6.S966 Final Exam Cheat Sheet

Group Theory (L1-2)

A **group** $(G, *)$ is a monoid with inverses. That is, it is closed, associative, there is an identity, and inverses.
The **order** of a (finite) group is $|G|$.

It is easier for a group to be represented as a **multiplication table** (or **Cayley table**) where the multiplication of groups is mapped.

If a group is **abelian** (ie. the elements commute) the multiplication table is symmetric.

Theorem 1 (Rearrangement Theorem)**.** *If we have* $G = \{E, A_1, \cdots, A_n\}$ *then* $\{A_k E, A_k A_1, \cdots, A_k A_n\} = G$. *That is, each row and column of the multiplication table of* G *contains each element once.*

A subset $H \subset G$ remains closed (and thus forms a group), we say $H \leq G$ is a subgroup of G.

An element $B \in G$ is said to be **conjugate** to $A \in G$ if $\exists X \in G$ such that $B = XAX^{-1}$. Conjugacy partitions the group G. In symmetry groups, each conjugacy class represents a distinct type of symmetry.

A **homomorphism** φ is a map $\varphi : G \to G$ such that $\varphi(xy) = \varphi(x)\varphi(y)$. A bijective homomorphism is called an **isomorphism**.

For a subset $B \subset G$, the **left cosets** of g are defined $gB = \{gb \mid \forall b \in B\}$. The **right cosets** are defined similarly.

A subgroup $H \leq G$ is said to be **normal** (or **self-conjugate**), denoted $H \triangleleft G$, if $\forall g \in G$, $gBg^{-1} = B$ (that is, $\forall b \in B, gbg^{-1} \in B$).

For a normal subgroup $H \triangleleft G$, the left and right cosets are equivalent. We thus define the **quotient group** (or **factor group**) G/H to be the cosets of H.

Theorem 2 (Lagrange's Theorem)**.** *For a group* G*, normal subgroup* $H \triangleleft G$*, we have* $|G| = |G/H||H|$. *That is, the order of the subgroup divides the order of the group.*

Linear Algebra (L3)

A **vector space** $(V, \mathbb{F}, +, \cdot)$ satisfies the following:

- $(V, +)$ forms an abelian group.
- Scalar Multiplication, Identity in $\mathbb{F}$, Distributivity (wrt both vectors and scalars)

The **Kroneker product** of $A \in \mathbb{F}^{m,n}$, $B \in \mathbb{F}^{p,q}$ is defined

$$A \overset{\text{kr}}{\otimes} B = \begin{bmatrix} a_{11}B & \cdots & a_{m,n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mn}B \end{bmatrix}$$

That is, $A \overset{\text{kr}}{\otimes} B \in \mathbb{F}^{mp,nq}$.
The **Kroneker sum** of $A \in \mathbb{F}^{n,n}$ and $B \in \mathbb{F}^{m,m}$ is given by:

$$A \overset{\text{kr}}{\oplus} B := (\mathbf{I}_{m,m} \overset{\text{kr}}{\otimes} A) + (B \overset{\text{kr}}{\otimes} \mathbf{I}_{n,n})$$

Theorem 3 (Vectorized Sylvester Equation)**.** *We have for* $A \in \mathbb{F}^{m,m}$, $B \in \mathbb{F}^{n,n}$, $X \in \mathbb{F}^{m,n}$, $C \in \mathbb{F}^{m,n}$, *the* ***Sylvester Equation***

$$AX + XB = C$$

can be rewritten as:

$$[(\boldsymbol{I}_{n,n} \overset{\text{kr}}{\otimes} A) + (B^T \overset{\text{kr}}{\otimes} \mathbf{I}_{m,m})]vec(X) = vec(C)$$

Two matrices $S \in \mathbb{F}^{m,m}$ and $R \in \mathbb{F}^{n,n}$ are said to be **similar** if $\exists Q \in \mathbb{F}^{m \times n}$ such that

$$SQ = QR$$

In general, to find Q, we can rewrite:

$$SQ - QR = [S \overset{\text{kr}}{\oplus} (-R^T)]\text{vec}(Q) = 0 \tag{1}$$

and use Gaussian elimination.

Representation of Finite Groups (L4-6)

Group Representations

We define a **group representation** D on a vector space V to be a group homomorphism $D : G \to \text{GL}(V)$. We refer to both the matrix, the vector space $\text{GL}(V)$, and the function D as the group representation. We define the **dimensionality** of that representation to be $|V|$.

Similarity Transforms: Group representations are not unique: namely, for any unitary $\mathcal{U}, \mathcal{U}D(g)\mathcal{U}^{-1}$ is also a group representation.

Direct Sums: for any two representations $D(g), D'(g)$, we can combine their vector spaces to get a new (block-diagonal) representation:

$$(D(g), V) \oplus (D'(g), V') = \begin{pmatrix} D(g) & 0 \\ 0 & D'(g) \end{pmatrix}$$

A useful theorem:

Theorem 4 (Maschke's Theorem)**.** *Every representation of a finite group* G *over a field* $\mathbb{F}$ *with characteristic not dividing the order of* G *is a direct sum of irreducible representations*

Irreducible and Unitary Representations

A group representation D is said to be **reducible** if there exists a similarity transform $\mathcal{U}$ such that $\forall g \in G, \mathcal{U}D(g)\mathcal{U}^{-1}$ can be brought into block-diagonal form.

Conversely, a group representation that is not reducible is said to be irreducible.

Group representations can be brought into unitary form:

Theorem 5 (Unitary Representation Theorem)**.** *Every group representation (with nonvanishing determinant) can be brought into unitary form by a similarity transform.*

Orthogonality Theorems

Schur's Lemma and the Wonderful Orthogonality Theorem serve as tests for determining irreducibility of group representations:

Lemma 6 (Schur's Lemma)**.** *We have the following irreducability relations:*

1. *If a matrix matrix* M *commutes with the representations of the group elements* $A_1, \cdots, A_h$ *(here* $D(g_i) = A_i$

$$MA_i = A_i M$$

   then either M *is a constant matrix or it is reducible.*

2. *If the matrix representations* $D^{(1)}(g_1), \cdots, D^{(1)}(g_h)$ *and* $D^{(2)}(g_1), \cdots, D^{(2)}(g_h)$ *are two irreducible representations of a given group of dimensionality* l_1 *and* l_2 *respectively, then if there exists a matrix* $M \in \mathbb{F}^{l_1 \times l_2}$ *such that*

$$MD^{(1)}(g_x) = D^{(2)}(g_x)M$$

   $\forall g_x \in G$*, then either:*
   (i) If $l_1 \neq l_2$, $M = 0$.
   (ii) If $l_1 = l_2$*, then either* $M = 0$ *or* $D^{(1)}$ *and* $D^{(2)}$ *differ by a similarity transform.*

This leads to the key orthogonality theorem for checking irreducibility:

Theorem 7 (Wonderful Orthogonality Theorem)**.** *Suppose we have two inequivalent, irreducible, group representations D^{Γ_j} and $D^{\Gamma_{j'}}$ of dimension l_j and l'_j respectively. Denote by $h = |G|$. We then have the following orthogonality relation:*

$$\sum_{g\in G} D^{(\Gamma_j)}_{\mu\nu}(g) D^{(\Gamma_{j'})}_{\nu'\mu'}(g^{-1}) = \frac{h}{l_j}\delta_{\Gamma_j\Gamma_{j'}}\delta_{\mu\mu'}\delta_{\nu\nu'} \tag{2}$$

If the representations are unitary (or brought into unitary form) this becomes:

$$\sum_{g\in G} D^{(\Gamma_j)}_{\mu\nu}(g)[D^{(\Gamma_{j'})}_{\mu'\nu'}(g)]^* = \frac{h}{l_j}\delta_{\Gamma_j\Gamma_{j'}}\delta_{\mu\mu'}\delta_{\nu\nu'} \tag{3}$$

This orthogonality relations in fact tells us that $\sum l_j^2 \leq h$. In fact this is an equality.for

Character of a Representation

The **character** of a matrix representation $D^{\Gamma_j}(g)$ for a group element $g$is the trace:

$$\chi^{\Gamma_j}(g) = \mathrm{tr} D^{(\Gamma_j)}(g) = \sum_{\mu=1}^{l_j} D^{(\Gamma_j)}(R)_{\mu\mu}$$

Theorem 8. *The character for each element in a class is the same.*

This leads us to a natural encoding of information of the group in the form of a **character table**, which has irreps as the rows and the conjugacy classes as the columns. For each row, column pair, we have the character of that conjugacy class. For example,

	$1C_1$ $X(E)$	$3C_2$ X(A,B,C)	$2C_3$ X(D, F)
Γ_1	1	1	1
Γ'_1	1	-1	1
Γ_2	2	0	-1

Figure 1: The character table of $P(3) \cong D_3$:

If a representation is *irreducible* we call the character *primitive.*

Orthogonality Relations for Character

We have the following re characterization of the WOT in terms of character:

Theorem 9 (Wonderful Orthogonality Theorem for Character)**.** *The primitive characters of an irreudcible reprsentation obey the orthogonality relation*

$$\sum_{g\in G} \chi^{(\Gamma_j)}(g)\chi^{(\Gamma_{j'})}(g^{-1}) = h\delta_{\Gamma_j,\Gamma_{j'}} \tag{4}$$

or for unitary representations:

$$\sum_{g\in G} \chi^{(\Gamma_j)}(g)[\chi^{(\Gamma_{j'})}(g)]^* = h\delta_{\Gamma_j,\Gamma_{j'}} \tag{5}$$

We also have the following theorem that shows equivalence of two irreps:

Theorem 10. *Two irreps are equivalent (ie. related by a similarity transform) iff they have the same characters.*

Some things to remark:

- Characters (namely the WOT) can tell us if a representation is irreducible or not.
- We can check if we have *all* irreps through the character table.

Reducible Representations

In general, we get that irreps serve as a "basis" of all reprsentations, given by the following theorem:

Theorem 11. *The reduction of representations into irreps is unique. Thus, characters are a unique linear combination of irrep characters:*

$$\chi^{\Gamma}(C_k) = \sum_{\Gamma_i} a_i \chi^{(\Gamma_i)}(C_k) \tag{6}$$

In particular we have the coefficients $a_j = S_j/h$ where

$$S_j = \sum_{g\in G}\chi^{(\Gamma_j)}(g)\chi^{(\Gamma)}(g) = \sum_{C_k\in\mathcal{C}} N_k[\chi^{(\Gamma_j)}(C_k)]^*\chi(C_k)$$

Corollary 12. *The number of irreps is equal to the number of conjugacy classes.*

We also in fact get the following relationship about characters of irreps:

Corollary 13 (Columnwise Orthogonality of Character)**.** *We have the following orthonormality relationship for character:*

$$\sum_i \chi^{(\Gamma_i)}(C_k)\left[\chi^{(\Gamma_i)}(C_{k'})\right] N_k = h\delta_{kk'} \tag{7}$$

That is, for fixed irreducible representations, the characters evaluated on different conjugacy classes are orthonormal when weighted by class size.

Regular Representations

We define a particular representation for a group G as follows: consider the Cayley Table defined by enumerating all the group elements with the identity element e being at the top left and the rows being enumerated in terms of the inverses of the row elements.

The **Regular Representation** is given for an element $g \in G$ by putting a 1 wherever g appears in the multiplication table. By construction, only the identity will have nonzero trace.

The regular representation essentially "stacks" the irreps based on their dimensionality as given by the following:

Theorem 14. *The regular representation contains each irrep a number of times equal to its dimensionality.*

From this we get directly the equivalence:

Corollary 15. *The order of a group h and dimensionality l_j of the irresp Γ_j are related by*

$$\sum l_j^2 = h \tag{8}$$

Finding Irreps of A Group

In general how do we actually find the irreps of a group?

Algorithm 16. *To find the irreps of a group G, suppose we have any given representation $\rho : G \to GL(V)$. Now:*

(a) *Use the vectorized Sylvester's equation to solve*

$$Q\rho(g) = \rho(g)Q$$

More specifically, find a solution space $\{Q_1, \cdots, Q_r\}$ and draw $\alpha \sim U([0,1])$ and let $Q = \sum_{i=1}^{r} \alpha_i Q_i$

(b) *Diagonalize the matrix $Q = S\Lambda S^{-1}$. Now the eignespaces W_i corresponding to the eigenvalues λ_i will with probability 1 will be minimally stable.*

(c) *Each eigenspace W_i gives the projector $P_i = B_i B_i^\dagger$. The restriction of ρ onto the eigenspace $\rho_i = B_i \rho B_i^\dagger$ will be an irrep.*

Why does this work? By part 1 of Schur's Lemma, if Q commutes with an irreducible S, it is constant. If S is reducible, then it can be taken to be block-diagonal through a similarity transform with irreps on the diagonal, into the form

$$\begin{pmatrix} c1\mathbb{I} & \cdots & 0 \\ & \ddots & \\ 0 & \cdots & c_m\mathbb{I} \end{pmatrix}$$

with the eigenvalues of this being precisely the c_js. Taking a random weighted combination will give (in practice) a Q that has c_js distinct from which the projection onto the eigenspaces are precisely the irreps.

Products of Representations

There are three main types of group products, split into three cases:

(a) The **Tensor Product** of two representations of the same group G:

$$D^{(\Gamma_i)}(g) \otimes D^{(\Gamma_j)}(g) = D^{(\Gamma_i \otimes \Gamma_j)}(g) \Leftrightarrow D^{(\Gamma_i)}_{\mu,\nu}(g) D^{(\Gamma_j)}_{\mu',\nu'} = D^{(\Gamma_i \otimes \Gamma_j)}(g)_{\mu\mu',\nu\nu'}$$

In general, even if Γ_i and Γ_j are irreducible, the tensor product is reducible.

(b) The **Direct Product** of two representations of commuting groups G_A and G_B is given by

$$D^{(\Gamma_i)}(g) \overset{\text{kr}}{\otimes} D^{(\Gamma_j)}(h) \quad g \in G_A, h \in G_B$$

This forms a representation of the direct product $G_A \times G_B = \{A_i B_j | A_i \in G_A, B_j \in G_B\}$.

(c) **Semi-Direct Product** of representations of two non commuting groups G_A and G_B which gives a group representation of $G_A \ltimes G_B$ (semi direct product of the groups).

Vibrational Modes (L7-8)

We use symmetry to study various types of vibrational modes of molecules. The **vibrational modes** are the *internal* movements/displacements of a physical object. Intuitively, these are all representation of displacements of the object mod those that are due to external translations and rotations. Vibrational analysis via symmetry is a shortcut to many interesting properties.

By decomposing the displacement space into invariant subspaces corresponding to the irreducible representations (irreps) of the system's symmetry group, we can predict how these vibrational modes are measurable by specific characterization methods (e.g. **Infrared Spectroscopy (IR)** or **Raman spectroscopy**) or split or shift during distortions or symmetry reductions.

A **phonon** is a quantized mode of lattice vibration in a crystalline solid. Translational degrees of freedom correspond to **acoustic modes** and **optical modes**, where the former refers to in-phase movements and the latter refer to out of phase movements.

Masses and Springs

The energy of a system of N masses connected by springs can be described by the following Hamiltonian:

$$H(\mathbf{x}, \mathbf{m}) = \frac{1}{2} \sum_{i=1} m_i \left(\frac{\partial x_i}{\partial t} \right)^2 + V(\mathbf{x}) \tag{9}$$

The first term is the kinetic energy and the second term is the potential energy. Now, given an equilibrium position $\mathbf{x}_0$, the potential energy V can be taylor expanded (with the linear term cancelling due to force equilbrium), leading to a Hamltonian with indices:

$$H(\xi, \mathbf{x}) = \frac{1}{2} \sum_i m_i \left(\frac{\partial \xi_i}{\partial t} \right)^2 + \frac{1}{2} \sum_{i,j} \frac{\partial^2 V}{\partial \xi_i \partial \xi_j} = \frac{1}{2} \dot{\xi}^T M \dot{\xi} + \frac{1}{2} \xi^T K \xi \tag{10}$$

where M is the mass matrix and $K = \frac{\partial V}{\partial \xi_i \partial \xi_j}$. Taking the derivative with respect to time (conservation of energy), we get

$$\dot{H} = 0 = M\ddot{\xi} + K\xi \tag{11}$$

which is precisely the spring oscillator with solution:

$$\xi = ae^{i\omega t} \tag{12}$$

which gives the **secular equation**:

$$(K - \omega^2 M)\xi = 0 \tag{13}$$

Intuitively, this implies around equilbrium, the model exhibits certain small vibrations.

Finding Vibrational Modes

Here, $\xi \in \mathbb{R}^{3n}$ and $K - \omega^2 M$ is a Hermitian matrix. Now, the generalized displacements ξ lie on a vector space acted on by $\Gamma^{\text{atomic sites}} \otimes \Gamma^{\text{3D vectors}}$.

We would like to find the *vibrational modes* of this space, ie. the the group representation with the external translations and rotations quotiented out, ie.

$$\Gamma^{a.s.} \otimes \Gamma^{vec} - \Gamma^{trans} - \Gamma^{rot} = \Gamma^{vib} \tag{14}$$

This vibrational mode can then be represented as a direct sum of irreps showing the "component parts" of the general vibrational mode.

Spectroscopy

Molecules can vibrate under infrared light. Under an IR source, we can test the frequencies that are missing in a process called **infrared spectroscopy**. In order for a molecule to be IR measurable, we require

$$\Gamma^{final} \otimes \Gamma^{vec} \otimes \Gamma^{initial} = A_1 \tag{15}$$

On the other hand, for **Raman Spectroscopy**, we must represent as a rank 2 tensor $\Gamma^{l=2}$ instead.

Symmetry Breaking Distortions

Irreps of G can become irreducible under a subgroup $H \subset G$. **Branching Rules** describe the exact mapping between the irreps of G and the irreps of H.

A simple algorithm to finding all subgroups preserving distortions as follows:

(a) Find all copies of the desired subgroup in G using `vib_modes.isomorphic_subgroups`
(b) For each non-scalar irrep of G see how the subgroup H transforms when restricted to H. This irrep will when restricted to H generally **branch** into a direct sum of irreps of H.
(c) Check whether the trivial representation, A_1^H appears in the restriction. This means there is a subspace invariant under H but not neccesarily under G.
(d) Find which vibrational modes of G correspond to these irreps.

These vibrational modes tell us which specific dispalcements preserve H.
Now, normally vibrational modes retain the symmetry of the objects (material or molecules). However, if the displacement Γ does not result in A_1, this can break symmetry in G. There can be many causes such as Temperature, Pressure, External Fields which cause **phase transitions**.

Now, given an equilibrium state, there can be many possible ways to fall into nonequilibrium states, which is a phenomenom called **symmetry breaking**.

Lie Algebra (L9-11)

Lie groups are groups defined smoothly on a set of parameters: $g(\alpha)$, ie. it is a differentiable manifold. Some examples include the $SO(3)$ (3D rotations) group, $SU(2)$ (complex 2D rotations) group, and the $SL(2,\mathbb{R})$ (real 2×2 matrices with det 2) group.

They have an identity element $\mathbb{1}$, namely at $\alpha = 0$. We can thus taylor expand way from $\alpha = 0$:

$$D(d\alpha) = \mathbb{1} + (d\alpha_a)X_\alpha + O((d^2\alpha)) \tag{16}$$

where $X_a = \frac{\partial}{\partial \alpha_a} D(\alpha)|_{a=1,\cdots,N}$ are the **generators** of the Lie Group. Here, we use the **Einstein Summation Notation** and so we are actually doing a sum across all X_a (all the generators). These X_a are the matrix "generators" of the group. Thus, for small α, the one step approximation

$$D(d\alpha) \approx \mathbb{1} + (d\alpha_a)X_\alpha \tag{17}$$

holds. Now for α far away from 0, we can imagine taking $d\alpha \approx \alpha/k$ for some small k, and then we get the expansion:

$$D(\alpha) = \lim_{k\to\infty} D(\alpha/k)^k = \lim_{k\to\infty}\left(\mathbb{1} + \alpha_a \frac{X_a}{k}\right)^k = e^{\alpha_a X_a} \tag{18}$$

Some notes about matrix exponentials $e^X = \sum_{k=0}^{\infty} \frac{X^k}{k!}$. They are always invertible, with inverse e^{-X}. An important matrix identity for exponential matrices:

Theorem 17 (Baker-Campbell-Hausdorff Formula)**.** *We have for matrices X, Y,*

$$e^X e^Y = e^Z \tag{19}$$

where

$$Z = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}[X,[X,Y]] - \frac{1}{12}[Y,[X,Y]] + \cdots \tag{20}$$

*and $[X,Y] = XY - YX$ is the **commutator** of X and Y (as it measures the degree of how much X and Y commute).*

Some properties about commutators:

Lemma 18. *The commutator is:*

1. ***Bilinear**: $[aX + bY, cZ] = [aX, cZ] + [bY, cZ]$*
2. ***Alternativity**: $[X,X] = 0$*
3. ***Anticommutativity**: $[X,Y] = -[Y,X]$*
4. ***Jacobi Identity**: $[X,[Y,Z]] + [Y,[Z,X]] + [Z,[X,Y]] = 0$*

This set of generators g along with the multiplications between the group elements $[\cdot,\cdot]$ define the corresponding **Lie Algebra** for this Lie Group and can be taken into full representation form through exponentiation.

Deriving Generators for SO(n)

The **special orthogonal group** $SO(n)$ is defined to be all orthogonal matrices $R \in \mathbb{R}^n$ with $\det R = 1$. As the exponential map (for matrices) is always invertible, set $R = e^A$ for some matrix A. By Baker-Campbell-Hausdorff, we thus get $R^T = e^{-A}$.

Some relevant exponential matrix identities:

- $(e^A)^T = e^{(A^T)}$
- For orthogonal matrices, we thus get $(e^A)^T = e^{-A} = e^{(A^T)}$ which gives $A^T = -A$

We thus get that the generators A are **skew-symmetric**. Now, the number of "free parameters" from this matrix due to the skew-symmetric structure is given by $n(n-1)/2$. Each free parameter, or degree of freedom will correspond to a generator, which corresponds to a basis matrix for A.

In general, one can show that group multiplication is well defined for this parameterization iff the generators are closed under commutation.

Properties of Exponential Matrices

We have that similarity transforms in the exponential correspond to just similarity transforms in general:

$$e^{\mathcal{U}X\mathcal{U}^{-1}} = \mathcal{U}e^X\mathcal{U}^{-1} \tag{21}$$

Similarly, we get for direct sums, we get

$$e^{A\oplus B} = e^A \oplus e^B \tag{22}$$

Fianlly, for tensor/Kroneker products we get

$$e^A \overset{\text{kr}}{\otimes} e^B = e^{A \overset{\text{kr}}{\oplus} B} \tag{23}$$

Generators for SO(2) and SO(3)

The standard generators we use for $SO(2)$ are given by $L = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ and for $SO(3)$ the standard generators are given by

$$L_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, L_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, L_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Representations of SO(2) and SO(3)

We have for $SO(2)$ the standard generator L can be brought into block-diagonal form by the similarity transform:

$$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = \mathcal{U} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \mathcal{U}^{-1} \tag{24}$$

where $\mathcal{U} = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ i/\sqrt{2} & -i/\sqrt{2} \end{pmatrix}$. We thus get that by the properties of direct sums:

$$e^{i\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\alpha} = \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix} = e^{i\alpha} \oplus e^{-i\alpha} \tag{25}$$

that is, the representation interms of exponential matrices is reducible and the irreps are *complex*. From this, we can rearrive at the common 2D rotation parameterization:

$$\begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}$$

Similarly, you can get the 3D rotation parameterizations by repeating the same process for $SO(3)$:

$$R_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{pmatrix}, \quad R_y = \begin{pmatrix} \cos\alpha & 0 & \sin\alpha \\ 0 & 1 & 0 \\ -\sin\alpha & 0 & \cos\alpha \end{pmatrix}$$

$$R_z = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

which we call the **Euler-Angle Representation**. These generators (L_x, L_y, L_z) turn out to be irreducible so in fact for $SO(3)$ we have generators for the irreducible representation. For Lie Alegbra, however, the more natural representation is in terms of the **axis-angle representation**, where we rotate about an arbitrary axis $\hat{v}$ by an angle θ:

$$e^{\mathbb{1}\times(\hat{v}\theta)} \neq e^{\theta(\hat{v}_x L_x + \hat{v}_y L_y + \hat{v}_z L_z)} \tag{26}$$

which corresponds to the actual "coefficients" of the exponential parameterization (unlike α in the Euler Angle).

Irreps of SO(2)

In 2D, we found the irreps were complex of the form $e^{im\alpha}$. The tensor products are of the form:

$$e^{im_1\alpha} \overset{\text{kr}}{\otimes} e^{im_2\alpha} = e^{i(m_1+m_2)\alpha} \tag{27}$$

Thus, all $e^{im\alpha}$ for $m \in \mathbb{Z}$ are irreps. The intuition is that objects that transform under the irrep $e^{im\alpha}$ has m-fold symmetry (ie. they repeat every $2\pi/m$ in rotation).

Irreps of SO(3)

As described above, L_x, L_y, and L_z are already irreducible. How do we get the other irreps? We will see that if we have the "smallest" (dimensionality-wise) faithful representation of irreps, we can take tensor products and decompose.

In general, the following algorithm does the trick:

Algorithm 19 (Finding Irreps of Lie Groups)**.** *Assume X are generators of the smallest faithful irrep of the group. If X and X^* (conjugate) are isomorphic keep only X (eg. $SU(2)$ and $SO(3)$). Then, repeat the following:*

(a) Keep two lists ρ_{todo}, ie. irreps to tensor product with X (and X^*), and ρ_{done}, irreps already tensor producted w/X (and X^*). Add the trivial irrep to ρ_{todo}.

(b) While $|\rho_{todo}| + |\rho_{done}| < n$:

i. $\rho = \rho_{todo}.\texttt{pop}(0)$, $\rho_{done}.\texttt{append}(\rho)$

ii. Tensor product ρ with X (and X^*)

iii. Decompose tensor product to irreps.

iv. Check for isomorphism, and if new append to ρ_{todo}

(c) Return $\rho_{todo} + \rho_{done}$

Angular Momentum and Dirac Notation

In quantum mechanics, the angular momentum operators $\mathbf{L} = (L_x, L_y, L_z)$ are precisely the generators of the Lie Group $SO(3)$, with the $2l+1$ dimensional representations being called the l-dimensional (or "spin-l") representations of these operators.

Now, one can show that the **irrep invariant**

$$(L^{(l)})^2 = (L_x^{(l)})^2 + (L_y^{(l)})^2 + (L_z^{(l)})^2 \tag{28}$$

commutes with all $L_i^{(l)}$, ie. $[L^{(l)}, L_i^{(l)}] = 0$. By Schur's Lemma, we thus have that $L^{(l)}$ is a constant matrix. For $l = 1$, we have $L^{(1)} = 2\mathbf{I}$.

Now, in general, one can not block-diagonalize all $L_i^{(l)}$ but we can instead choose to diagonalize one of the generators, namely $L_z^{(l)}$, and then label the angular momentum states based on the eigenvalues of $L^{(l)}$ and $L_z^{(l)}$. More specifically, we typically take $\lambda^{(l)} = -l(l+1)$ to be the eigenvalue of $L^{(l)}$ and m to be the eigenvalue of $L_z^{(l)}$ and label quantum states as kets $|l, m\rangle$.

Ladder Operators

TODO.

Irreps of O(2)

We now consider the more general **orthogonal groups**, denoted $O(n)$.

We have that for $n = 2$, $O(2) = SO(2) \rtimes Z_2$ where $Z_2 = \{e, i\}$ where e is the identity and i is the mirror. These groups, $SO(2)$ and Z_2 do not commute so we require the use of the semidirect product. For this group, we find that the irreps are the trivial irrep of all 1s, 1s for all rotations and -1 for all rotoinversions, and

$$\begin{pmatrix} \cos(m\alpha) & \sin(m\alpha) \\ -\sin(m\alpha) & \cos(m\alpha) \end{pmatrix}$$

Irreps of O(3)

We have from Dresselhaus, that

$$O(3) = SO(3) \times Z_2 \tag{29}$$

ie. Z_2 commutes with $SO(3)$. For the higher order n, the irreps are more complicated. As described before, we can use ladder operators L_+ and L_- to move between different quantum states. From these, we get that there exists some m_{max} such that $L^+|l, m_{max}\rangle = 0$ so that $-l \leq m \leq l$.

Clebsch-Gordon Coefficients and Selectino Rules

We thus get computing tensor products of generators, eg. $(l = 1) \otimes (l = 1)$ can be written as a (normalized) direct sums of **paths** of higher irreps where the coefficients are called the **Clebsch-Gordon coefficients** and each irrep has

$|l_1 - l_2| \leq l_3 \leq l_1 + l_2$.

The rules that govern these decompositions are called the **selection rules**:

(a) **SO(2)** $m_3 = m_1 + m_2$
(b) **O(2)** $m_3 = m_1 \pm m_2$
(c) **SO(3)** $|L_1 - L_2| \leq L_3 \leq L_1 + L_2$
(d) **O(3)** $|L_1 - L_2| \leq L_3 \leq L_1 + L_2$, $p_1 p_2 = p_3$

Cartesian Tensors (L12)

Cartesian Tensors

Cartesian Tensors are tensors defined in terms of an orthonormal coordinate system in Euclidean Space. For example, vectors $\mathbf{e}_i$, matrices $\mathbf{e}_i \otimes \mathbf{e}_j$, tensors $\mathbf{e}_i \otimes \mathbf{e}_j \otimes e_k$ and so on. The number of indices is called the **order** of the tensor.

How do you rotate a Cartesian Tensor? We can rotate each matrix or flatten the matrix and then rotate. General matrices have 9 degrees of freedom (dof) as $1 \otimes 1 = 0 \oplus 1 \oplus 2$.

For many tensors, however, there are less degrees of freedoms due to constraints, such as symmetry `ij = ji` which gives $(1 \otimes 1)_{symm} = 0 \oplus 2$. Other examples include the elasticity tensor `ijkl = klij` and the Levi-Cevita tensor `ijk = jki = kij = -jik = -ikj = -kji`.

How do we go from one such general formula to the cartesian tensor decomposition?

Algorithm 20. *Given a general symmetry formula for a set of matrices:*

(a) Take formula indicating (generators of) index permutation and value sign change (if any) and generate full permutation and sign group with ***grids.formula_to_perm_and_sign_group*** *by extracting signs and permutations represented by formulas, and then running* ***groups.generate_groups*** *on signs $\oplus$ perms and then separating back out.*
(b) Take perm group on indices and construct perm group on grid of values (i.e. how index permutations permute tensor entries)
(c) Given perm group on tensor basis, multiply each element by corresponding sign, sum, and get orthogonal basis (and projector)
(d) Apply the projector onto the tensor product and see how it decomposes.

Branching Rules

Given a cartesian tensor describing a symmetry $H \subset O(3)$, *only* the entries that transform as A_1 (or A_{1g}) will be non-zero. This can dramatically reduce the number of independent parameters in the tensor. For example, a four dimensional tensor has $3^4 = 81$ degrees of freedom but with the typically constrains of an elasticity tensor this drops to 21.

Spherical Harmonics, Fourier Transforms (L15-16)

Signals on Spheres

A **signal on sphere** is a map $f : S^2 \to \mathbb{R}$. It turns out that the irreps of $SO(3)$, Y_m^l (where $-l \leq m \leq l$ serve as an orthonormal basis for all signals on the sphere.

In a similar way, the **Fourier Transform** is an invertible decomposition of a function into its "frequencies" and "amplitudes"

$$\hat{f}(x) = \int_{-\infty}^{\infty} f(x) e^{-2i\pi\xi x} dx \tag{30}$$

while the inverse is

$$f(x) = \int_{-\infty}^{\infty} \hat{f}(\xi) e^{-2i\pi\xi x} x d\xi \tag{31}$$

For signals on a sphere, integrals are replaced by tensor products of irreps. A **harmonic function** on a manifold is one that satisfies $\nabla^2 f = 0$. Spherical harmonics are the *eigenvalues* of the Laplacian.

How many components k do you need to represent a signal on a sphere? We have the following theorem:

Theorem 21 (Nyquist-Shannon)**.** *To sample without aliasing we require roughly twice the frequency,* $2\pi/\theta_{feature} = L$

This is the notion of **bandwith** on a sphere, to seperate features on a sphere that differ by some angle.

Power Spectra, Bispectra

Often when dealing with spherical harmonic expansions of signals on a sphere, the raw coefficients a_{lm} can be quite complicated. Often, we look at *invariant terms* that are retained under symmetry operations that do not change under rotations (of $SO(3)$ or $O(3)$).

Some examples of this are the **power spectrum** and **bispectrum** which correspond to the scalar and pseudoscalar parts of the tensor products of the spherical harmonic coefficients, ie. the power spectrum is the scalar part (`0e`) of $x \otimes x$, the bispectrum is the scalar/pseudoscalar parts of $x \otimes x \otimes x$ and so on. These quantities are invariant under symmetry operations

Group Convolutions, Spherical CNNs (L17-18)

Spherical CNNs

For images, we often consider cross-correlation (referred to as convolution in the ML literature) of a planar signal $f : \mathbb{R}^2 \to \mathbb{R}$ (an image) with some filter $\psi : \mathbb{R}^2 \to \mathbb{R}$:

$$[f \star \psi](x) = \int_y f(y)\psi(x - y) \tag{32}$$

We now consider functions on the sphere $f : S^2 \to \mathbb{R}$ which are commonly used in many applications such as omnidirectional vision. To do this, we must extend the idea of a convolution between functions on the plane to functions on a group G:

$$[f \star \psi](g) = \langle f, L_g \psi \rangle = \sum_{h \in G} f(h)\psi(g^{-1}h) \tag{33}$$

Group Convolutions in Real Space

One way to paramterize Equation 33 is through the regular representation. Since by the rearrangement theorem, we have $g^{-1}G = G$ for any $g \in G$, we can write:

$$\begin{aligned}
[f \star \psi](g) = \langle f, L_g \psi \rangle &= \sum_{h \in G} f(h)\psi(g^{-1}h) && (34)\\
&= \sum_{h \in G}\sum_{j \in G} f(h)\psi(j)\mathbb{1}[g^{-1}h = j] && (35)\\
&= \sum_{h \in G}\sum_{j \in G} f(h)\psi(j)D^{reg}(g^{-1})_{j,h} && (36)\\
&= \sum_{h \in G}\sum_{j \in G} f(h)\psi(j)D^{reg}(g)_{h,j} && (37)
\end{aligned}$$

That is to say, the regular representation $D^{reg}(g)$ is our change of basis from $f \otimes g$ tensor product rep to the regular representation vector space. In practical terms, for an input f of size `[batch, c_in, reg_rep]`, `'zci'`, filter ψ of size `[c_out, c_in, reg_rep]`, `'dcj'`/, and the regular representation $D(g)$ with size `[reg_rep, reg_rep, reg_rep]`, `'kij'` we get an output `'zdk'`.

Group Convolutions in Fourier Space

Now, doing this convolution in real space is rather inefficient. One can instead speed this up by doing a Discrete Fourier Transform using a generalized version of the Convolution Theorem which we recall states that for two signals $f, \psi : \mathbb{Z}^2 \to \mathbb{R}$ that

$$\widehat{f \star \psi} = \hat{f} \odot \hat{\psi} \tag{38}$$

where $\hat{f} : \mathbb{Z}^2 \to \mathbb{C}$ refers to the Fourier transform of f. In a similar vein, recall how we defined the general fourier transform of rotations on a sphere to be the set of coefficients onto the Wigner-D basis $\{D^l_{m,n}(g)\}$. The spherical harmonics satisfy a generalized Fourier Theorem:

$$\widehat{\psi \star f} = \hat{f}\hat{\psi}^\dagger \tag{39}$$

Thus, to get the convolution for any given $g \in G$, we can simply first take the Fourier Transform of f and $\psi^\dagger$ onto the Wigner-D matrix basis $D^l_{mn}(R)$ to get a set of coefficients $\hat{f}$ and $\hat{\psi}^\dagger$ and then matrix multiplying to get the Fourier Transform of $\psi \star f$. To get the final convolution

$$\psi \star f = \hat{f}\hat{\psi}D(g) \tag{40}$$

Group Convolutions in Practice

In practice, how do you get group equivariant deep networks? In practice, you simply rotate the filter and then convolve around the input and then stack the resulting outputs in what we call a **lifting convolution**. This is done by using the permutation representation above.

Steerable Convolution (L19)

We can imagine that the approach in real space where we make a filter bank of possible roto-translations of the kernel and then applying them to our input in real space is extremely inefficient. For general Lie groups, it also requires discretizations which can become inaccurate. To go to more general groups such as Lie Groups ($SO(3)$) we require more machinery. As explained above, by sticking in Fourier space and building up from basis functions in Fourier space can allow us to generalize.

This motivates **steerable filters** as follows: a *steerable basis* for a group G is a set of basis functions $\{B_i\}$ such that for any $g \in G$ and any group element transformed by g, the function also transforms as g, ie.

$$B_b(D^{vec}(g)x) = D^{filt}(g)B_b(x) \tag{41}$$

Suppose you have a set of points $\{x_i\}$ that transform under a rotation $g \in G$ as $D^{\rho_{vec}}(g)x_i$ and features $\{f_i\}$ that transform as $D^{\rho_{in}}(g)f_i$. Next, consider a filter $\psi : \mathbb{R}^2 \to W$ that takes relative vectors $x_{ij} = x_i - x_j$. Now, define a convolution operators on these features to get $f \star \psi$:

$$(f \star \psi)(x_a) = \sum_{b \in \mathcal{N}(a)} f_b \otimes \psi(x_{ab}) \tag{42}$$

We would like to have the property that:

$$D^{\rho_{in}}(g)f_j \otimes \psi(D^{vec}(g)x_{ij}) = D^{\rho_{in}\otimes\rho_{filter}}(g)[f_j \otimes \psi(x_{ij})] \tag{43}$$

Now suppose our filter ψ is built from steerable basis functions $\{B_i\}$ so

$$\psi(x_{ab}) = \sum_i c_i B_i(x_{ab}) \tag{44}$$

We thus get

$$\psi(D^{\rho_{vec}}(g)x_{ab}) = \sum_i c_i B_i(D^{\rho_{vec}}(g)x_{ab}) = cD^{filt}(g)B(x_{ab}) \tag{45}$$

where $c = \text{diag}(c_1, \cdots, c_j)$. By Schur's Lemma, for c to commute with $D^{filt}(g)$ we need c to be constant with respect to each irrep of $D^{filt}(g)$. This would then give:

$$\psi(D^{\rho_{vec}}(g)x_{ab}) = cD^{\rho_{filter}}(g)B(x_{ab}) \tag{46}$$

$$= D^{\rho_{filter}}(g)cB(x_{ab}) = D^{\rho_{filter}}(g)\psi(x_{ab}) \tag{47}$$

which gives

$$D^{\rho_{in}}(g)f \otimes \psi(D^{\rho_{filt}}(g)x_{ij}) = D^{\rho_{in}\otimes\rho_{filt}}(g)[f \otimes \psi(x)] \tag{48}$$

Thus, any steerable group convolution is block-diagonal/constant on each irrep.