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1

a)

definition: $\rho(g_1 g_2) = \rho(g_1)\rho(g_2)$, $g_1, g_2 \in G$

1. show $\rho(e) = I$

set $g_1 = e$:

$$\rho(g_2) = \rho(e\, g_2) = \rho(e)\,\rho(g_2) \Rightarrow \rho(e) = I$$

2. show $\rho(a^{-1}) = \rho(a)^{-1}$

set $g_1 = a^{-1}$, $g_2 = a$

$$I = \rho(e) = \rho(a^{-1}a) = \rho(a^{-1})\,\rho(a) \Rightarrow \rho(a^{-1}) = \rho(a)^{-1}$$

b)

$$A' = R A R^T = \frac{1}{3} T_r(T)\, R\, I_3 R^T = \frac{1}{3} T_r(T)\, I_3 \overset{T_r(T) = T_r(T')}{=} \frac{1}{3} T_r(T')\, I_3$$

$$B' = R B R^T = R\, \frac{1}{2}(T - T^T)\, R^T = \frac{1}{2}\left(R T R^T - R T^T R^T\right) = \frac{1}{2}\left(T' - (R T R^T)^T\right) = \frac{1}{2}(T' - T'^T)$$

$$C' = R C R^T = R\, \frac{1}{2}\left(T + T^T - \frac{2}{3} T_r(T)\, I_3\right) \overset{\text{same steps as in A and B}}{=} \frac{1}{2}\left(T' + T'^T - \frac{2}{3} T_r(T')\, I_3\right)$$

$\Rightarrow$ A, B, C transform according to decomposition of T'

c)

$$T - T^T = \begin{pmatrix} 0 & T_{12}-T_{21} & T_{13}-T_{31} \\ T_{21}-T_{12} & 0 & T_{23}-T_{32} \\ T_{31}-T_{13} & T_{32}-T_{23} & 0 \end{pmatrix} = \varepsilon_{ijk} \underbrace{\begin{pmatrix} T_{12}-T_{21} \\ T_{13}-T_{31} \\ T_{23}-T_{32} \end{pmatrix}}_{=:v}$$

Antisym tensors have the following properties:

- 0 in diagonal
- Upper triangle is negative of lower triangle $\Rightarrow$ in total three different absolute values contained

$\Rightarrow$ ε_{ijk} fulfills form, v gives the three values

$$\begin{aligned} R_{li} B_{ij} R_{mj} &= R_{li}\, \varepsilon_{ijk}\, v_k\, R_{mj} \\ &= v_n\, I_{3kn}\, R_{li} R_{mj}\, \varepsilon_{ijk} \\ &= v_n\, R^{-1}_{no} R_{ok} R_{li} R_{mj}\, \varepsilon_{ijk} \\ &= v_n\, R^{-1}_{no} \det(R^T)\, \varepsilon_{lmo} \\ &= v_n\, R^{-1}_{no}\, \varepsilon_{lmo} \quad , \quad R^{-1} = R^T \\ &= \varepsilon_{lmo} R_{on} v_n \end{aligned}$$

d)

$$\underline{3} \otimes \underline{3} \otimes \underline{3} = \underline{3} \otimes (\underline{1} \oplus \underline{3} \oplus \underline{5})$$

$$2l_1+1 \otimes 2l_2+1 = \bigoplus_{L=|l_1-l_2|}^{l_1+l_2} 2L+1$$

$$= \underline{3} \otimes \underline{1} \oplus \underline{3} \otimes \underline{3} \oplus \underline{3} \otimes \underline{5}$$

$$= \underline{3} \oplus \underline{1} \oplus \underline{3} \oplus \underline{5} \oplus \underline{3} \oplus \underline{5} \oplus \underline{7}$$

$$= \underline{1} \oplus \underline{3} \oplus \underline{3} \oplus \underline{3} \oplus \underline{5} \oplus \underline{5} \oplus \underline{7}$$

e)

The l_1 of $3 \otimes k$ is $l_1 = 1$. The resulting maximum l is $l_1 + l_2 = 1 + l_2$.

Starting with $k = 3$ $l_2 = 1$. For every additional $\otimes 3$ l becomes larger by 1.

$\Rightarrow$ n-times $3 \otimes \ldots \otimes 3$ results in $l = n$ exactly only one time as only the prior largest l can decompose in the new largest l.

f)

Stars and Bars problem solution:

number of ways to put n indistinguishable stars into k distinguishable bins $= \binom{n+k-1}{k-1}$

Symmetry of Tensor $\Rightarrow$ indistinguishable indices

way to put n indistinguishable indices into $\underset{\text{(consider 3 d as stated in exercise)}}{3 \text{ dims}}$ $= \binom{n+3-1}{3-1} = \binom{n+2}{2}$

$\Rightarrow$ fully symmetric Tensor has $\binom{n+2}{2}$ components

Question for Tutor:

What is an intuitive explanation for the fact that the way of putting the indices in the dimension is the number of components?

Looking at the constraints of trace:

number of possible traces (= number of constraints) = choose 2 out of n indices $= \binom{n}{2}$

$\Rightarrow$ number of independent components $= \binom{n+2}{2} - \binom{n}{2}$

$$= \frac{(n+2)!}{2!\,(n+2-2)!} - \frac{n!}{2!\,(n-2)!}$$

$$= \frac{(n+2)!\;2!\,(n-2)!}{2!\;n!\;2!\,(n-2)!} - \frac{n!\;2!\;n!}{2!\,n!\,2!\,(n-2)!}$$

$$= \frac{(n+2)\,(n+1)\;n!\;2!\,(n-2)! - n!\;2!\;n\,(n-1)(n-2)!}{2!\,n!\,2!\,(n-2)!}$$

$$= \frac{((n+2)(n+1) - n\,(n-1))\;n!\;2!\,(n-2)!}{2!\,n!\,2!\,(n-2)!}$$

Perfect

$$= \frac{n^2+3n+2 - n^2+n}{2}$$

$$= \frac{4n+2}{2} = 2n+1$$

$\Rightarrow$ symmetric traceless tensor has same number of free dims as the $l = n$ decomposition part.

2

a)

$$h(x) = h(\rho(g)\, x) = \rho(g)\, h(x)$$

$\Rightarrow$ $h(x)$ has same symmetry as x

b)

Ellipsoids have no single vectorial quantity that can describe them. Due to the symmetric sampling no direction is implied. Therefore, the only resulting option is the zero vector, as it ensures the equivariance property.

Exactly

c)

sheet11

January 26, 2025

0.1 2 Equivariant neural networks

0.1.1 (c)

1.

[1]:
```
import torch
from e3nn.o3 import wigner_D

# Define a rotation: use YXY Euler angles (alpha, beta, gamma) (YXY seems to be␣
↪the order of rotations) (values arbitratily chosen)
alpha = torch.tensor(0.1)  # Rotation around Y-axis
beta = torch.tensor(0.2)   # Rotation around X-axis
gamma =torch.tensor(0.3)  # Rotation around Y-axis

D_matrix = wigner_D(1, alpha, beta, gamma)

print("Wigner-D Matrix for l=1 (rotation matrix):")
print(D_matrix)

# Verify equivalence to a standard 3D rotation matrix
from scipy.spatial.transform import Rotation as R
rotation_matrix = R.from_euler('YXY', [alpha,beta,gamma]).as_matrix()

print("\nStandard 3D Rotation Matrix:")
print(rotation_matrix)


print("\nDifference between Wigner-D and 3D Rotation Matrix:")
print(D_matrix.numpy() - rotation_matrix)


assert torch.allclose(torch.tensor(rotation_matrix,dtype=torch.float),␣
↪D_matrix, atol=1e-6)
print("Verified: Wigner-D matrix matches the Scipy rotation matrix.")
```

```
Wigner-D Matrix for l=1 (rotation matrix):
tensor([[ 0.9216,  0.0198,  0.3875],
        [ 0.0587,  0.9801, -0.1898],
        [-0.3836,  0.1977,  0.9021]])
```

```
Standard 3D Rotation Matrix:
[[ 0.92164908  0.01983384  0.38751721]
 [ 0.0587108   0.98006658 -0.18979606]
 [-0.38355705  0.19767681  0.902113  ]]

Difference between Wigner-D and 3D Rotation Matrix:
[[ 3.75588739e-07 -3.17601971e-08 -1.96742878e-06]
 [-4.79310225e-07  2.02125393e-08  2.26262875e-07]
 [ 1.94006552e-06 -2.75109682e-07  4.38595927e-07]]
Verified: Wigner-D matrix matches the Scipy rotation matrix.
```

For l=1 the wigner-d matrix corrspons to the rotation matrix. Therefore l=1 is the vecor representation.

2.

[2]:
```python
for l in [2, 3, 4]:
    D_matrix = wigner_D(l, alpha, beta, gamma)
    print(f"Wigner-D matrix for l = {l} has shape: {D_matrix.shape}")
    assert D_matrix.shape == (2 * l + 1, 2 * l + 1), "Dimension mismatch!"
```

```
Wigner-D matrix for l = 2 has shape: torch.Size([5, 5])
Wigner-D matrix for l = 3 has shape: torch.Size([7, 7])
Wigner-D matrix for l = 4 has shape: torch.Size([9, 9])
```

The Shapes of the wigner-d matrixces corrsponds to the expectations.

3. For equivariance proof show:

$$Y_l(R \cdot \mathbf{r}) = D_l(R) \cdot Y_l(\mathbf{r})$$

[3]:
```python
from scipy.special import sph_harm
import numpy as np

def transform_angles_yxy(theta, phi, alpha, beta, gamma):
    """
    Transform the angular components of spherical coordinates (theta, phi)
    using Euler angles (alpha, beta, gamma) in the YXY convention while keeping␣
 ↪the radius unaffected.

    Parameters:
    - theta: Polar angle (colatitude in radians)
    - phi: Azimuthal angle (longitude in radians)
    - alpha: First Euler angle (rotation around Y-axis)
    - beta: Second Euler angle (rotation around X-axis)
    - gamma: Third Euler angle (rotation around Y-axis)

    Returns:
```

```
    - theta_new: Transformed polar angle
    - phi_new: Transformed azimuthal angle
    """

    # Rotation matrices for the YXY Euler angle convention:
    Ry_alpha = np.array([
        [np.cos(alpha), 0, np.sin(alpha)],
        [0, 1, 0],
        [-np.sin(alpha), 0, np.cos(alpha)]
    ])

    Rx_beta = np.array([
        [1, 0, 0],
        [0, np.cos(beta), -np.sin(beta)],
        [0, np.sin(beta), np.cos(beta)]
    ])

    Ry_gamma = np.array([
        [np.cos(gamma), 0, np.sin(gamma)],
        [0, 1, 0],
        [-np.sin(gamma), 0, np.cos(gamma)]
    ])

    # Overall rotation matrix (YXY convention)
    R = np.dot(Ry_gamma, np.dot(Rx_beta, Ry_alpha))

    # Convert spherical coordinates (theta, phi) to Cartesian coordinates (x,␣
↪y, z)
    x = np.sin(theta) * np.cos(phi)
    y = np.sin(theta) * np.sin(phi)
    z = np.cos(theta)

    # Apply the rotation to the Cartesian coordinates
    xyz_new = np.dot(R, np.array([x, y, z]))

    # Convert the rotated Cartesian coordinates back to spherical coordinates
    theta_new = np.arccos(xyz_new[2])  # Polar angle
    phi_new = np.arctan2(xyz_new[1], xyz_new[0])  # Azimuthal angle

    return theta_new, phi_new


def compute_spherical_harmonics(l, theta, phi):
    """Compute all spherical harmonics Y_lm for a given l at (theta, phi)."""
    Y = []
    for m in range(-l, l + 1):
        Y_lm = sph_harm(m, l, phi, theta)
```

```python
        Y.append(Y_lm)
    return torch.tensor(Y, dtype=torch.complex64)

for l in [1, 2, 3, 4]:
    theta, phi = np.pi / 3, np.pi / 4  # Example spherical coordinates␣
 ↪arbitraily chosen
    alpha, beta, gamma = torch.tensor([0.1, 0.2, 0.3])  # Rotation angles in␣
 ↪radians arbitrarily chosen

    Y_l = compute_spherical_harmonics(l, theta, phi)

    theta_new, phi_new = transform_angles_yxy(theta, phi, alpha, beta, gamma)

    Y_l_rotated = compute_spherical_harmonics(l, theta_new, phi_new)

    D_l = torch.tensor(wigner_D(l, alpha, beta, gamma), dtype=torch.complex64)

    Y_l_transformed = D_l @ Y_l

    # Check if equivariance holds: Y_l(R * r) == D_l(R) * Y_l(r)
    assert torch.allclose(Y_l_rotated, Y_l_transformed, atol=1e-5),␣
 ↪f"Equivariance failed for l = {l}"
    print(f"Equivariance verified for l = {l}")
```

```
/var/folders/f4/8n1xlsxx5159pp44m83ldz5w0000gn/T/ipykernel_38131/1467973469.py:7
6: UserWarning: To copy construct from a tensor, it is recommended to use
sourceTensor.clone().detach() or
sourceTensor.clone().detach().requires_grad_(True), rather than
torch.tensor(sourceTensor).
  D_l = torch.tensor(wigner_D(l, alpha, beta, gamma), dtype=torch.complex64)
```

```
        ␣
 ↪---------------------------------------------------------------------------

        AssertionError                            Traceback (most recent call␣
 ↪last)

        Cell In[3], line 81
         78 Y_l_transformed = D_l @ Y_l
         80 # Check if equivariance holds: Y_l(R * r) == D_l(R) * Y_l(r)
    ---> 81 assert torch.allclose(Y_l_rotated, Y_l_transformed, atol=1e-5),␣
 ↪f"Equivariance failed for l = {l}"
         82 print(f"Equivariance verified for l = {l}")


        AssertionError: Equivariance failed for l = 1
```

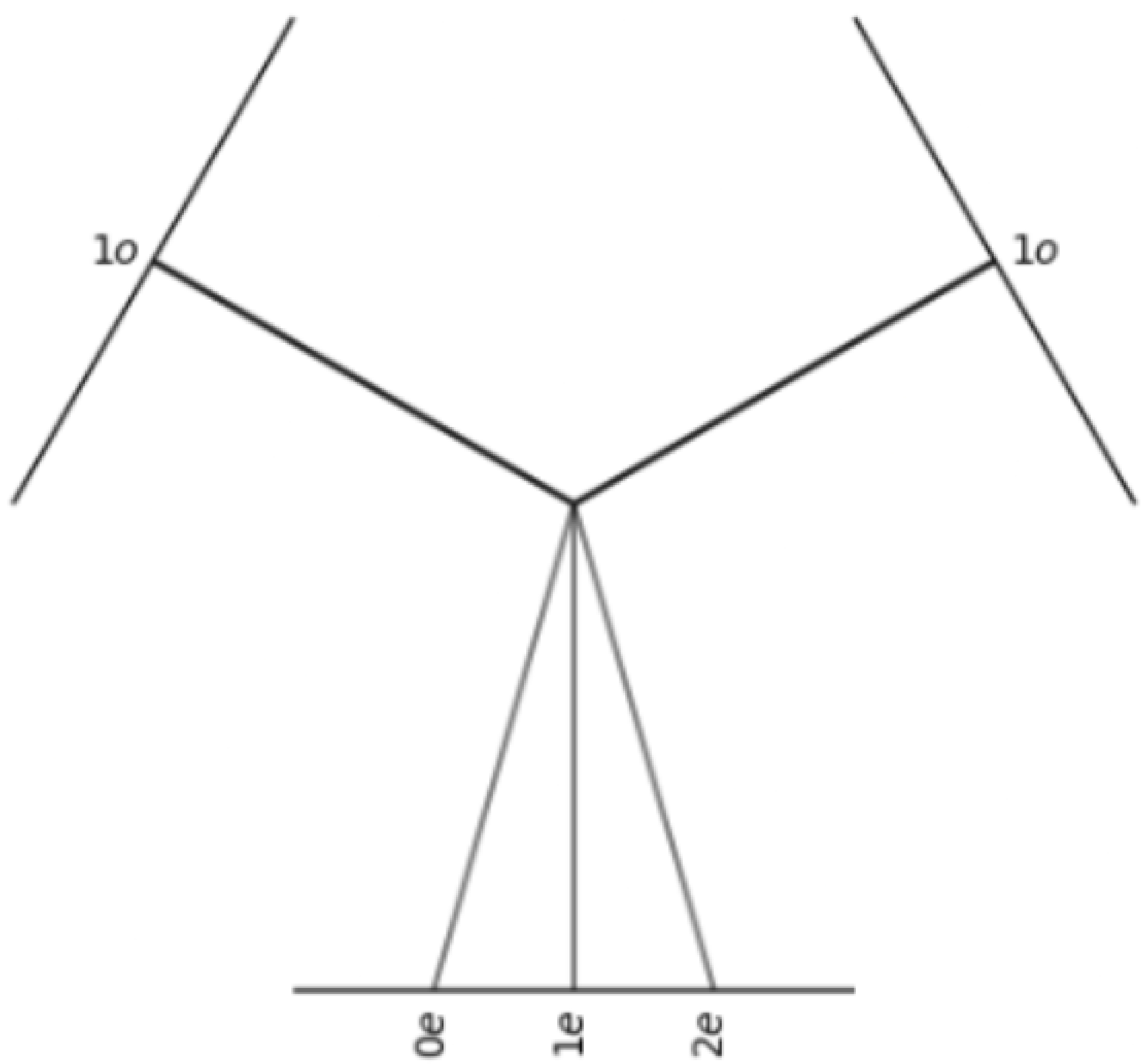
The Equivariance is not confirmed. Most likely there is a mistake in the code, which could not be found. I would be thankful if the Tutor recognises the mistake.

4.

Maybe in the transformation? Main parts look correct

[4]:
```
from e3nn.o3 import Irreps
import e3nn


l1 = Irreps("1x1o")
l2 = Irreps("1x1o")

tensor_product = e3nn.o3.FullTensorProduct(l1, l2)
tensor_product.visualize()
```

[4]:
```
(<Figure size 640x480 with 1 Axes>, <Axes: >)
```



According to equation 3 the resulting diensions are 1, 3 and 5 with l=1, 2 and 5.

5.

[5]:
```
v = np.array([1, 2, 3])
w = np.array([4, 5, 6])
```

```
rotation = R.random()  # This generates a random rotation object

tensor_product = np.outer(v, w)
print("Tensor product of v and w (outer product) and rotation:")
print(np.dot(rotation.as_matrix(), np.dot(tensor_product, rotation.as_matrix().
 ↪T)))

v_rotated = rotation.apply(v)
w_rotated = rotation.apply(w)

tensor_product_rotated = np.outer(v_rotated, w_rotated)
print("\nTensor product after of rotated vectors:")
print(tensor_product_rotated)

equivariance_check = np.allclose(tensor_product_rotated, np.dot(rotation.
 ↪as_matrix(), np.dot(tensor_product, rotation.as_matrix().T)))
print("\nEquivariance check result:", equivariance_check)
```

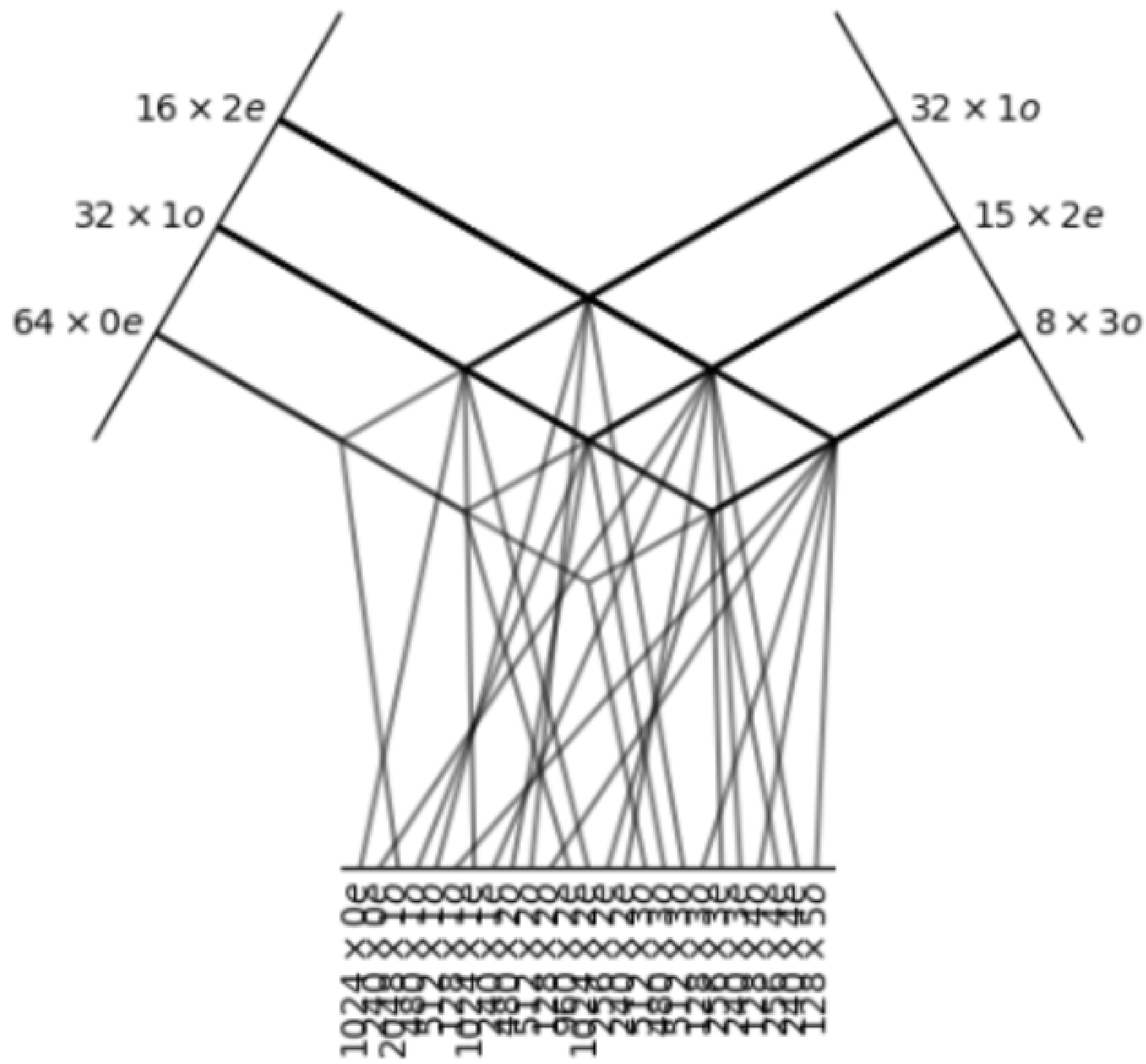
```
Tensor product of v and w (outer product) and rotation:
[[ 2.11504475e-01  1.33095101e-02 -1.06349922e+00]
 [ 1.08030554e+00  6.79812444e-02 -5.43205572e+00]
 [-6.30844914e+00 -3.96976789e-01  3.17205143e+01]]

Tensor product after of rotated vectors:
[[ 2.11504475e-01  1.33095101e-02 -1.06349922e+00]
 [ 1.08030554e+00  6.79812444e-02 -5.43205572e+00]
 [-6.30844914e+00 -3.96976789e-01  3.17205143e+01]]

Equivariance check result: True
```

Applying the rotation before or after the outer product gives an equivariant result.

6.

[6]:
```
rep1 = Irreps("64x0e + 32x1o + 16x2e")
rep2 = Irreps("32x1o + 15x2e + 8x3o")
tensor_product = e3nn.o3.FullTensorProduct(rep1, rep2)
tensor_product.visualize()
```

[6]:
```
(<Figure size 640x480 with 1 Axes>, <Axes: >)
```



[13]:
```python
import re
import pandas as pd

def parse_irrep_string(irrep_str):
    """
    Parse the input string of irreps into a list of tuples representing
    the multiplicity and angular momentum (l) for each irrep.

    Example input: '64x0e + 32x1o + 16x2e'

    Returns:
    - List of tuples: [(64, 0, 'e'), (32, 1, 'o'), (16, 2, 'e')]
    """
    irrep_pattern = r'(\d+)x(\d+)([eo])'
    matches = re.findall(irrep_pattern, irrep_str)
    parsed_irreps = [(int(m[0]), int(m[1]), m[2]) for m in matches]
    return parsed_irreps


def calculate_tensor_product_from_irreps(irrep_str1, irrep_str2):
```

```
    """
    Calculate the tensor product between two input string representations of␣
↪irreps
    and return the resulting dimensions in the same format as the input string.

    Args:
    - irrep_str1: The first string representing a direct sum of irreps (e.g.,␣
↪'64x0e + 32x1o + 16x2e')
    - irrep_str2: The second string representing a direct sum of irreps

    Returns:
    - result_str: String of the resulting irreps in the same format as the input
    """
    # Parse the irreps from the input strings
    irreps1 = parse_irrep_string(irrep_str1)
    irreps2 = parse_irrep_string(irrep_str2)

    result_irreps = []

    # For each combination of irreps from the two input representations
    for mult1, l1, parity1 in irreps1:
        for mult2, l2, parity2 in irreps2:
            # Calculate the tensor product of the two irreps with angular␣
↪momenta l1 and l2
            result_dimensions= calculate_tensor_product_dimensions(l1, l2)

            # Multiply the multiplicities from both irreps
            for l in result_dimensions:
                parity = 'o' if l%2 else 'e'
                result_irreps.append([mult1 * mult2, l, parity])

    # Convert the result list to a string format
    result_str = ' + '.join([f"{mult}x{l}{parity}" for mult, l, parity in␣
↪result_irreps])

    return result_str


def calculate_tensor_product_dimensions(l1, l2):
    """
    Calculate the dimensions of the resulting irreps when taking the tensor␣
↪product
    of two irreps with angular momenta l1 and l2.

    Parameters:
    - l1: The angular momentum quantum number of the first irrep
    - l2: The angular momentum quantum number of the second irrep
```

```
    Returns:
    - result_dimensions: List of the dimensions of the resulting irreps
    """
    result_dimensions = []
    for L in range(abs(l1 - l2), l1 + l2 + 1):
        result_dimensions.append(L)

    return result_dimensions


# Example usage
irrep_str1 = '64x0e + 32x1o + 16x2e'  # First representation
irrep_str2 = '32x1o + 16x2e + 8x3o'  # Second representation

result_str = calculate_tensor_product_from_irreps(irrep_str1, irrep_str2)

print(f"Resulting tensor product: {result_str}")
```

```
Resulting tensor product: 2048x1o + 1024x2e + 512x3o + 1024x0e + 1024x1o +
1024x2e + 512x1o + 512x2e + 512x3o + 256x2e + 256x3o + 256x4e + 512x1o + 512x2e
+ 512x3o + 256x0e + 256x1o + 256x2e + 256x3o + 256x4e + 128x1o + 128x2e + 128x3o
+ 128x4e + 128x5o
```

The output should be equal to the one of the figure.

[ ]:

```

```

3

a) $n(x) = \left(\sum_r p_r w_r(x)\right)^2$ ensures nonnegativity or $n(x) = \exp\left(\sum_r p_r w_r(x)\right)$

als a penalty can be used

$L_{penalty} = \lambda \int \max(-n(x), 0)^2 \, dx$, with λ being a hyperparameter for regularization strength.

b)

- non-linearity is more comlicated in gradients $\Rightarrow$ more computational intensive
- non-linearity in parameters leads to worse and more complicated convergence
- interpretability is lost due to complex non-linear interactions

Very good