Tensor Rank and the Spherical Harmonic Degree ℓ

Lecture 12 supplement: reading Cartesian tensors as SO(3) irreducible representations

One-sentence summary. Tensor rank counts Cartesian indices. The degree ℓ labels a minimal block of components that only mix with each other under rotation. A general rank-r tensor decomposes into several ℓ blocks; the symmetric traceless rank-r part is the $\ell = r$ block.

1. Two Different Languages

Cartesian tensor language	SO(3) irrep language
Counts how many indices an object has.	Describes how components mix under rotation.
v_i: rank 1, T_{ij}: rank 2	$0, 1, 2, \ldots$, or $0e, 1o, 2e, \ldots$ in e3nn
A general rank-r tensor is usually reducible.	Each ℓ block is irreducible.

2. Groups and Irreps

A group is a collection of symmetry transformations. For 3D rotations, the group is $SO(3)$, and each element is a rotation matrix R. A representation turns each rotation R into a matrix $D(R)$ acting on a feature vector. An irreducible representation, or irrep, is a representation that cannot be split into smaller rotation-closed blocks. The irreps of $SO(3)$ are labeled by $\ell = 0, 1, 2, \ldots$. In e3nn, blocks such as `0e`, `1o`, and `2e` are these SO(3) irreps with an extra parity label e/o.

$$\text{number of components in one } \ell \text{ block} = 2\ell + 1.$$

ℓ	components	intuition
0	1	scalar
1	3	rotates like a vector
2	5	rotates like a symmetric traceless rank-2 tensor
3	7	rotates like a symmetric traceless rank-3 tensor

3. The Rank-2 Example

Take two vectors and form

$$T_{ij} = a_i b_j.$$

This is a Cartesian rank-2 tensor with $3 \times 3 = 9$ components. But as a representation of rotations, it splits into three independent blocks:

$$\underbrace{1 \otimes 1}_{9\text{ components}} = \underbrace{0}_{1} \oplus \underbrace{1}_{3} \oplus \underbrace{2}_{5}.$$

The three pieces are:

$$\begin{aligned}
\ell = 0: &\quad \text{tr}(T) = T_{kk} = \vec{a} \cdot \vec{b}, \\
\ell = 1: &\quad T_{ij} - T_{ji} \quad \text{same information as } \vec{a} \times \vec{b}, \\
\ell = 2: &\quad \frac{1}{2}(T_{ij} + T_{ji}) - \frac{1}{3}\text{tr}(T)\delta_{ij}.
\end{aligned}$$

So “rank-2 tensor” and “$\ell = 2$” are not the same statement. A general rank-2 tensor contains $\ell = 0, 1, 2$. Only its symmetric traceless part is the $\ell = 2$ piece.

4. The Decomposition Is Fixed

Which ℓ blocks appear is fixed by the representation theory of rotations. It is not a modeling choice.

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

Examples:

$$\begin{aligned} 1 \otimes 1 &= 0 \oplus 1 \oplus 2, \\ 2 \otimes 1 &= 1 \oplus 2 \oplus 3, \\ 2 \otimes 2 &= 0 \oplus 1 \oplus 2 \oplus 3 \oplus 4. \end{aligned}$$

What can vary is the basis, normalization, and sign convention inside each block. That is why e3nn may return

$$\frac{\vec{a} \cdot \vec{b}}{\sqrt{3}}$$

instead of exactly $\vec{a} \cdot \vec{b}$. The physical content is the same; the coordinate convention is different.

5. Where Spherical Harmonics Enter

The spherical harmonics $Y_\ell^m(\hat{r})$ provide a standard basis for the ℓ irrep. For fixed ℓ, the index m runs from $-\ell$ to $+\ell$, giving $2\ell + 1$ functions.

Under a rotation, these $2\ell + 1$ functions mix only among themselves:

$$Y_\ell(R\hat{r}) = D^\ell(R) Y_\ell(\hat{r}).$$

For example, the five $\ell = 2$ spherical harmonics rotate into linear combinations of the same five functions. They do not leak into $\ell = 0$ or $\ell = 1$. This is why e3nn stores features in blocks such as

$$0e,\ 1o,\ 2e,\ 3o, \ldots$$

6. How e3nn Uses This

The e3nn feature declaration

```
"32x0e + 8x1o + 8x2e"
```

means:

block	copies	components per copy	total components
`0e`	32	1	32
`1o`	8	3	24
`2e`	8	5	40
total			96

To carry higher-order tensor information, add higher-ℓ channels:

```
"32x0e + 8x1o + 8x2e + 4x3o + 4x4e".
```

This increases compute cost. In molecular graph neural networks, practical choices are often $\ell_{\text{max}} = 2$ or 3.

What to remember. Cartesian rank counts indices in the original coordinate system. ℓ labels a minimal rotation block. e3nn does not carry arbitrary Cartesian tensors directly; it decomposes them into these rotation blocks and computes with those.