} = \epsilon_{ji}$$

4.1 Decomposition

The GL decomposition of a rank-two tensor space is the usual symmetric-antisymmetric decomposition of a matrix M.

$$M_{ij} = S_{ij} + A_{ij}$$

with:

$$\begin{aligned} S_{ij} &= \frac{1}{2}(M_{ij} + M_{ji}) \quad \Rightarrow \quad S_{ij} = S_{ji} \\ A_{ij} &= \frac{1}{2}(M_{ij} - M_{ji}) \quad \Rightarrow \quad A_{ij} = -A_{ji} \end{aligned}$$

which correspond to the Young diagrams below:

$$\begin{array}{|c|}\hline \\ \hline \\ \hline \end{array} \qquad \begin{array}{|c|c|}\hline & \\ \hline \end{array} .$$

Since the dielectric tensor ϵ is symmetric, we are left then only with the unique tableaux below, corresponding to the fully symmetric part S.

$$\begin{array}{|c|}\hline x_1 \\ \hline x_2 \\ \hline \end{array}$$

Indeed, the corresponding Young symmetrizer $\mathcal{S}(ij)$ acts as identity on a dielectric tensor. Note that we may also form a trace by way of contraction with g_{ij}, since the dielectric tensor is not traceless. However, this is unnecessary in our algebraic derivation of harmonic components, as discussed above.

5 Piezoelectric Tensors

The piezoelectric strain constants $(d_{ijk})_T$ are defined (at constant temperature) by the thermodynamic relation:

$$\left(d_{ijk}\right)_T = \left(\frac{\partial \epsilon_{ij}}{\partial E_k}\right)_{\sigma,T}$$

where ϵ is the strain tensor, and the partial derivative is taken at constant stress σ and temperature T.

These strain constants d_{ijk} are related to the piezoelectric stress constants e_{ijk} via the elastic tensor C_{ijkl} according to:

$$\left(e_{ijk}\right)_T = \left(d_{ilm}\right)\left(C_{ijkl}\right)_{E,T}$$

with e_{ijk} defined as:

$$\left(e_{ijk}\right)_T = \left(\frac{\partial D_i}{\partial \epsilon_{jk}}\right)_{\sigma,T}$$

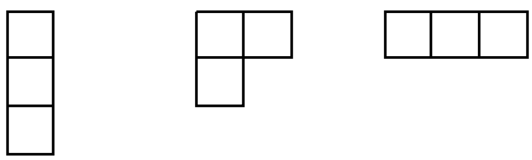
and where D is the resulting electric displacement vector in the material. We now will generally neglect the explicit notation of constant parameters.

The piezoelectric strain components d_{ijk} are symmetric under i, j due to the symmetry of the strain tensor ϵ_{ij}, so that we have:

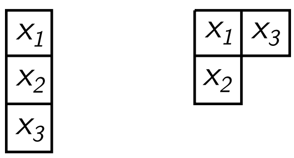
$$d_{ijk} = d_{jik}$$

5.1 Decomposition

The Young diagrams for a rank-three tensor are as follows:



according to the symmetry$d_{ijk} = d_{ikj}$, we can again see that all Young tableaux but the following will disappear, since the rest are asymmetric in the last two indices.



where the totally symmetric component tensor here we define as S and the mixed symmetry component tensor we define A, so that we have the Young decomposition:

$$d_{ijk} = S_{ijk} + A_{ijk}$$

defined component-wise in terms of strain components:

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

The fully symmetric part S is of an adequate form for harmonic decomposition, with those relations given in the next section.

The mixed symmetry part A however requires further decomposition with respect to $SO(3)$, so that we have a set of symmetric tensors describing it. It's 8 independent components can be described by a $5 \oplus 3$ dimensional space consisting of a symmetric rank-2 tensor and a trace vector.

The trace vector v^i, describing A's 3-dimensional $SO(3)$ invariant subspace, can be formed from the contraction of the metric tensor g along A's first and second indices. That is, we define:

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

Note that this choice is somewhat arbitrary, since we could define the trace part to correspond to the contraction along the first and third indices, or the second and third. However, it can be shown that for the mixed symmetry of A, these two potential trace vectors are linearly dependent (related by an overall factor of 1 and -2, respectively).

Rather simply then, we can reconstruct a third-rank tensor V, corresponding to this rank-one invariant subspace, by defining V component-wise as:

$$V_{ijk} = \frac{1}{4}\left[v_i g_{jk} + v_j g_{ik} - 2 v_j g_{ik}\right]$$

The rank-2 invariant subspace of A then may be constructed by symmetrizing the partial contraction with ϵ along the first and second indices (the anti-symmetric pair). Note that the antisymmetric part of this partial contraction corresponds to the trace vector space accounted for here by u. Explicitly, we define:

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

which is a traceless symmetric rank-2 tensor. And from which we may reconstruct the corresponding rank-3 tensor B, defined by:

$$B_{ijk} = \frac{1}{3}\left[\epsilon_{ik}^{p} b_{pj} + \epsilon_{ij}^{p} b_{pk}\right]$$

Thus, we may provide a total harmonic decomposition for A in terms of the invariant subspaces of the rank-1 u and the rank-2 b, such that:

$$A_{ijk} = V_{ijk} + B_{ijk}$$

And so, as mentioned above, the symmetric part S is readily decomposed in the spherical bases into $\mathcal{H}^{(1)} \oplus \mathcal{H}^{(3)}$. And then the mixed-symmetry part inhabits the space $\mathcal{H}^{(1)} \oplus \mathcal{H}^{(2)}$.

6 Elasticity Tensor

The elasticity (or simply, elastic) tensor C of a material relates it's Cauchy strain to some small applied stress . This may be described, component-wise, as the linear relation below:

$$\epsilon_{ij} = C_{ijkl} \tau_{kl}$$

As should be clear by the number of indices, the elastic tensor is a fourth rank tensor. The symmetries of the elastic tensor are discussed below, as they are relevant for our application. However, it is worth noting here that the total number of independent components of the elastic tensor is 21 in general.

The elastic tensor has several symmetries, but is not, in general, symmetric upon any swapping of indices. For all systems, C satisfies the so-called 'minor symmetries' below:

$$C_{ijkl} = C_{jikl}$$

$$C_{ijkl} = C_{ijlk}$$

resulting from the symmetry of the strain and stress tensors ($\tau_{ij} = \tau_{ji}$ and $\epsilon_{ij} = \epsilon_{ji}$) under the assumption of equilibrium. This reduces the number of independent components from 81 to 36.

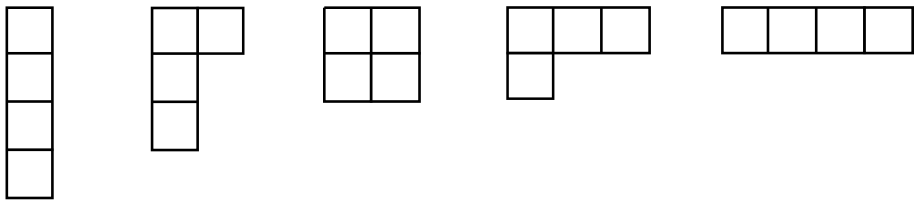
Furthermore, for conservative systems in which the elastic deformation is describable in terms of some potential energy function (and which we shall henceforth assume for our application), C has the additional 'major symmetry':

$$C_{ijkl} = C_{klij}$$

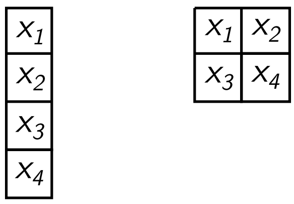
This further reduces the number of independent components from 36 (from the minor symmetries) to 21 in total.

6.1 Decomposition

If we examine the Young diagrams of a fourth rank tensor, as below:



We can immediately notice that the symmetries of C require that all but the totally symmetric tensor S and one mixed symmetry tensor A must vanish. S has 15 independent components, and A has 6. Furthermore, A has corresponding symmetrizer $\mathcal{C}S(x_1x_2)S(x_3x_4)A(x_1x_3)A(x_2x_4)$. Thus, A is exactly the tensor symmetric under permutation of i, j and k, l but antisymmetric under exchanges i, k and j, l.



Note that this mixed-symmetry subspace A corresponds to Backus' [Bac70] asymmetric tensor A. With S and A being defined component-wise as:

$$S_{ijkl} = \frac{1}{3}\big(C_{ijkl} + C_{ikjl} + C_{klij}\big)$$

$$A_{ijkl} = \frac{1}{3}\big(2C_{ijkl} - C_{ikjl} - C_{klij}\big)$$

The fully symmetric part can of course be converted to spherical harmonic components via a Clebsch-Gordon expansion. The mixed symmetry A, however requires further decomposition.

All six components can be described by the symmetric (but not traceless) tensor t, defined as the double partial contraction of A with the totally antisymmetric tensor ϵ as:

$$t_{ij} = \epsilon_i^{mk}\epsilon_j^{nl}A_{mnkl}$$

which can be reconstructed as the subtensor N as:

$$N_{ijkl} = \frac{1}{2}\big(\epsilon\epsilon - \epsilon\epsilon\big)t_{mn}$$

This tensor t then has a harmonic decomposition according to the rank-two Clebsch-Gordon transformation between the J_z basis and the harmonic basis y_ℓ^m.

References

[Bac70] George Backus. A geometrical picture of anisotropic elastic tensors. *Reviews of geophysics*, 8(3):633–671, 1970.

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[HXG22] Hongyu Yu Hongjun Xiang, Yang Zhong and Xinggao Gong. A general tensor prediction framework based on graph neural networks. 2022.

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[IR22] Yakov Itin and Shulamit Reches. Decomposition of third-order constitutive tensors. *Mathematics and Mechanics of Solids*, 27(2):222–249, 2022.

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[LM20] Francisco Gonzalez Ledesma and Matthew Mewes. Spherical harmonic tensors. 2020.

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[PEC23] Teerachote Pakornchote, Annop Ektarawong, and Thiparat Chotibut. Straintensornet: Predicting crystal structure elastic properties using se(3)-equivariant graph neural networks. 2023.

StrainTensorNet predicts the components of the elastic tensor using an equivariant network by predicting the Strain-Energy Density (SED) components (an invariant representation) for various stresses and using these to extract elastic properties.

[VWP23] Maxwell C Venetos, Mingjian Wen, and Kristin A Persson. Machine learning full nmr chemical shift tensors of silicon oxides with equivariant graph neural networks. *The Journal of Physical Chemistry A*, 127(10):2388–2398, 2023.

This paper applies symmetry and harmonic decompositions to the NMR spectra shift tensor to predict them equivariantly. Also, pretty much exactly what I'm doing.

[WHM+23] Mingjian Wen, Matthew K. Horton, Jason M. Munro, Patrick Huck, and Kristin A. Persson. A universal equivariant graph neural network for the elasticity tensors of any crystal system. 2023.

This paper by the materials project team is our original punchline, giving Backus' spherical harmonic decomposition of the elastic tensor and reading it off of the irreps of the equivariant output.