Sheet#11 Proposed Solution MLPH_W24

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1 Sheet 11

1.1 Ex 1

(a) Check that the definition of a group representation $\rho : G \to GL(V)$ implies that the representation of the identity element corresponds to the identity matrix, $\rho(e) = I$.

Proof: Let $a \in G$. $\rho(a) = \rho(ae) = \rho(a)\rho(e) = \rho(ea) = \rho(e)\rho(a)$. Thus, $\rho(e) = I$.

Secondly, show that the definition implies $\rho(a^{-1}) = \rho(a)^{-1}$.

Proof: a as above, then $I = \rho(e) = \rho(a^{-1}a) = \rho(a^{-1})\rho(a) \implies \rho(a^{-1}) = \rho(a)^{-1}$

(b) Consider separetely the transformation behavior of the decomposition of $T = A + B + C$ and show that $T' = A' + B' + C'$.

Proof:

$$T' = \frac{1}{3}Tr(RTR^T)I_3 + \frac{1}{2}(RTR^T - (RTR^T)^T) + \frac{1}{2}(RTR^T + (RTR^T)^T) - \frac{2}{3}Tr(RTR^T)) \tag{1}$$

$$= \frac{1}{3}Tr(T)I_3 + \frac{1}{2}(RTR^T - (RTR^T)^T) + \frac{1}{2}(RTR^T + (RTR^T)^T - \frac{2}{3}Tr(T)) = \tag{2}$$

$$= \frac{1}{3}Tr(T)RR^TI_3 + \frac{1}{2}(RTR^T - RT^TR^T + \frac{1}{2}(RTR^T + RT^TR^T - \frac{2}{3}Tr(T)RR^T) \tag{3}$$

$$= \frac{1}{3}Tr(T)RI_3R^T + \frac{1}{2}(RTR^T - RT^TR^T + \frac{1}{2}(RTR^T + RT^TR^T - \frac{2}{3}RTr(T)R^T) \tag{4}$$

$$= R(A + B + C)R^T \tag{5}$$

$$= A' + B' + C' \tag{6}$$

We used that the trace of a tensor transforms like a scalar under $SO(3)$ i.e. it is invariant as shown in the lecture, the orthonormal property $I = R^TR = RR^T$, and $(AB)^T = B^TA^T$.

(c) Due to the alternating property $B_{ij} = -B_{ji}$ we can write in components $B = \varepsilon_{ijk}v_k$. Then v_k transforms like a vector under transformation of $B' = RBR^T$.

Proof using the hint and $\det(R) = 1$:

$$B'_{ij} = R_{ik}B_{kl}R_{lj} = R_{ik}\varepsilon_{klm}v_mR_{lj}$$

$$= R_{ik}\varepsilon_{klo}R_{on}R_{nm}v_mR_{lj} = \det(R)\varepsilon_{ijn}R_{nm}v_m = \varepsilon_{ijn}R_{nm}v_m$$

(d)

$$3 \otimes 3 \otimes 3 = 3 \otimes (2 \cdot 0 + 1 \oplus 2 \cdot 1 + 1 \oplus 2 \cdot 2 + 1)$$
$$= 3 \otimes (1 \oplus 3 \oplus 5) = (3) \oplus (1 \oplus 3 \oplus 5) \oplus (3 \oplus 5 \oplus 7) = \underline{1} \oplus 3\underline{3} \oplus 2\underline{5} \oplus \underline{7}$$

(e) For the product of the first two irreps, $l_1 = l_2 = 1$. Thus the largest value that L can attain is $L = 2$, meaning there is exactly one irrep in the decomposition with order 2. Multiplying the result with an additional $l = 1$ irrep yields a sum whose largest index is $L' = L + 1 = 3$, which is the number of factors in the multiplication. Any additional factor will only raise the order of the highest irrep in the decomposition of the product by 1 exactly, meaning that the highest order irrep of the order n tensor will be n with multiplicity 1.

1.2 Ex 2

(a) Show that for a general equivariant function $h(x)$ that the output has the same symmetries as the input, e.g.

$$\rho(g)x = x \implies \rho'(g)h(x) = h(x).$$

Proof: The defining property of equivariance is here $\rho(g)h(x) = h(\rho'(x))$. Thus

$$h(x) = h(\rho(g)x) = \rho'(g)h(x).$$

(b) We consider an $SO(3)$-equivariant GNN f taking as input a set P of p vectors $x_i \in \mathbb{R}^3$. It is further invariant w.r.t. permutations of the input by means of message passing (cf. Ch. 4.2.2 https://cs.mcgill.ca/~wlh/comp766/files/chapter4_draft_mar29.pdf). The GNN maps the set of vectors to an 3-vector,

$$f : \mathbb{R}^{3\times p} \to \mathbb{R}^3.$$

Assume that the input P is sampled evenly from an ellipsoid and that the output $f(P)$ ought to transform like a vector. Argue that the output can only be the zero vector,

$$f(P') = Rf(P) \implies f(P) = 0.$$

Argument: Consider the discrete group under matrix multiplication with elements that have representations of the kind $Diag(\pm 1, \pm 1, \pm 1) \in \mathbb{R}^3$ in the principal basis of the ellipsoid. Since the point clouds are sampled evenly from the ellispoid, they are invariant under this discrete symmetry group up to noise. By (a), f must preserve the discrete symmetry in the output, implying

$$f(P) = f(-P) = -f(P).$$

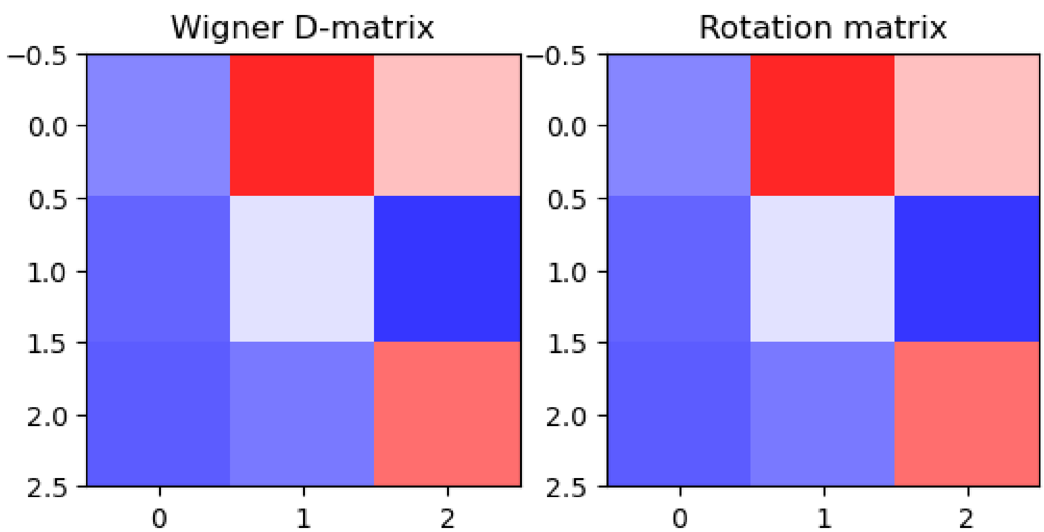
and hence $f(P) = 0 \ \forall \ P$.

(c)

[1]:
```
from e3nn.o3 import Irrep, Irreps
from e3nn import o3
import matplotlib.pyplot as plt
import torch
```

1.

[2]:
```
# get random element of O#
rot = o3.rand_matrix().to(dtype=torch.float64)
irreps = Irreps("1e")
# calculate the Wigner D-matrix

D = irreps.D_from_matrix(rot)

fig, (ax1,ax2) = plt.subplots(1,2)
ax1.imshow(D, cmap='bwr', vmin=-1, vmax=1)
ax1.set_title("Wigner D-matrix")
ax2.imshow(rot, cmap='bwr', vmin=-1, vmax=1)
ax2.set_title("Rotation matrix");
```



2.

[3]:
```
for l in [2,3,4]:
    irrep = Irrep(str(l)+"e") # e = even = no inversion = proper SO3 with␣
 ↪determinant +1
    expected_matrix_dimension = (2*l + 1, 2*l + 1)
    actual_matrix_dimension = tuple(irrep.D_from_matrix(rot).shape)
    print("Expected",expected_matrix_dimension, "Found",␣
 ↪actual_matrix_dimension)
```

```
Expected (5, 5) Found (5, 5)
Expected (7, 7) Found (7, 7)
Expected (9, 9) Found (9, 9)
```

Checks out.

3.

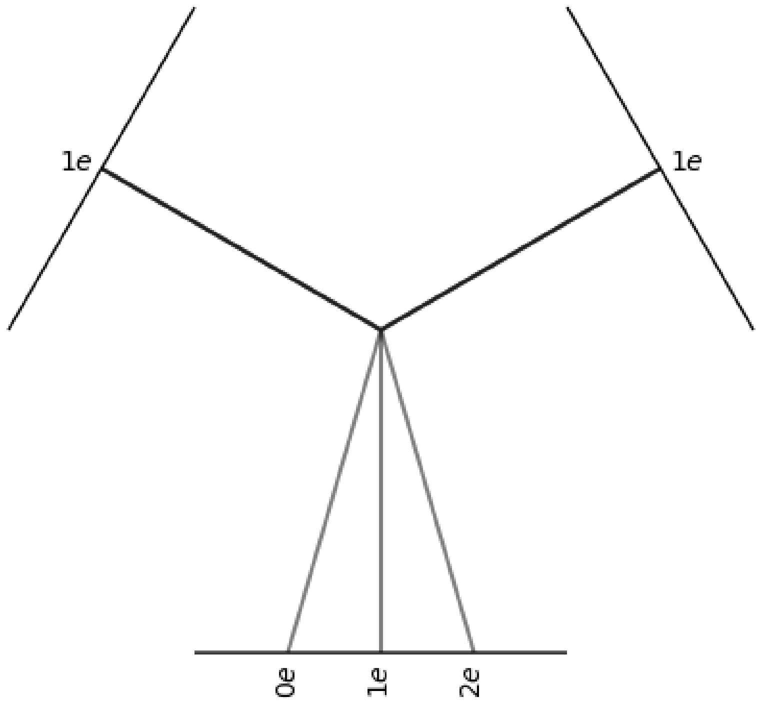
[4]:
```python
x = random_vec = torch.randn(3).to(dtype=torch.float64)
for l in [1,2,3,4]:
    # 1. Rotate before calculating SH
    y = rotated_input = rot @ random_vec
    # 2. Calculate SH of rotated input
    u = o3.spherical_harmonics(l, y, normalize=True)

    # 3. Calculate SH of input
    _v = o3.spherical_harmonics(l, x, normalize=True)
    # 4. Rotate after calculating SH
    WDmat = Irreps(str(l)+"e").D_from_matrix(rot)
    v = WDmat @ _v

    # 5. Compare
    print(f"l={l}, deviation = ", torch.norm(u-v))
```

```
l=1, deviation =  tensor(1.4984e-07, dtype=torch.float64)
l=2, deviation =  tensor(3.4881e-07, dtype=torch.float64)
l=3, deviation =  tensor(6.3489e-07, dtype=torch.float64)
l=4, deviation =  tensor(9.9959e-07, dtype=torch.float64)
```

Commutes up to floating point precision.

4.

[5]:
```python
irrep_a = Irreps("1e")
irrep_b = Irreps("1e")
product = o3.FullTensorProduct(irrep_a, irrep_b)
product.visualize();
```



Indeed, the tensor product has three summands, where the number is ℓ. Applying $2\ell+1$ yields the excpected decomposition

$$2 \cdot 0 + 1 \oplus 2 \cdot 1 + 1 \oplus 2 \cdot 2 + 1 = 1 + 3 + 5.$$

5. We calculate $R(v \otimes u)R^T$ and compare it to $(Rv) \otimes (Ru)$

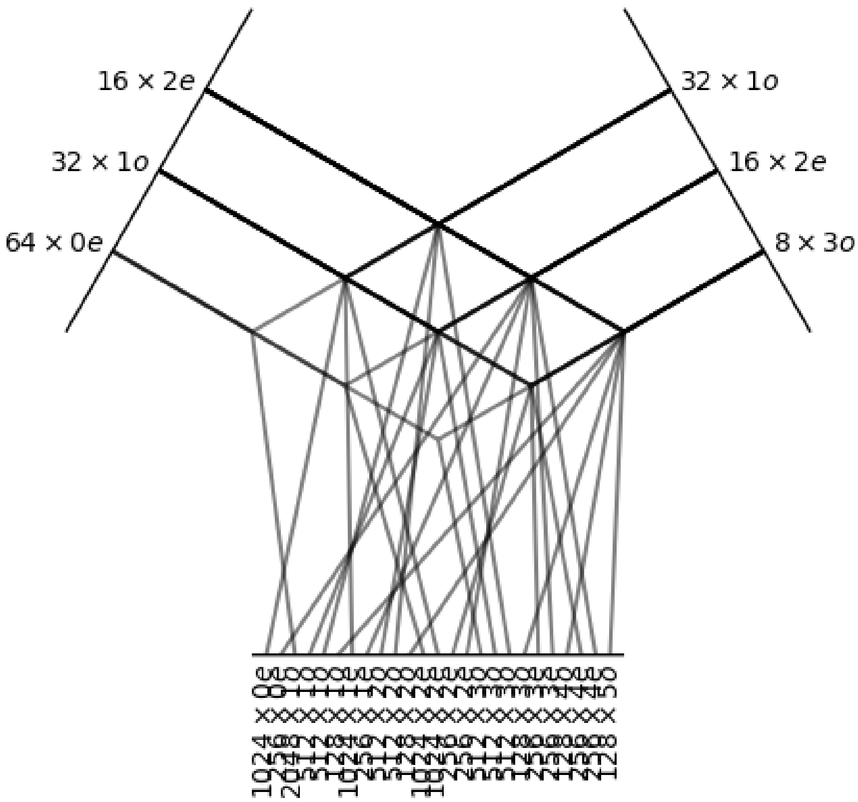
[6]:
```
rot = o3.rand_matrix().to(dtype=torch.float64)

u = torch.tensor([1,2,3], dtype=torch.float64)
v = torch.tensor([4,5,6], dtype=torch.float64)

product = torch.outer(u, v)
rotated_product = torch.matmul(torch.matmul(rot, product), rot.T)

product2 = torch.outer(torch.matmul(rot, u), torch.matmul(rot, v))

rotated_product - product2
```

[6]:
```
tensor([[0., 0., 0.],
        [0., 0., 0.],
        [0., 0., 0.]], dtype=torch.float64)
```

6. Full Tensor Product

[7]:
```python
in1 = Irreps("64x0e+32x1o+16x2e")
in2 = Irreps("32x1o+16x2e+8x3o")

product = o3.FullTensorProduct(in1, in2)
product.visualize()
```

[7]:
```
(<Figure size 640x480 with 1 Axes>, <Axes: >)
```



[8]:
```python
calculated_output_irreps = {l:0 for l in range(0,6)}
for multiplicity, l1 in ((16,2), (32, 1), (64, 0)):
    for m2, l2 in ((32, 1), (16,2), (8,3)):
        for L in range(abs(l1-l2), l1+l2+1):
            calculated_output_irreps[L] += multiplicity * m2


true_output_irreps = dict()
for L in range(0,6):
    true_output_irreps[L] = product.irreps_out.count(f"{L}e") + product.
 ↪irreps_out.count(f"{L}o")
```

[9]:
```
calculated_output_irreps, true_output_irreps
```

[9]:
```
({0: 1280, 1: 4480, 2: 3712, 3: 2176, 4: 640, 5: 128},
 {0: 1280, 1: 4480, 2: 3712, 3: 2176, 4: 640, 5: 128})
```

1.3 3 Electron densities

(a) There are multiple ways of addressing this problem. For instance, one might introduce a regularization term that penalizes negative densities somehow, for instance by integrating the density on the grid where it is negative. Another, more scalable way, would be to check if its possible to make some of the components of p_μ dependent parameters such that positive densities everywhere are guaranteed, but this loses degrees of freedom. Finally, one could use

$$\hat{n}(x) = \max(0, n(x))$$

to ensure positive densities.

(b) By setting

$$n(x) = (\sum_\mu p_\mu \omega_\mu)^2,$$

the basis functions lose expressivity because the square in the exponent essentially turns linear regions into quadratic ones. Think of something like

$$\omega \propto |x| \rightarrow \omega^2 \propto |x|^2$$

Since the discontinuity conveniently models sharp transitions, thus squaring the orbital loses expressivity at the origin.