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Equivariant GNNs

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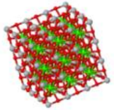
Geometric Graph Neural Networks

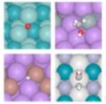
Why we care about geometric GNNs? There are many systems with geometric & relational structures.


Small Molecules


Proteins

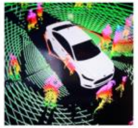

DNA/RNA


Inorganic Crystals

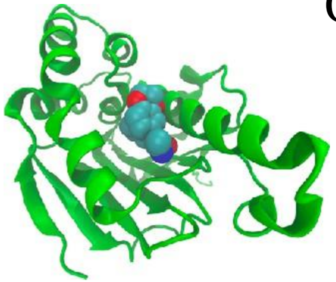

Catalysis Systems


Transportation & Logistics


Robotic Navigation


3D Computer Vision

Geometric GNNs is a fundamental tool for machine learning on geometric (3D) graphs.



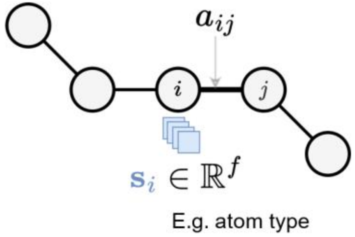
Geometric Graph → Geometric GNN → Prediction

- Functional properties?
- Ligand binding affinity?
- Ligand efficacy?

Image Credit: A Hitchhiker's Guide to Geometric GNNs for 3D Atomic Systems, Duvel et al.. and their presentation slides

Graphs and Geometric Graphs

Graphs are purely topological objects.



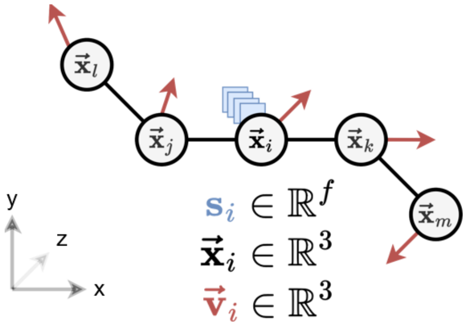
$G = (A, S)$

$A \in \mathbb{R}^{n \times n}$: Adjacency matrix

$S \in \mathbb{R}^{n \times a}$: Scalar features

a is the dimension or number of scalar feature channels.

Geometric graphs are a type of graphs where nodes are additionally endowed with geometric information.



$G = (A, S, X, V)$

$A \in \mathbb{R}^{n \times n}$: Adjacency matrix

$S \in \mathbb{R}^{n \times a}$: Scalar features

$X \in \mathbb{R}^{n \times d}$: Coordinates

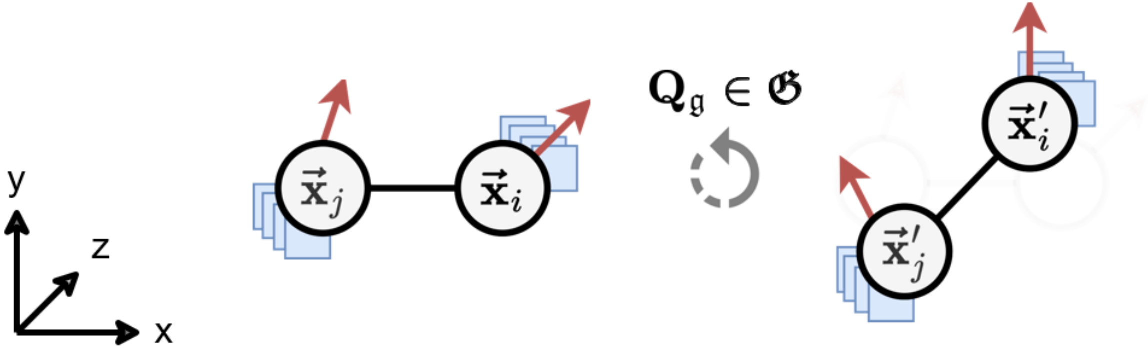
$V \in \mathbb{R}^{n \times b \times d}$: Geometric features

b is the dimension or number of geometric feature channels.

Image Credit: A Hitchhiker's Guide to Geometric GNNs for 3D Atomic Systems, Duvel et al.. and their presentation slides

Physical Symmetries

We have two types of features: **Scalar features** and **Geometric features**. **Geometric features transform with Euclidean transformations** of the system (equivariance); **Scalar features remain unchanged** (invariance).



$$\mathbf{s}_i' = \mathbf{s}_i$$

$$\vec{\mathbf{x}}_i' = \mathbf{Q}_{\mathfrak{g}} \vec{\mathbf{x}}_i$$

$$\vec{\mathbf{v}}_i' = \mathbf{Q}_{\mathfrak{g}} \vec{\mathbf{v}}_i$$

Image Credit: A Hitchhiker's Guide to Geometric GNNs for 3D Atomic Systems, Duvel et al.. and their presentation slides

Review: Equivariance and Invariance

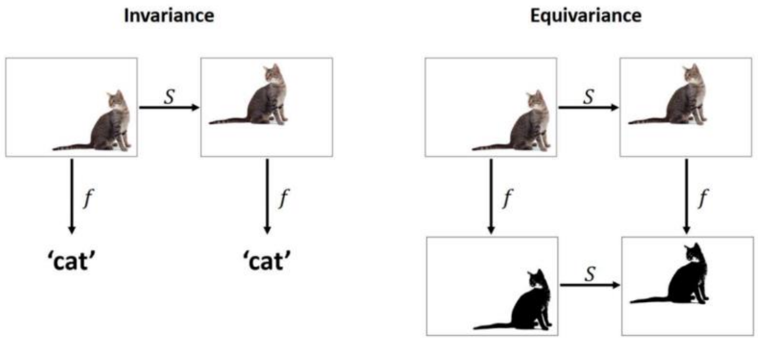
Equivariance is a property of an operator $\Phi : X \to Y$ (such as a neural network layer) by which it commutes with the group action:

$$\Phi \circ \rho^X(g) = \rho^Y(g) \circ \Phi,$$

Invariance is a property of an operator $\Phi : X \to Y$ (such as a neural network layer) by which it remains unchanged after the group action:

$$\Phi \circ \rho^X(g) = \Phi,$$

- $\rho^X(g)$: group representation action on X
- $\rho^Y(g)$: group representation action on Y
- Invariance is a special case of equivariance when $\rho^Y(g)$ is the identity.



Geometric GNNs should account for physical symmetries

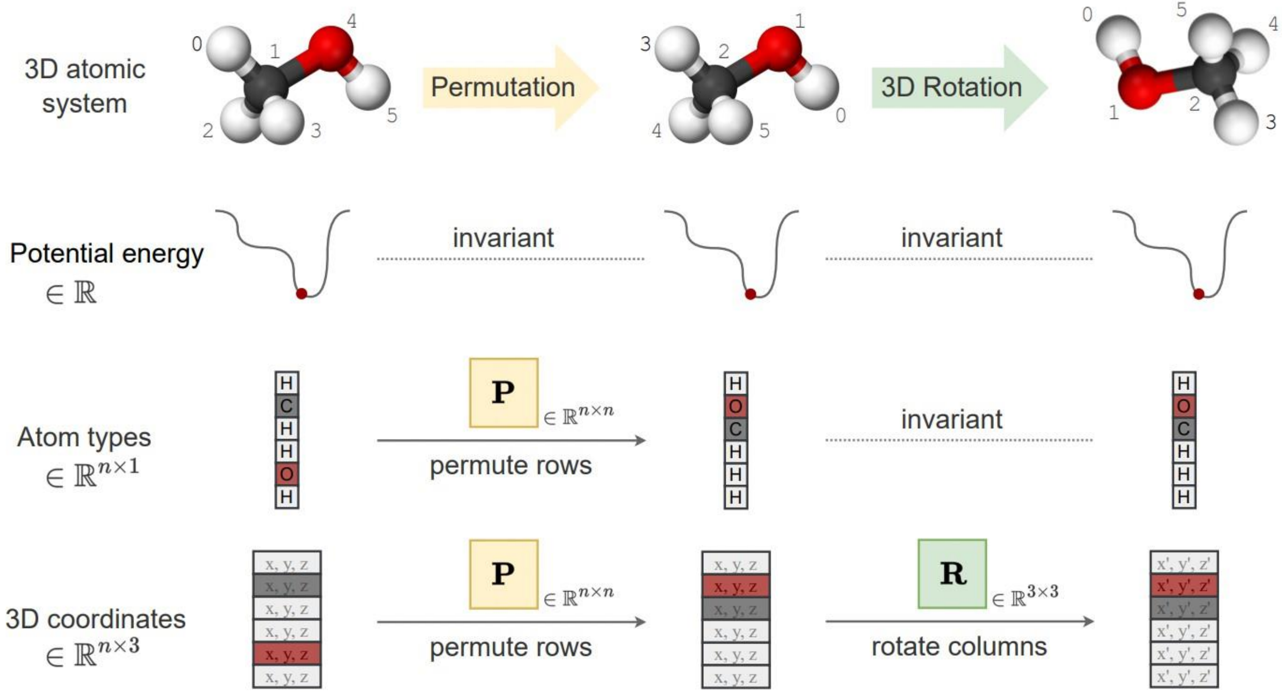
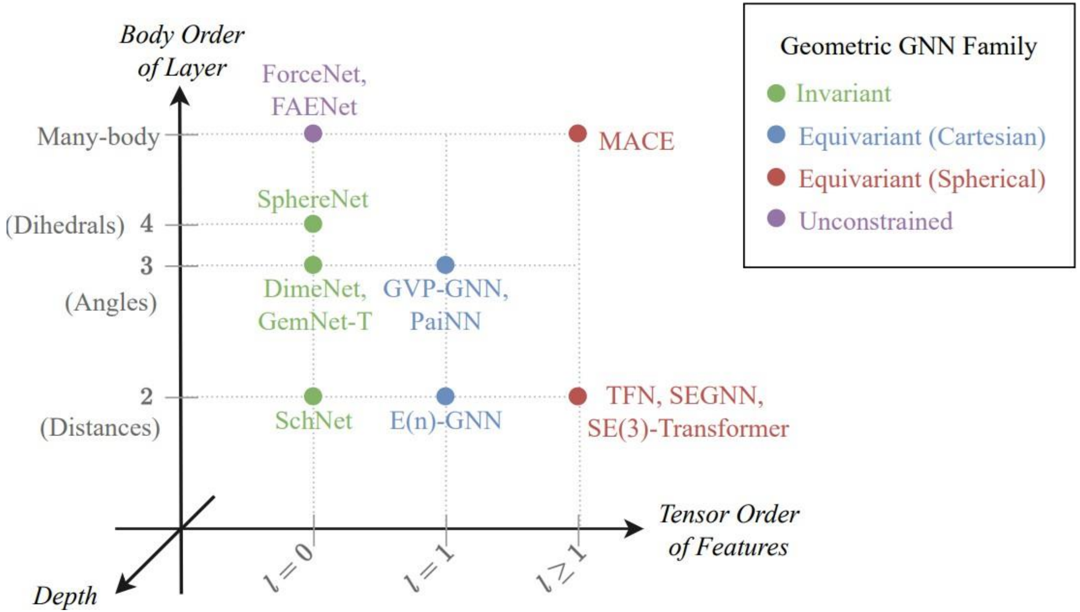


Image Credit: A Hitchhiker's Guide to Geometric GNNs for 3D Atomic Systems, Duvel et al.. and their presentation slides

Building blocks of Geometric GNNs

- Scalar features must be updated in an invariant manner.
- Geometric features must be updated in an equivariant manner.



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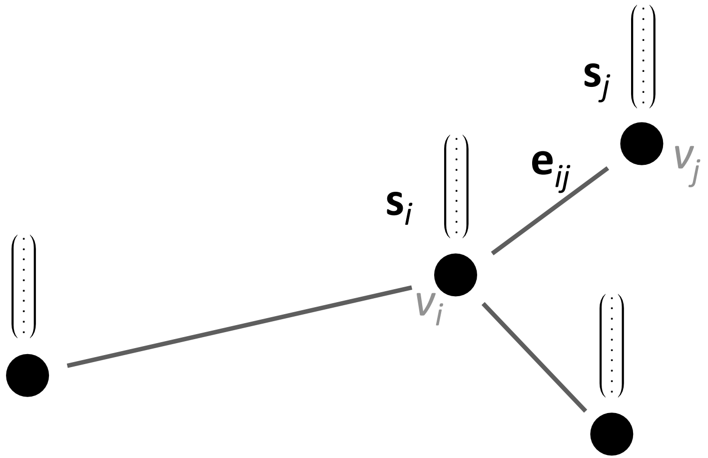
Review: The Message Passing Framework



$G = (A, S, E)$

$A \in \mathbb{R}^{n \times n}$: Adjacency matrix

$S \in \mathbb{R}^{n \times a}$: Node features

$E \in \mathbb{R}^{n \times n \times b}$: Edges features

Goal of Message Passing: iteratively update node features to obtain useful hidden representations

Review: The Message Passing Framework

Input Graph

↓ Node-wise transformation (MLP)

Initial Node Embeddings

↓ Message Passing

Final Node Embeddings

↓ Pooling

Graph Embedding (Optional)

↓ Transformation (MLP)

Final Predictions

Message passing layer:

- Messages

$$\mathbf{m}_{ij} = f_1\left(\mathbf{s}_i, \mathbf{s}_j, \mathbf{a}_{ij}\right),$$

- Aggregate + node updates

$$\mathbf{s}'_i := f_2\left(\mathbf{s}_i, \sum_{j \in \mathcal{N}(i)} \mathbf{m}_{ij}\right),$$

or equivalently,

$$\mathbf{s}'_i := f_2\left(\mathbf{s}_i, \sum_{j \in \mathcal{N}(i)} f_1\left(\mathbf{s}_i, \mathbf{s}_j, \mathbf{a}_{ij}\right)\right),$$

where f_1, f_2 are message and updating functions (MLPs).

$$\mathbf{s}'_i := f_2\left(\mathbf{s}_i, \sum_{j \in \mathcal{N}(i)} f_1\left(\mathbf{s}_i, \mathbf{s}_j, \mathbf{a}_{ij}\right)\right),$$

Geometric Message Passing

For geometric message passing, we condition on geometries. As an illustrative example, assume we have the coordinate information and let a_{ij} contain geometric information, we can have the following message passing schemes:

$$\mathbf{m}_{ij} = f_1\left(\mathbf{s}_i, \mathbf{s}_j, x_j - x_i\right)$$

To make it equivariant (invariant) to E(3), there are in general two directions: Scalarization and Using Steerable Tensor Features. We term them as invariant GNNs (scalarization) and equivariant GNNs (Tensor Operations). Invariant GNNs constraint the geometric information that can be utilized, while the other constraints the model operations.

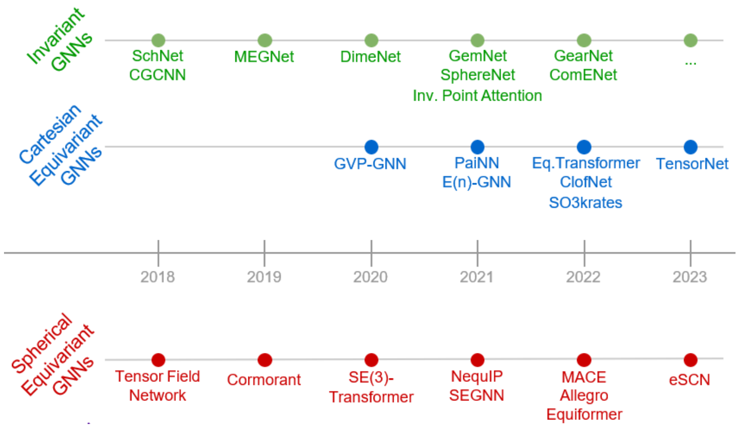


Image Credit: A Hitchhiker's Guide to Geometric GNNs for 3D Atomic Systems, Duvel et al.. and their presentation slides

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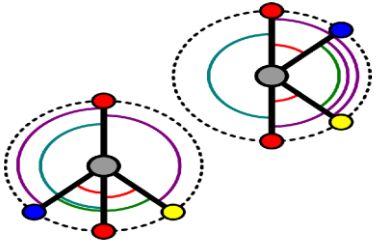
Invariant GNNs

1. Using relative distances (1-hop; body order 2): $\mathbf{m}_{ij} = f_1\left(\mathbf{s}_i, \mathbf{s}_j, d_{ij}\right)$, where $d_{ij} = ||x_j - x_i||$. This is $E(3)$-equivariant, but we limit the expressivity of the model as we cannot distinguish different local geometries. We cannot distinguish two local neighbourhoods apart using the unordered set of distances only.
2. Using relative distances and bond angles (2-hop; body order 3): $\mathbf{m}_{ij} = f_1\left(s_i, s_j, d_{ij}, \sum_{k \in \mathcal{N}_j \setminus \{i\}} f_3\left(s_j, s_k, d_{ij}, d_{jk}, \measuredangle ijk\right)\right)$. This is $E(3)$-equivariant, but again we limit the expressivity of the model.
3. Using relative distances, bond angles, and torsion angles (3-hop; body order 4):

$$\boldsymbol{m}_{ij} = f_1\left(s_i, s_j, d_{ij}, \sum_{k \in \mathcal{N}_j \setminus \{i\}, l \in \mathcal{N}_k \setminus \{i,j\}} f_3\left(s_k, s_l, d_{kl}, d_{ij}, d_{jk}, \measuredangle ijk, \measuredangle jkl, \measuredangle ijkl\right)\right).$$

This is $E(3)$-equivariant and complete.



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Invariant GNNs

In summary, invariant GNNs update latent representations by scalarizing local geometry information. This is efficient, and we can achieve invariance with simple MLP without specific constraints on the operations or activations we can take.

Pros:
- Simple usage of non-linearities on many-body scalars.
- Great performance on some use-cases (e.g. GemNet on OC20).

Cons:
- Scalability of scalar's pre-computation. The accounting of higher-order tuples is expensive.
- Making invariant predictions may still require solving equivariant sub-tasks.
- May lack generalization capabilities (equivariant tasks, multi-domain).

GemNet (Torsion) in theory is complete; however, it requires a complete graph and a certain discretization scheme to be universal.

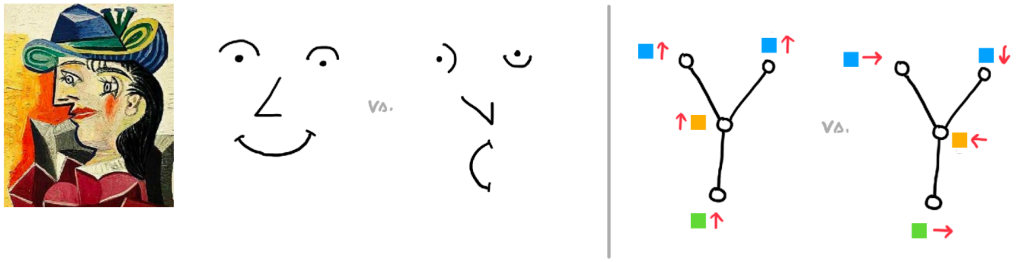
So far, the precise body order of scalars at which all geometric graphs can be uniquely identified remains an open question.

Equivariant GNNs

- In invariant GNNs, invariants are ‘fixed’ prior to message passing.
- Equivariant GNNs build up invariants ‘on the go’ during message passing. More layers of message passing can lead to more complex invariants being built up. Furthermore, equivariant quantities remain available.

Intuition: **The Picasso Problem**

Making invariant predictions may still require solving equivariant sub-tasks



Relative orientation of eyes, nose, mouth is important
(**orientation of sub-graphs w.r.t. one another**),
not just their presence (**invariant quantities**)!

Equivariant GNNs

- In invariant GNNs, we work with only scalars $f\ (s_1, s_2, \ldots, sn)$.
- In equivariant GNNs, we work with vectors $f\ (s_1, s_2, \ldots s_n, v_1, \ldots, v_m)$.

Example: “Scalar-vector” GNNs

Scalar message:

$$\mathbf{m}_i := \quad f_1\left(\mathbf{s}_i, \|\mathbf{v_i}\|\right) + \sum_{j \in \mathcal{N}_i} f_2\left(\mathbf{s}_i, \mathbf{s}_j, \|\vec{\boldsymbol{x}}_{ij}\|, \|\boldsymbol{v}_j\|, \vec{\boldsymbol{x}}_{ij} \cdot \mathbf{v}_j, \vec{\boldsymbol{x}}_{ij} \cdot \mathbf{v}_i, \mathbf{v}_i \cdot \mathbf{v}_j\right)$$

Vector message:

$$\begin{aligned}\vec{\mathbf{m}}_i := f_3\left(\mathbf{s}_i, \|\mathbf{v_i}\|\right) \odot \mathbf{v}_i &+ \sum_{j \in \mathcal{N}_i} f_4\left(\mathbf{s}_i, \mathbf{s}_j, \|\vec{\boldsymbol{x}}_{ij}\|, \|\boldsymbol{v}_j\|, \vec{\boldsymbol{x}}_{ij} \cdot \mathbf{v}_j, \vec{\boldsymbol{x}}_{ij} \cdot \mathbf{v}_i, \mathbf{v}_i \cdot \mathbf{v}_j\right) \odot \mathbf{v}_j \\ &+ \sum_{j \in \mathcal{N}_i} f_5\left(\mathbf{s}_i, \mathbf{s}_j, \|\vec{\boldsymbol{x}}_{ij}\|, \|\boldsymbol{v}_j\|, \vec{\boldsymbol{x}}_{ij} \cdot \mathbf{v}_j, \vec{\boldsymbol{x}}_{ij} \cdot \mathbf{v}_i, \mathbf{v}_i \cdot \mathbf{v}_j\right) \odot \vec{\boldsymbol{x}}_{ij},\end{aligned}$$

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Equivariant GNNs

The high-level ideas in equivariant GNNs is that we keep track of the “types” of the objects and apply equivariant operations. Here, we introduce some concepts, Cartesian tensors, Spherical tensors, tensor product, Wigner-D matrices, and CG coefficients.

A tensor is a multi-dimensional array with directional information.

We have two key operators for Cartesian tensors: tensor product and tensor contraction. They allow us to move up and down the rank of Cartesian tensors to produce tensors of higher ranks or contract them down to lower ranks. Intuitively, we are creating new tensors using the indices.

Equivariant GNNs

We get two vectors in 3D space

```
irreps_x = o3.Irreps('1o')
irreps_y = o3.Irreps('1e')

x = irreps_x.randn(-1)
y = irreps_y.randn(-1)
print(x)
print(y)
```

```
tensor([-0.1222, -0.7573,  1.0416])
tensor([ 0.3303,  0.5315, -1.0235])
```

Equivariant GNNs

We get their outer, inner, and cross products.

```
[12] outter = torch.einsum('i,j', x, y)
     inner = torch.einsum('i,i', x, y)
     cross = torch.linalg.cross(x, y)
     print("======== Outter, Inner, Cross ========")
     print(outter)
     print(inner)
     print(cross)
```

```
======== Outter, Inner, Cross ========
tensor([[-0.0404, -0.0650,  0.1251],
        [-0.2501, -0.4025,  0.7750],
        [ 0.3440,  0.5536, -1.0661]])
tensor(-1.5089)
tensor([0.2214, 0.2189, 0.1851])
```

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Equivariant GNNs

We get a random rotation matrix in O(3) and rotate x,y and get the outter, inner, and cross

```
[13] R = o3.rand_matrix()
     print(R)
     r_x = torch.einsum('ij,j', R, x)
     r_y = torch.einsum('ij,j', R, y)
     r_outter = torch.einsum('i,j', r_x, r_y)
     r_inner = torch.einsum('i,i', r_x, r_y)
     r_cross = torch.linalg.cross(r_x, r_y)
     print("======== Outter, Inner, Cross after Rotation ========")
     print(r_outter)
     print(r_inner)
     print(r_cross)
```

```
tensor([[ 0.1437, -0.9875,  0.0642],
        [ 0.9593,  0.1549,  0.2360],
        [-0.2430,  0.0276,  0.9696]])
======== Outter, Inner, Cross after Rotation ========
tensor([[-0.4329,  0.1256, -0.8433],
        [-0.0061,  0.0018, -0.0119],
        [-0.5532,  0.1606, -1.0778]])
tensor(-1.5089)
tensor([-0.1725,  0.2900,  0.1317])
```

```
print(r_x)
print(r_y)
```

```
tensor([0.7971, 0.0112, 1.0188])
tensor([-0.5431,  0.1576, -1.0580])
```

Equivariant GNNs

All of them transform in a certain way, or, all of these operations are equivariant. Outter product will transform with the "outter product" of the rotation matrices (i.e. Kronecker product if we flatten the resulting outter product of the vectors). Inner product are invariant. Cross product will transform with the original rotation matrix.

```python
R_outter = torch.einsum('ij,kl', R, R)
rotate_outter = torch.einsum('ijkl,jl', R_outter, outter)
rotate_inner = inner
rotate_cross = torch.einsum('ij,j', R, cross)
print("======== Rotate Outter, Inner, Cross ========")
print(rotate_outter)
print(rotate_inner)
print(rotate_cross)
```

```
======== Outter, Inner, Cross after Rotation ========
tensor([[-0.4329,  0.1256, -0.8433],
        [-0.0061,  0.0018, -0.0119],
        [-0.5532,  0.1606, -1.0778]])
tensor(-1.5089)
tensor([-0.1725,  0.2900,  0.1317])
```

```
======== Rotate Outter, Inner, Cross ========
tensor([[-0.4329,  0.1256, -0.8433],
        [-0.0061,  0.0018, -0.0119],
        [-0.5532,  0.1606, -1.0778]])
tensor(-1.5089)
tensor([-0.1725,  0.2900,  0.1317])
```

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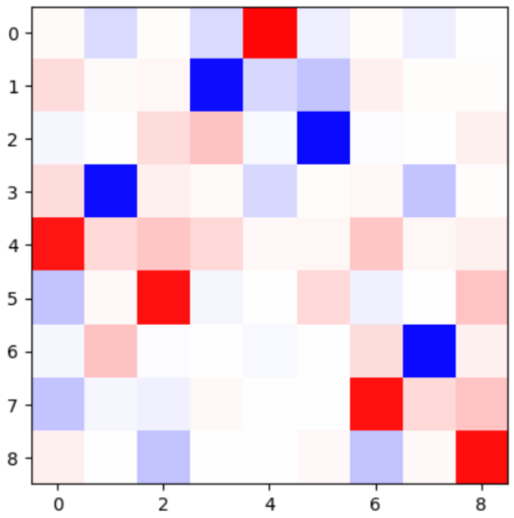
Equivariant GNNs

Visualize this rotation tensor for the outter product (a 3x3x3x3 tensor, we visualize as a 9 by 9 matrix)

```
plt.imshow(torch.kron(R, R), cmap='bwr', vmin=-1, vmax=1);
```



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Equivariant GNNs

Now, for the outter product and the rotated one, we do a change of basis, and represent them in spherical basis.

```
[17] tp = o3.FullTensorProduct(irreps_x, irreps_y)
     # print(tp)
     irreps_xy = tp(x, y)
     irreps_rxy = tp(r_x, r_y)
     print("======== Spherical Outter ========")
     print(irreps_xy )
     print("======== Spherical Rotated Outter ========")
     print(irreps_rxy)
```

```
======== Spherical Outter ========
tensor([-0.8712,  0.1566,  0.1548,  0.1309,  0.3317, -0.2228,  0.1231,  0.9395,
        -0.7253])
======== Spherical Rotated Outter ========
tensor([-0.8712, -0.1220,  0.2051,  0.0932, -0.9875,  0.0845,  0.6182,  0.1052,
        -0.4561])
```

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Equivariant GNNs

Now, for the outter product and the rotated one, we do a change of basis, and represent them in spherical basis.

```
[17] tp = o3.FullTensorProduct(irreps_x, irreps_y)
     # print(tp)
     irreps_xy = tp(x, y)
     irreps_rxy = tp(r_x, r_y)
     print("======== Spherical Outter ========")
     print(irreps_xy )
     print("======== Spherical Rotated Outter ========")
     print(irreps_rxy)
```

```
======== Spherical Outter ========
tensor([-0.8712,  0.1566,  0.1548,  0.1309,  0.3317, -0.2228,  0.1231,  0.9395,
        -0.7253])
======== Spherical Rotated Outter ========
tensor([-0.8712, -0.1220,  0.2051,  0.0932, -0.9875,  0.0845,  0.6182,  0.1052,
        -0.4561])
```

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Equivariant GNNs

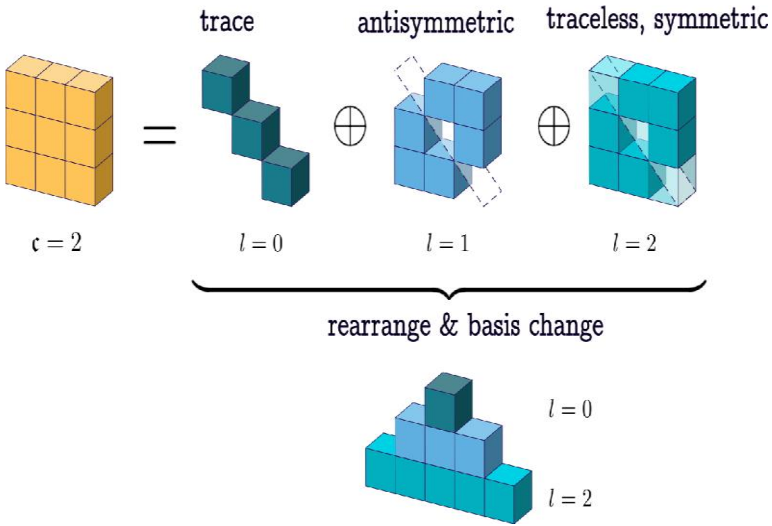

Image Credit: A Hitchhiker's Guide to Geometric GNNs for 3D Atomic Systems, Duvel et al.. and their presentation slides

Equivariant GNNs

This spherical outter product is also equivariant, and the transformation matrix is the Wigner-D matrix

```
[18] D = tp.irreps_out.D_from_matrix(R)
     print("======== Rotate Spherical Outter by Wigner-D ========")
     irreps_rotate_xy = torch.einsum('ij,j', D, irreps_xy)
     print(irreps_rotate_xy)
```

```
======== Rotate Spherical Outter by Wigner-D ========
tensor([-0.8712, -0.1220,  0.2051,  0.0932, -0.9875,  0.0845,  0.6182,  0.1052,
        -0.4561])
```

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Equivariant GNNs

Visualize this rotation tensor for the spherical outter product:

```
plt.imshow(D, cmap='bwr', vmin=-1, vmax=1);
```