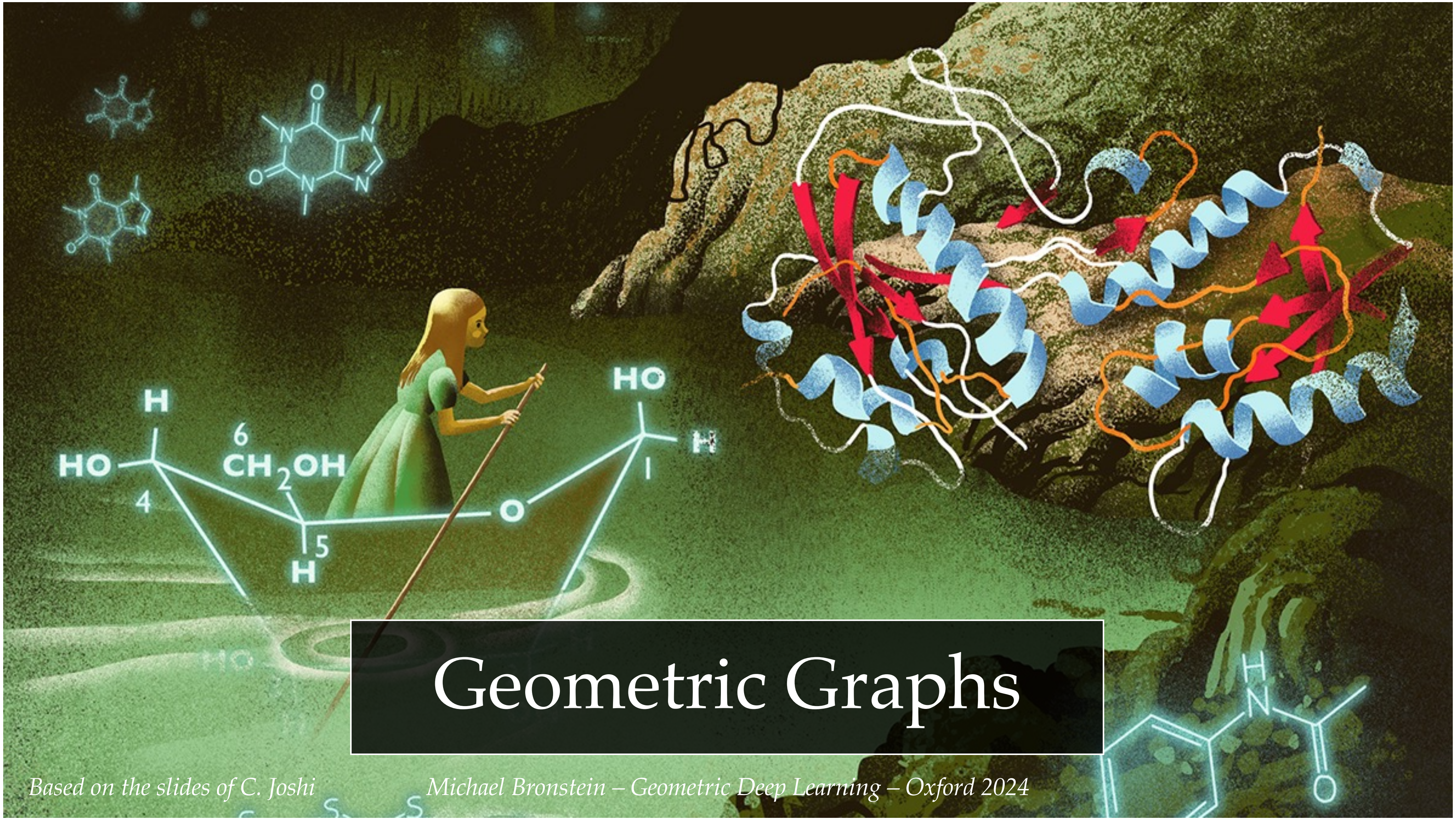
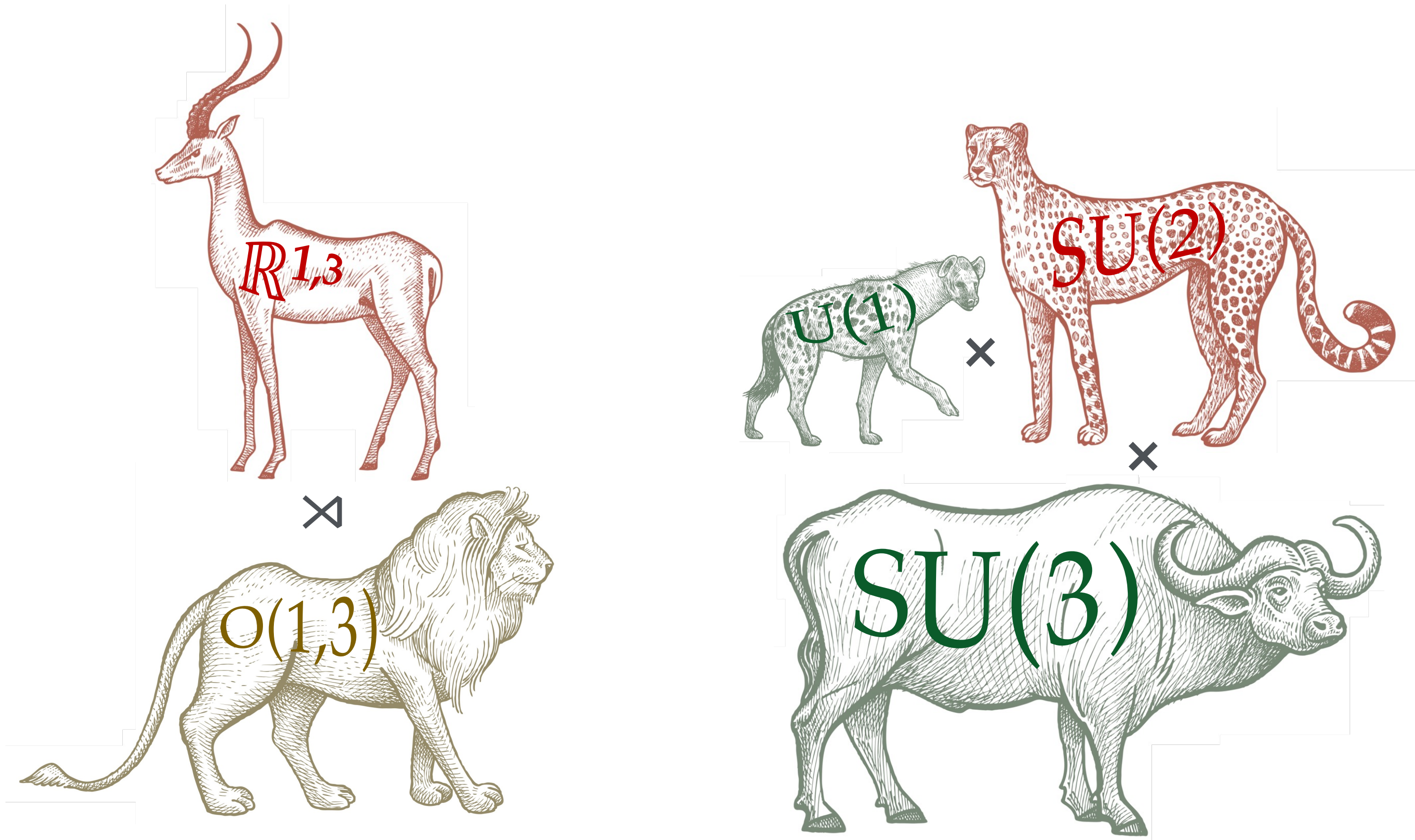


Geometric Graphs

Based on the slides of C. Joshi

Outline

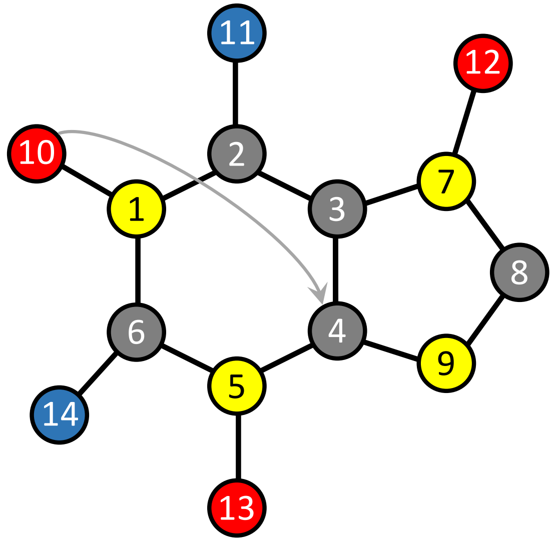
- Geometric graphs are decorated with geometric features such as 3D coordinates, velocities, etc.
- Geometric features transform with the Euclidean transformations
- Geometric GNNs account for these transformations appropriately
- Interactions can be of different *"body order"*: pairwise, triplets, or multibody
- Features can be of different *"tensor order":* scalars, cartesian vectors, or spherical tensors.
- Expressive power of Geometric GNNs



External symmetry **Internal symmetry**

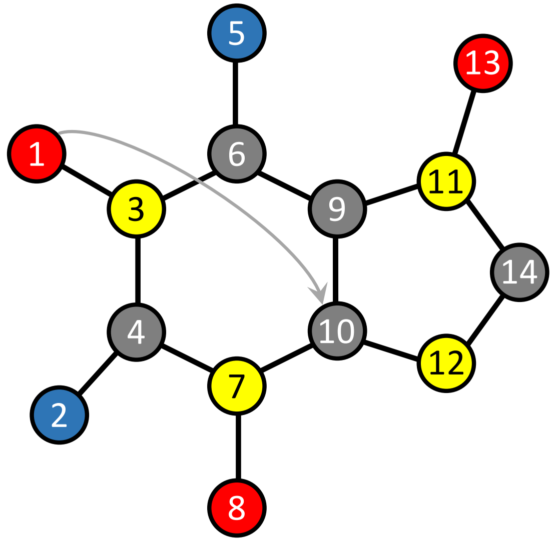
Internal vs External Symmetry

Group S_n
acting on the **domain**
(node *index permutation*)



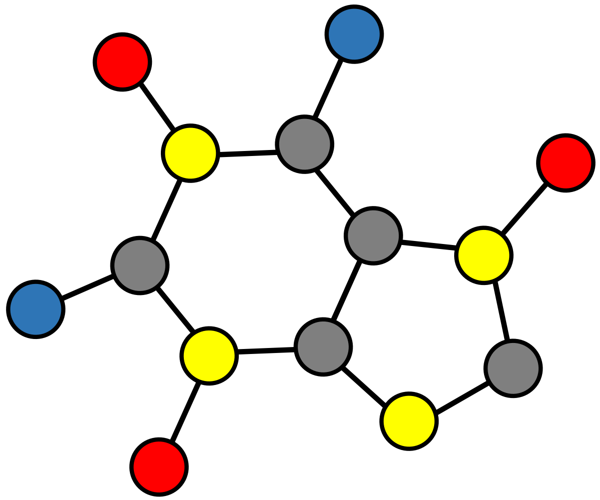
Internal vs External Symmetry

Group S_n
acting on the **domain**
(node *index permutation*)



Internal vs External Symmetry

Group S_n
acting on the **domain**
(node *index permutation*)

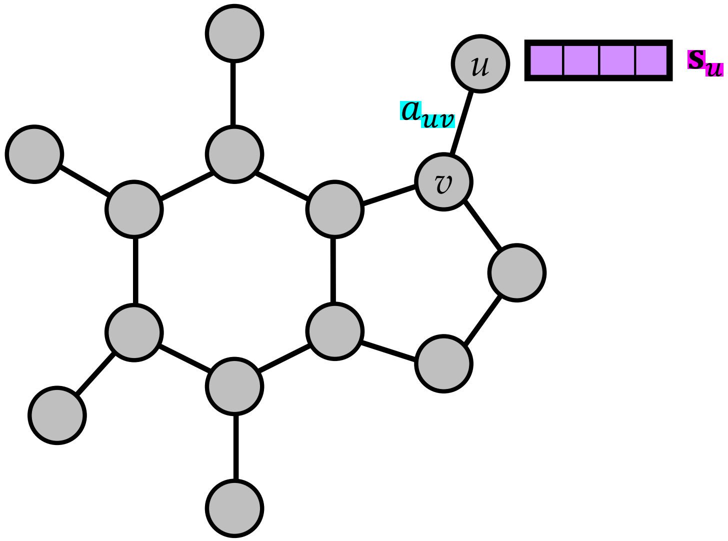


Group SO(3)
acting on the **data**
(node *coordinate rotation*)

GEOMETRIC GRAPHS

Graphs

- Set of *nodes* connected by *edges* (represented by adjacency matrix)
- Nodes have some d-dimensional features (“*d channels*”)



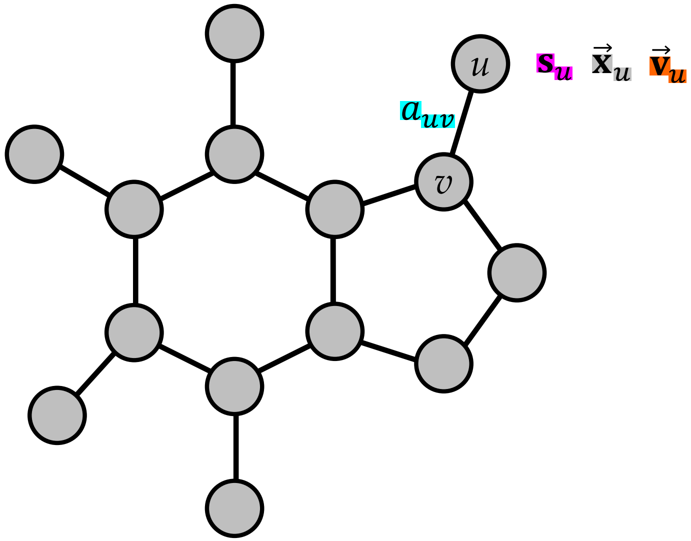
$$\mathcal{G} = (\mathbf{A}, \mathbf{S})$$

$n \times n$ adjacency matric

$n \times d$ scalar node features

Geometric Graphs

- Set of *nodes* connected by *edges* (represented by adjacency matrix)
- Nodes also have *geometric positions* (e.g. atoms in 3D) + *geometric features* (e.g. velocities)



$n\times3$ coordinate matrix

$n\times3$ geometric features

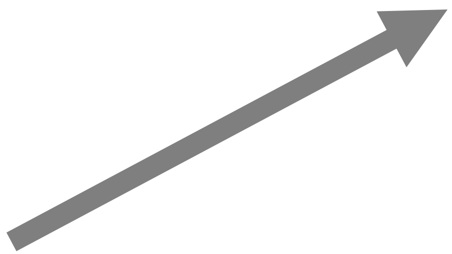
$$\mathcal{G} = (\mathbf{A}, \mathbf{S}, \vec{\mathbf{X}}, \vec{\mathbf{V}})$$

$n\times n$ adjacency matric

$n\times d$ scalar node features

Note: we limit our attention here to vectors for simplicity, but geometric features can be tensors of higher order

What is a Vector?

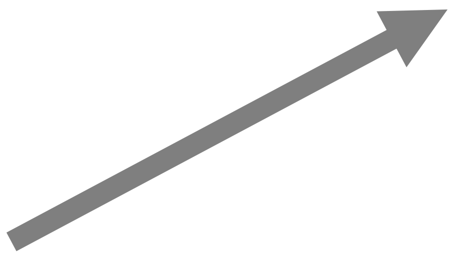


(0.75,0.5)

"Arrow" **"Array of numbers"**

"Element of a vector space"
(addition & scalar multiplication)

What is a Vector?



$(0.75, 0.5)$

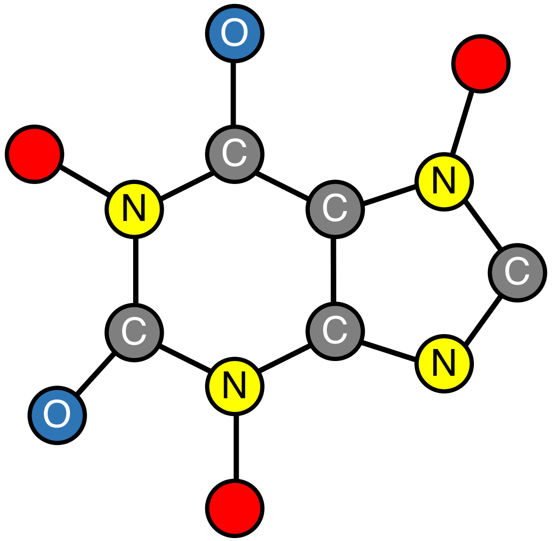
“Arrow”

“Array of numbers”

”An object that transforms like a vector”

Transformations of Geometric Graphs

- Euclidean transformations act differently on different features



$O(3)$

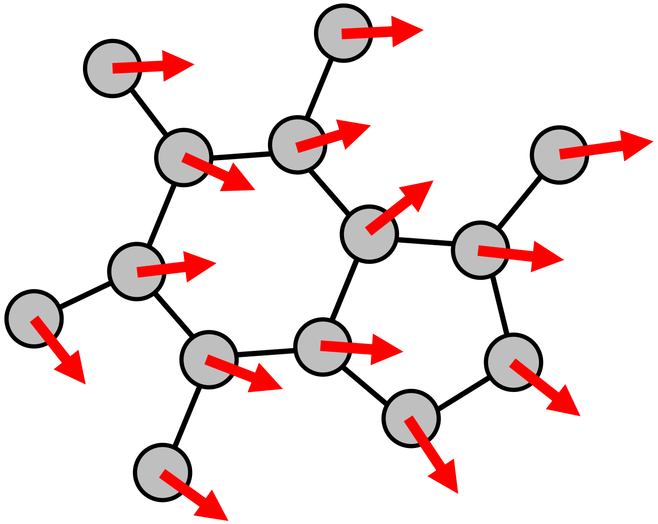
Rotation &
Reflection

$\mathbf{s}_u \rightarrow \mathbf{s}_u$

Scalar features (e.g. atom types) remain *invariant*

Transformations of Geometric Graphs

- Euclidean transformations act differently on different features



$O(3)$

Rotation & Reflection

$\mathbf{s}_u \rightarrow \mathbf{s}_u$

$\vec{\mathbf{x}}_u \rightarrow \mathbf{R}\vec{\mathbf{x}}_u$

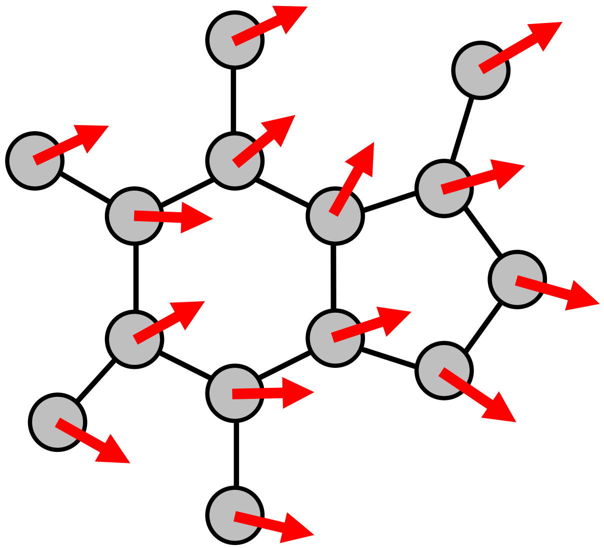
$\vec{\mathbf{v}}_u \rightarrow \mathbf{R}\vec{\mathbf{v}}_u$

Scalar features (e.g. atom types) remain *invariant*

Positions and geometric features are transformed

Transformations of Geometric Graphs

- Euclidean transformations act differently on different features

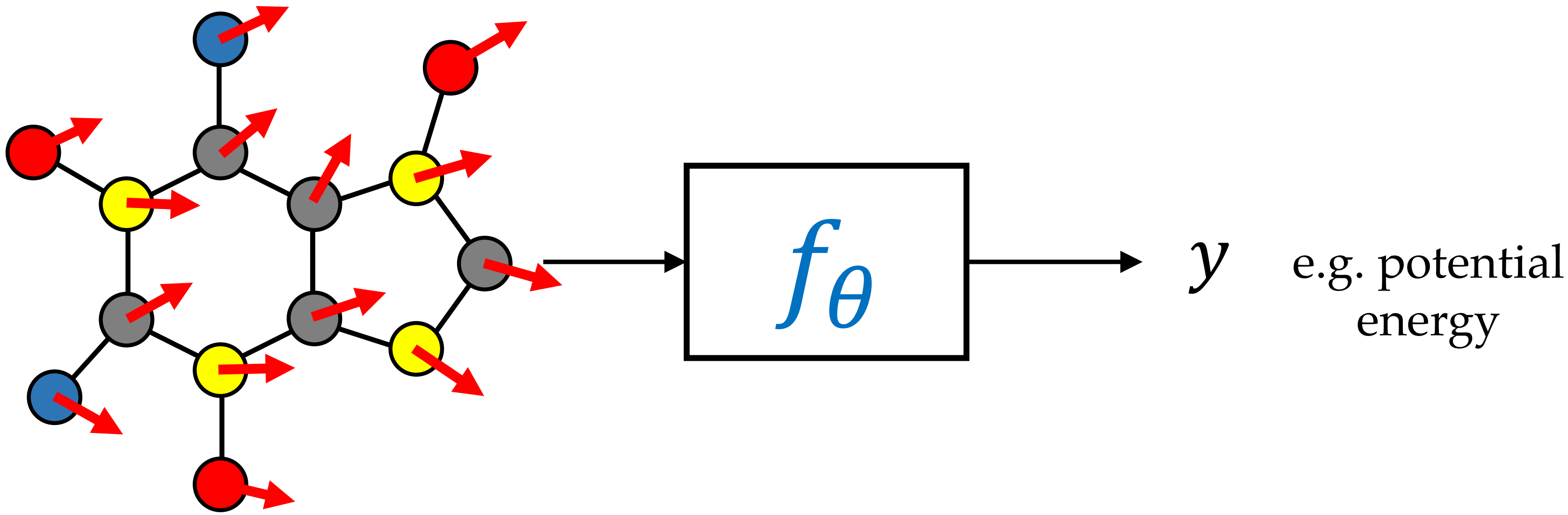


$O(3)$ **Rotation & Reflection**	$T(3)$ **Translation**
$\mathbf{s}_u \to \mathbf{s}_u$	$\mathbf{s}_u \to \mathbf{s}_u$
$\vec{\mathbf{x}}_u \to \mathbf{R}\vec{\mathbf{x}}_u$	$\vec{\mathbf{x}}_u \to \vec{\mathbf{x}}_u + \mathbf{t}$
$\vec{\mathbf{v}}_u \to \mathbf{R}\vec{\mathbf{v}}_u$	$\vec{\mathbf{v}}_u \to \vec{\mathbf{v}}_u$

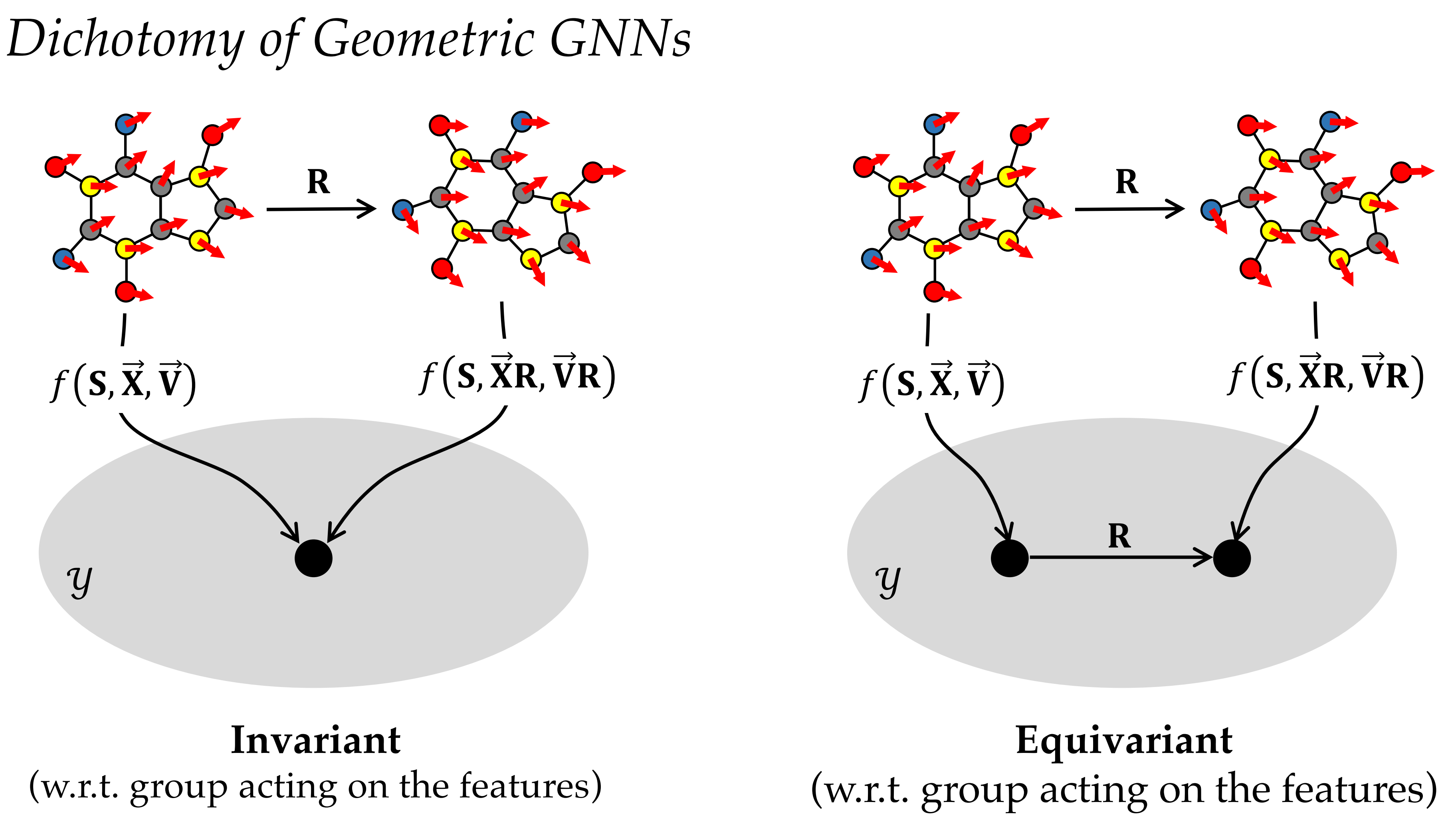
Geometric features invariant under translation

GEOMETRIC GNNs

Geometric GNNs

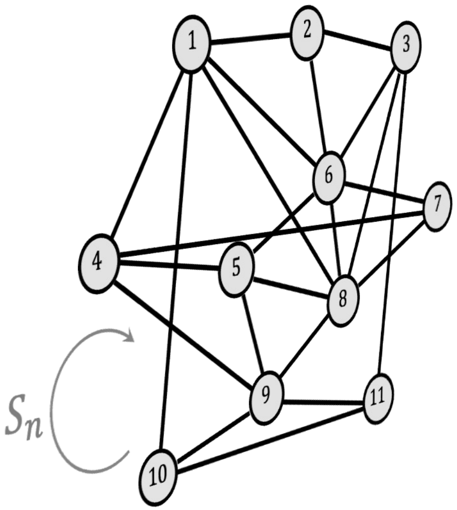


Graph (atoms+bonds)
Scalar features (atom types)
Positions of atoms
Geometric features (e.g. forces)


Dichotomy of Geometric GNNs
R
$f(\mathbf{S}, \vec{\mathbf{X}}, \vec{\mathbf{V}})$
$f(\mathbf{S}, \vec{\mathbf{X}}\mathbf{R}, \vec{\mathbf{V}}\mathbf{R})$
$\mathcal{Y}$
Invariant
(w.r.t. group acting on the features)
R
$f(\mathbf{S}, \vec{\mathbf{X}}, \vec{\mathbf{V}})$
$f(\mathbf{S}, \vec{\mathbf{X}}\mathbf{R}, \vec{\mathbf{V}}\mathbf{R})$
R
$\mathcal{Y}$
Equivariant
(w.r.t. group acting on the features)

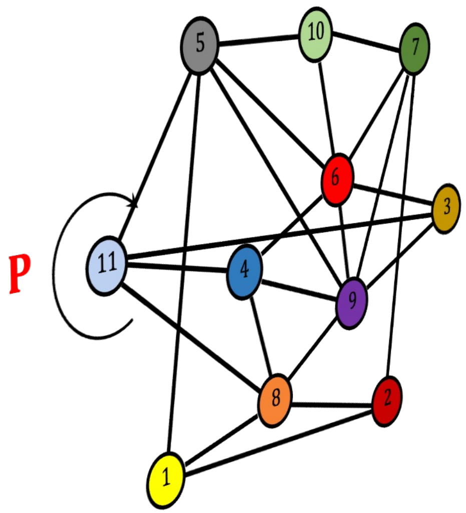
Graph Neural Networks

Graph $G = (V, E)$



Permutation group S_n

Node features $\mathcal{X}(G)$



Permutation matrix P

$$\mathbf{PX} = \left(x_{\pi^{-1}(i),j}\right)$$

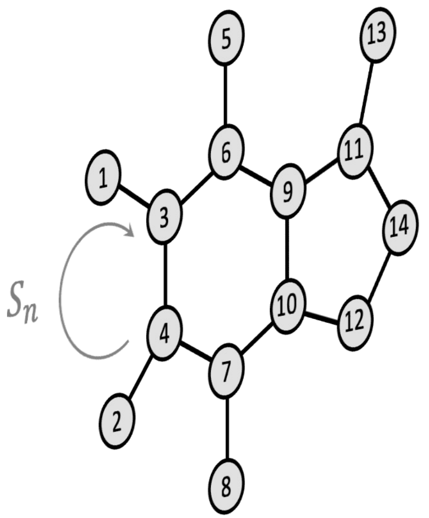
Functions $\mathcal{F}\left(\mathcal{X}(\Omega)\right)$

Message passing

$$\mathbf{F}\left(\mathbf{PX}, \mathbf{PAP}^\top\right) = \mathbf{PF}(\mathbf{X}, \mathbf{A})$$

Geometric ("Equivariant") Graph Neural Networks

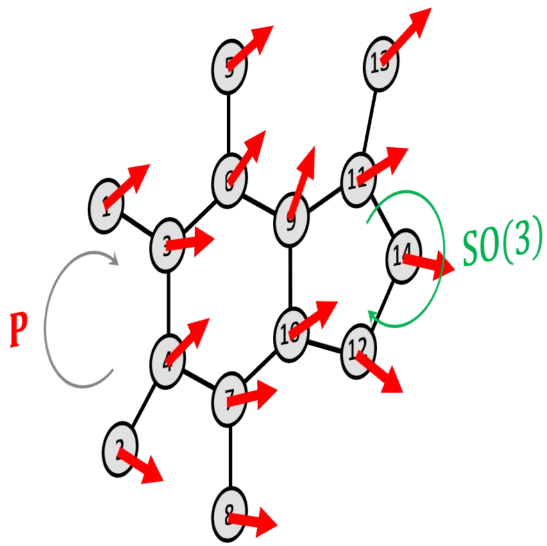
Geometric Graph G



Permutation group S_n

"domain symmetry"

Node features $\mathcal{X}(G)$



Permutation matrix P

Rotation R

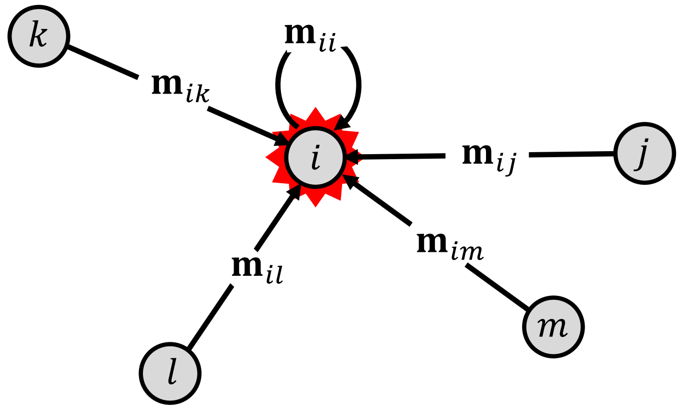
"data symmetry"

Functions $\mathcal{F}(\mathcal{X}(\Omega))$

Geometric message passing

$$\mathbf{F}(\mathbf{PXR}, \mathbf{PAP}^\top) = \mathbf{PF}(\mathbf{X}, \mathbf{A})\mathbf{R}$$

Standard Message Passing

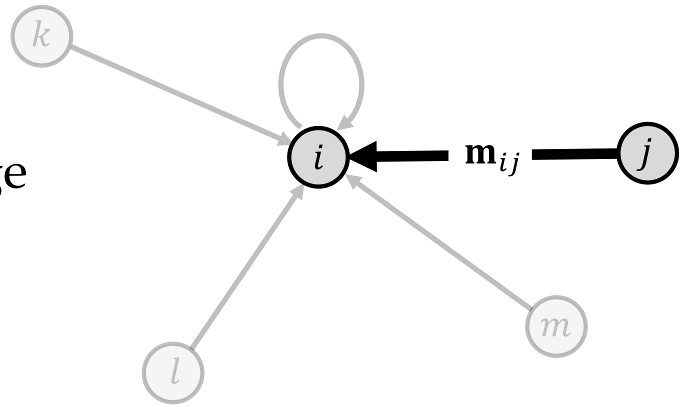


$$\phi\left(\mathbf{s}_i, \boxed{\sum_{j \in \mathcal{N}_i} \psi(\mathbf{s}_i, \mathbf{s}_j)}\right)$$

Permutation-invariant aggregation
to respect *domain symmetry*

Standard Message Passing

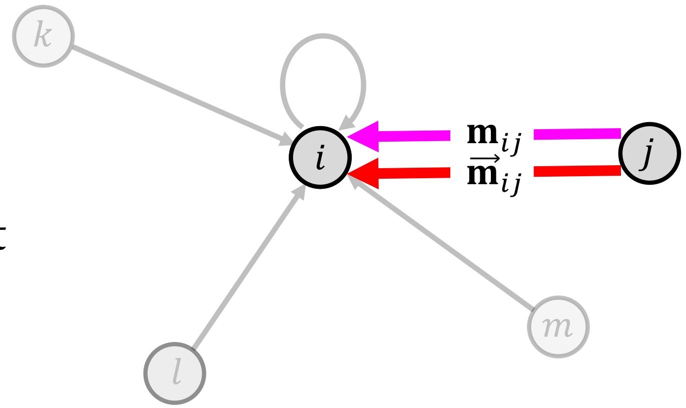
No constraints on message passing function ψ and update ϕ: features can be transformed arbitrarily



$$\phi\left(\mathbf{s}_i, \boxed{\sum_{j\in\mathcal{N}_i} \psi(\mathbf{s}_i, \mathbf{s}_j)}\right)$$

Permutation-invariant aggregation
to respect *domain symmetry*

Geometric Message Passing



Different transformation & update for features that transform differently (scalars and vectors) to respect *data symmetry*

$$\phi\left(\mathbf{s}_i, \vec{\mathbf{x}}_i, \vec{\mathbf{v}}_i, \sum_{j \in \mathcal{N}_i} \psi\left(\mathbf{s}_i, \vec{\mathbf{x}}_i, \vec{\mathbf{v}}_i, \mathbf{s}_j, \vec{\mathbf{x}}_j, \vec{\mathbf{v}}_j\right)\right)$$

Permutation-invariant aggregation to respect *domain symmetry*

Timeline

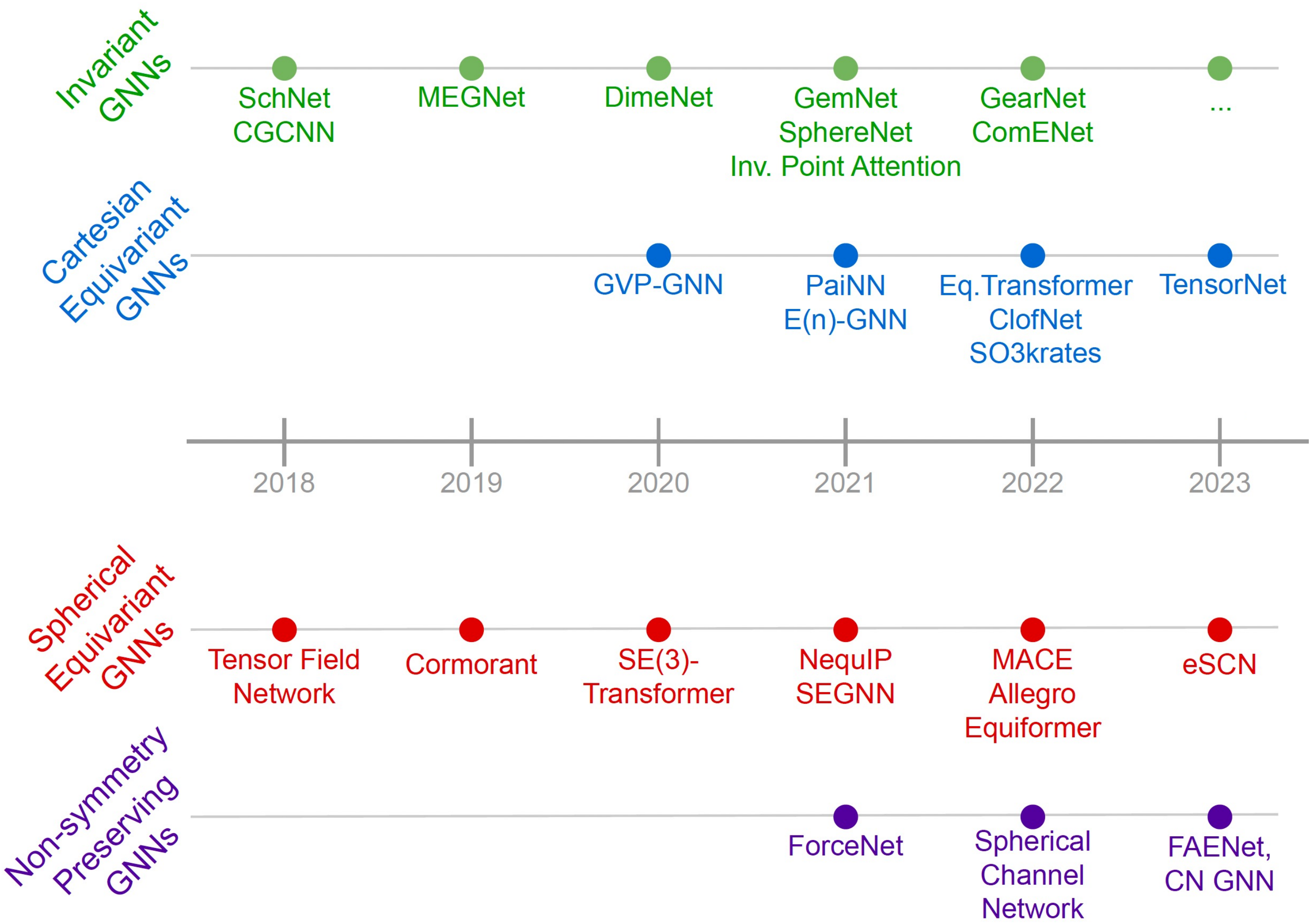


Figure: Duval et al. 2023

Dichotomy of Geometric GNNs

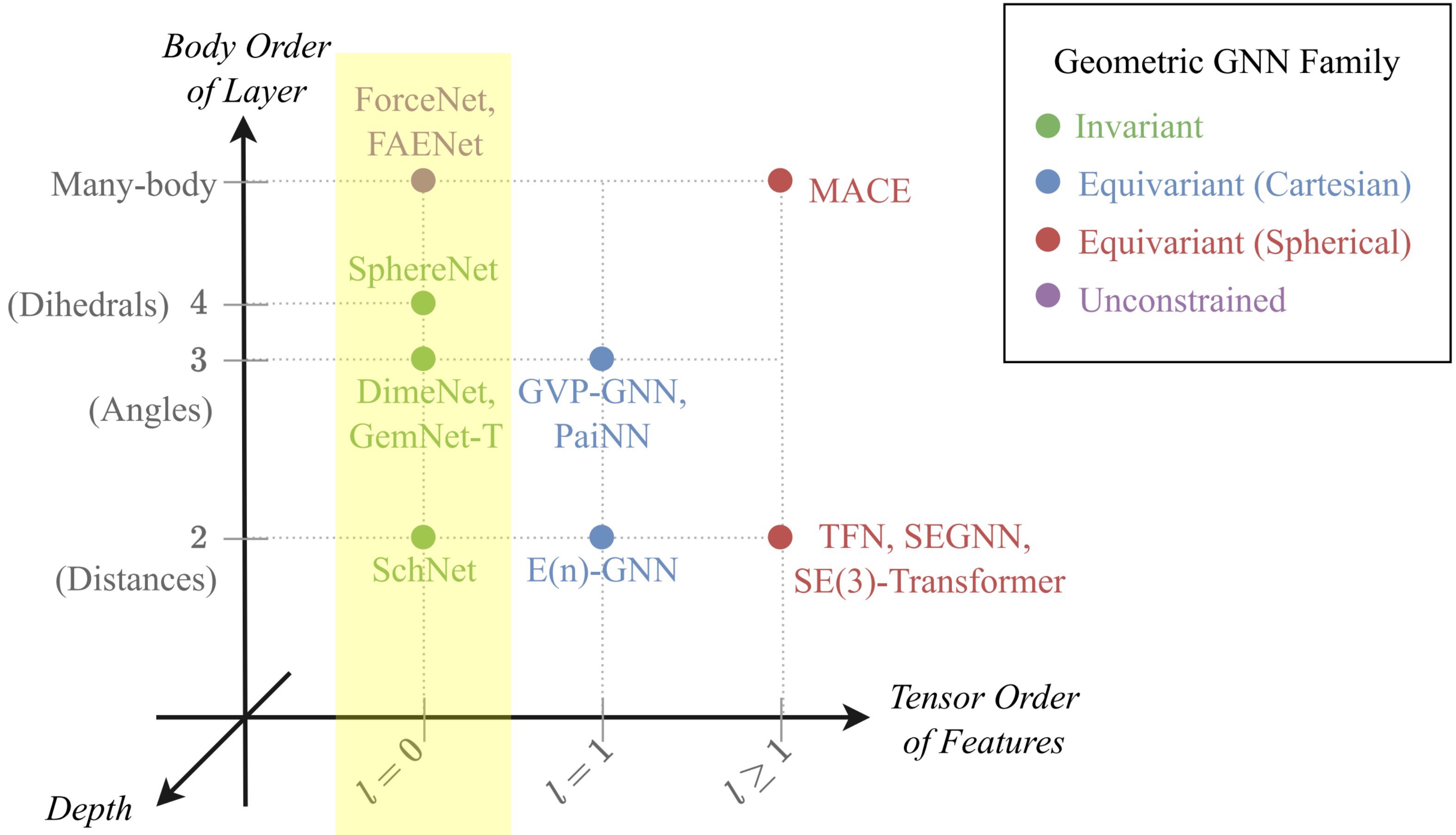
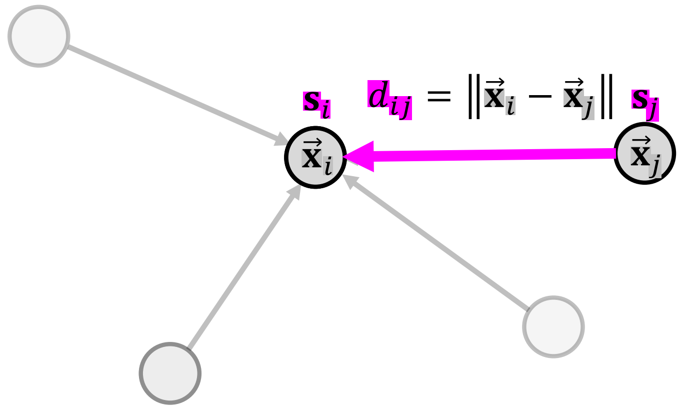


Figure: Duval et al. 2023

INVARIANT GEOMETRIC GNNs

SchNet: second-order invariants

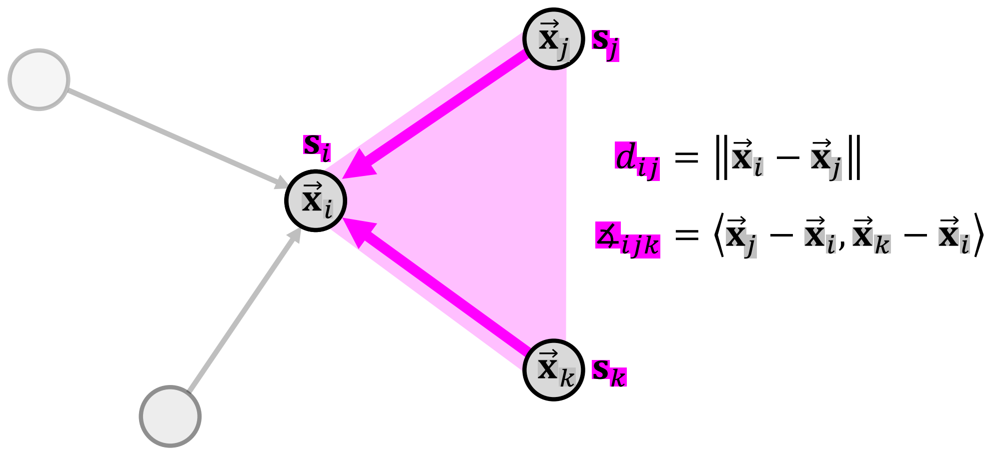


$$\mathbf{s}_i \leftarrow \mathbf{s}_i + \sum_{j \in \mathcal{N}_i} \psi(\mathbf{s}_j, d_{ij})$$

- Use relative distances to scalarise local geometry
- Relative distances are invariant to global rotations & translations

Schütt et al. 2018 (SchNet); also Xie & Grossman 2018 (CGCNN); Lie et al. 2020; Sanchez-Gonzalez 2020

DimeNet: third-order invariants

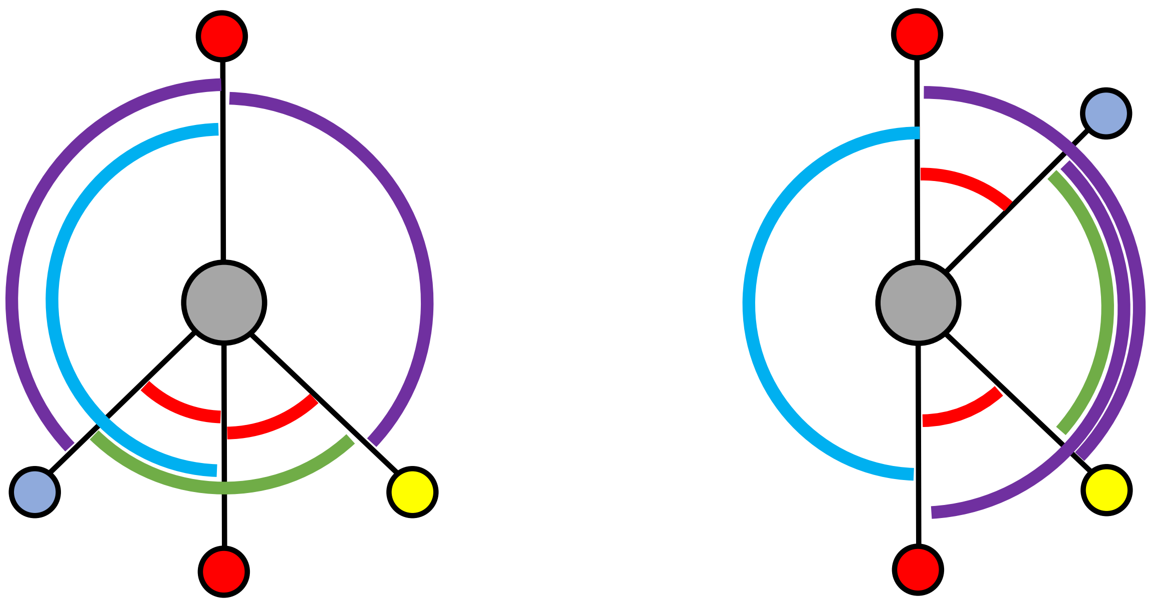


$$\mathbf{s}_i \leftarrow \sum_{j \in \mathcal{N}_i} \phi\left(\mathbf{s}_i, \mathbf{s}_j, d_{ij}, \sum_{j \in \mathcal{N}_i \setminus \{j\}} \psi(\mathbf{s}_j, \mathbf{s}_k, d_{ij}, \measuredangle_{ijk})\right)$$

- Use relative distances (second body order) and angles (third body order)
- Relative distances & angles are invariant to global rotations & translations

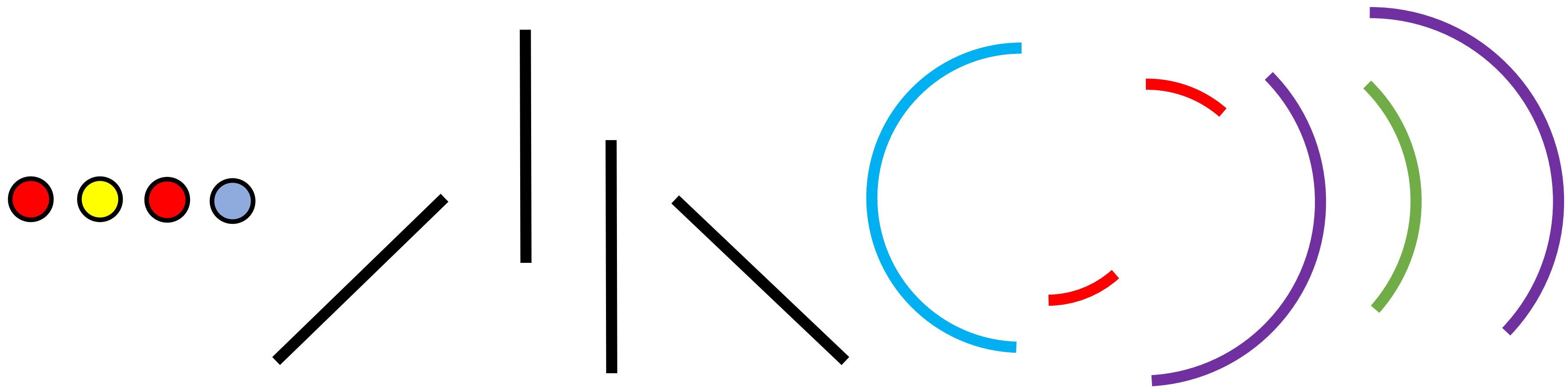
Gasteiger et al. 2020 (DimeNet)

Distinguishing Geometric Graphs



Bartok et al. 2013; Pozdnyakov 2020

Distinguishing Geometric Graphs

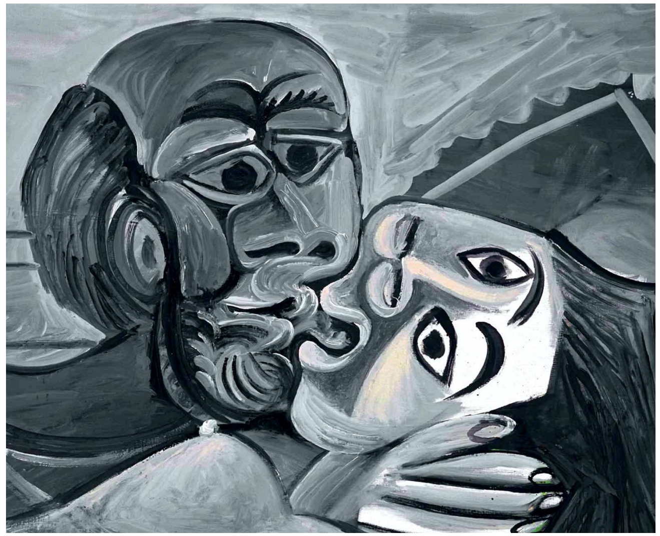


Can these neighbourhoods be distinguished
using unordered set of *distances & angles* only?

Bartok et al. 2013; Pozdnyakov 2020

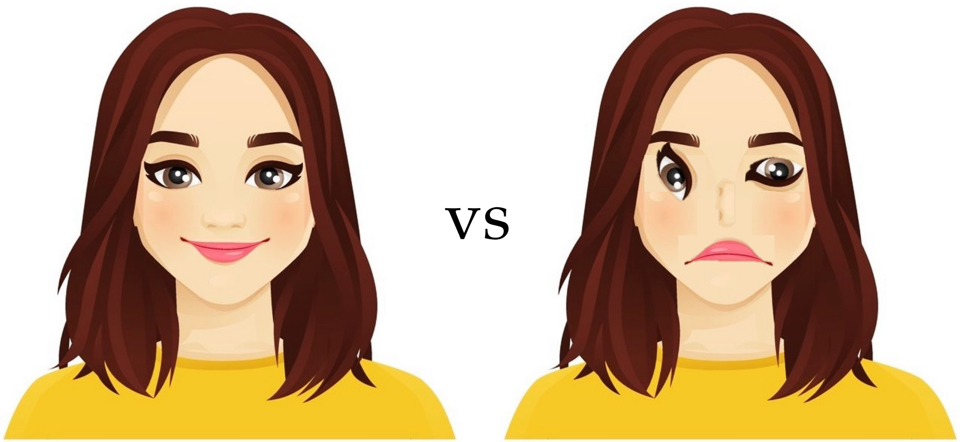
Invariance vs Equivariance

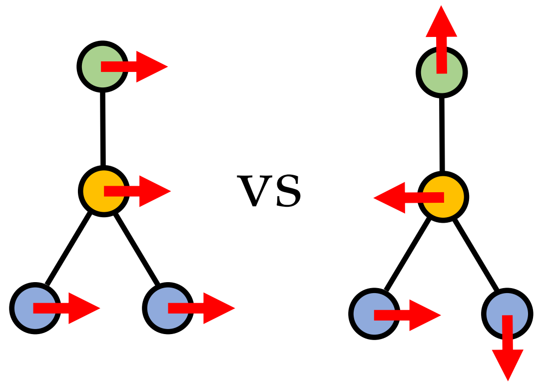
vs



"Picasso phenomenon"

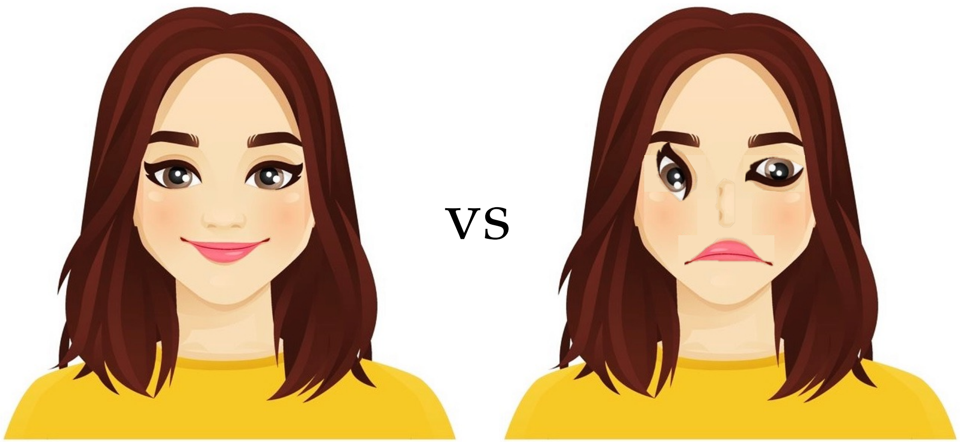
Invariance vs Equivariance

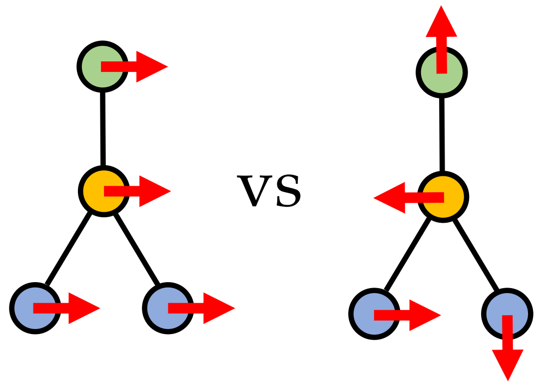




Relative orientations of features are important,
not only their presence!

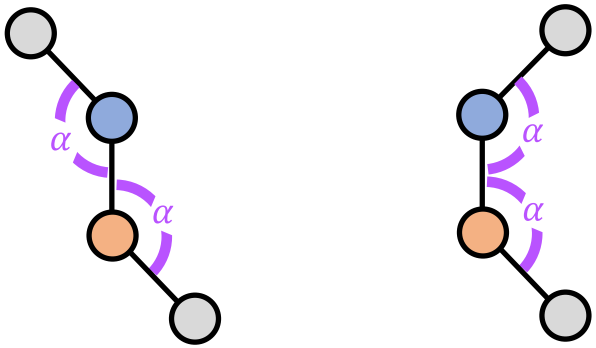
Invariance vs Equivariance



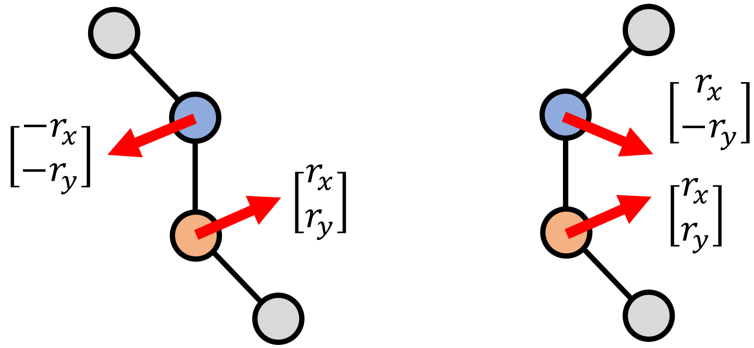


Making invariant predictions may still require solving equivariant sub-tasks

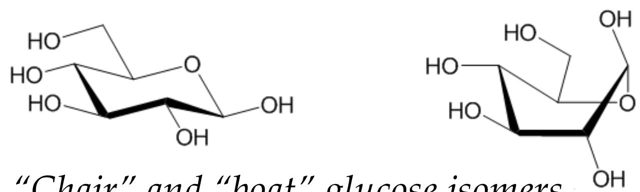
Distinguishing Geometric Graphs



Scalars only cannot distinguish these graphs



We need geometric features representing relative orientations!



"Chair" and "boat" glucose isomers

Schütt et al. 2021

Dichotomy of Geometric GNNs

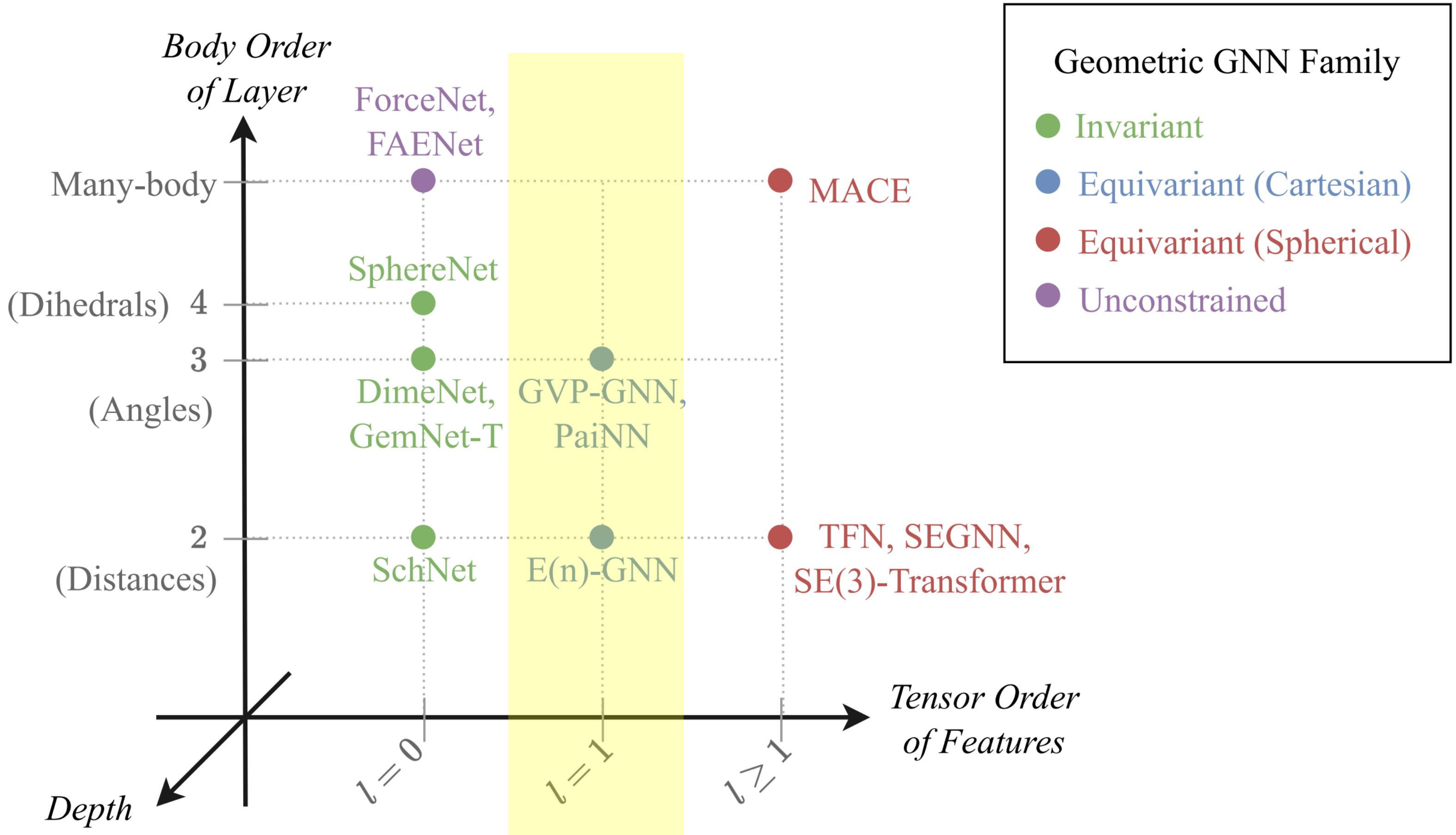
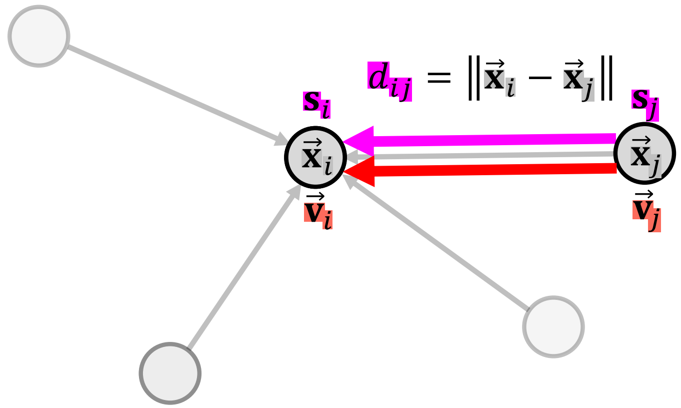


Figure: Duval et al. 2023

“CARTESIAN” EQUIVARIANT GEOMETRIC GNNs

PaiNN: separate message passing for scalars & vectors



$$\mathbf{s}_i \leftarrow \sum_{j \in \mathcal{N}_i} \psi(\mathbf{s}_j, d_{ij}) \qquad \mathbf{v}_i \leftarrow \sum_{j \in \mathcal{N}_i} \phi(\mathbf{s}_j, d_{ij})\mathbf{v}_j + \sum_{j \in \mathcal{N}_i} \phi(\mathbf{s}_j, d_{ij})(\vec{\mathbf{x}}_i - \vec{\mathbf{x}}_j)$$

- Separate update for scalar & vector features
- Not any function is equivariant! Gated nonlinearity (no ReLU), sum, & vector products

Schütt et al. 2021 (PaiNN); also Satorras et al. 2021 (E(n)-GNN); Jing et al. 2020 (GVP-GNN)

Beyond Scalars & Vectors: Tensors

- We have seen that different objects transform differently under rotations ("acted upon by different *representations* of the rotation group")
  - Scalars: $s \to s$
  - Vectors: $\vec{v} \to \mathbf{R}\vec{v}$
- We can also mix features in different ways
  - Scalar-vector: $\vec{w} = s \cdot \vec{v}$
  - Vector-vector: $s = \langle \vec{v}, \vec{w} \rangle$
  - Tensor: $\vec{M} = \vec{v} \otimes \vec{w}$ a matrix with elements $\vec{m}_{ij} = \vec{v}_i \vec{w}_j$, which transforms as

$$\vec{M} \to \mathbf{R}\vec{M}\mathbf{R}^{\mathrm{T}}$$

Note: We have seen this already with graphs. Rotation matrix $\rho(g) = \mathbf{R}$ here is the representation of $g \in SO(3)$. The representation of a tensor product is $(\rho \otimes \rho)(g)\vec{M} = \rho(g)\vec{M}\rho(g)^{\mathrm{T}}$.

Tensor-type features

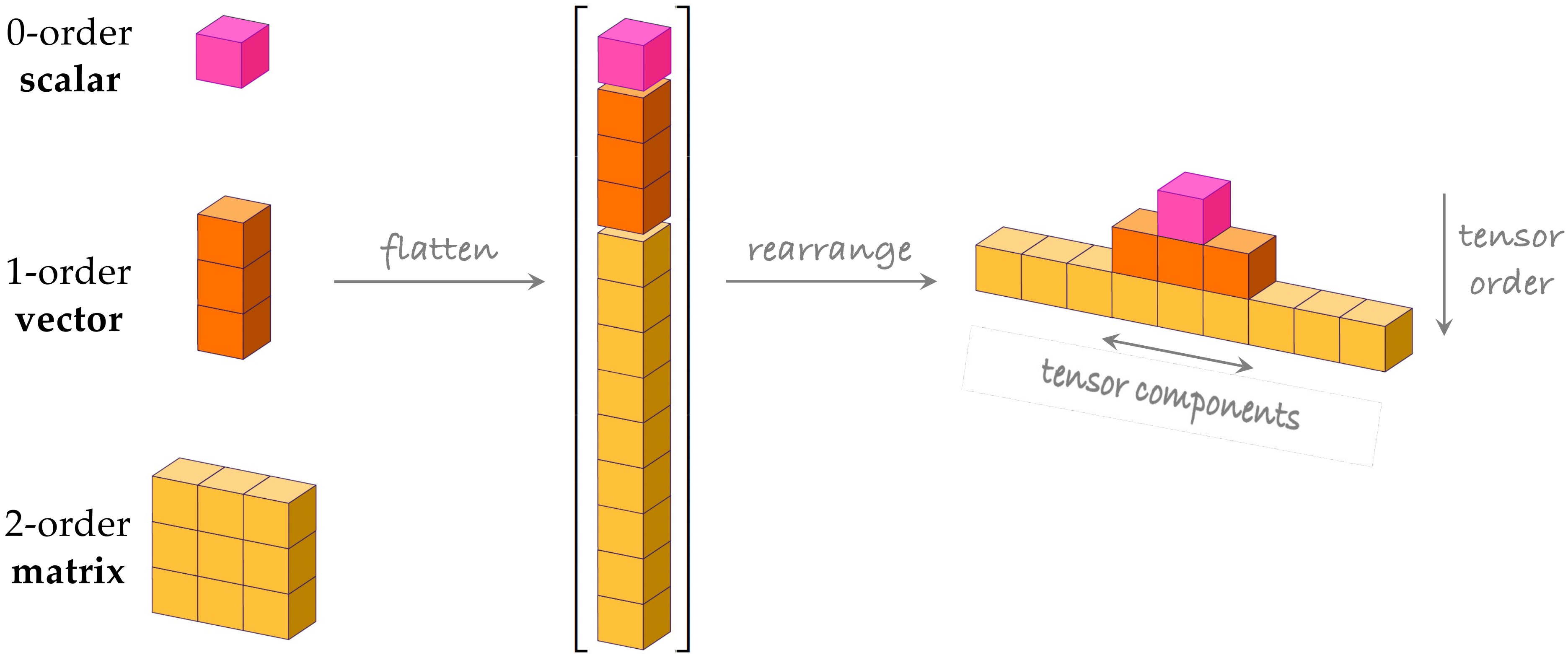
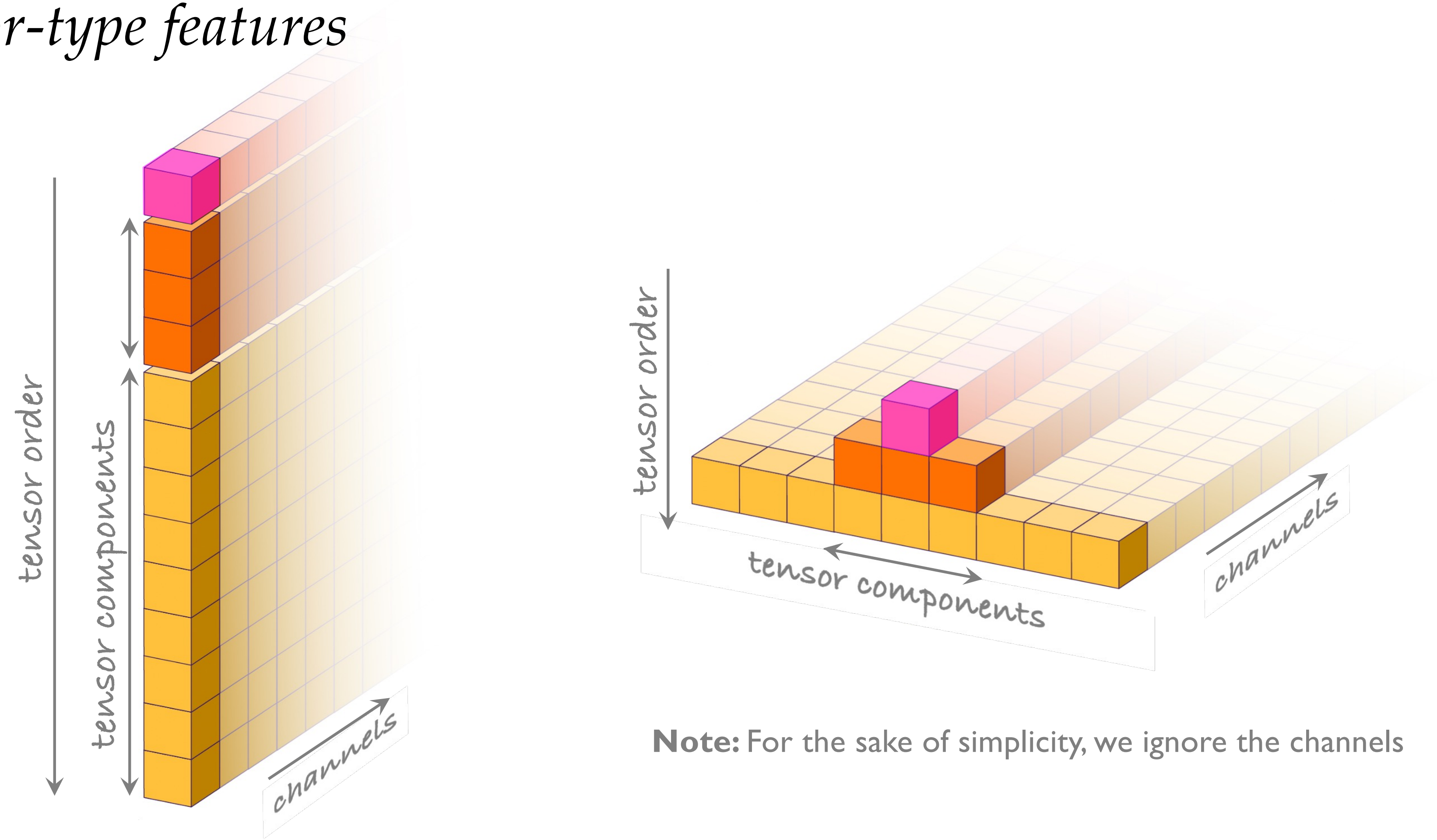


Figure: S. Mathis (from Duval et al. 2023)

Tensor-type features



Note: For the sake of simplicity, we ignore the channels

Figure: S. Mathis (from Duval et al. 2023)

How Tensor-type features transform?

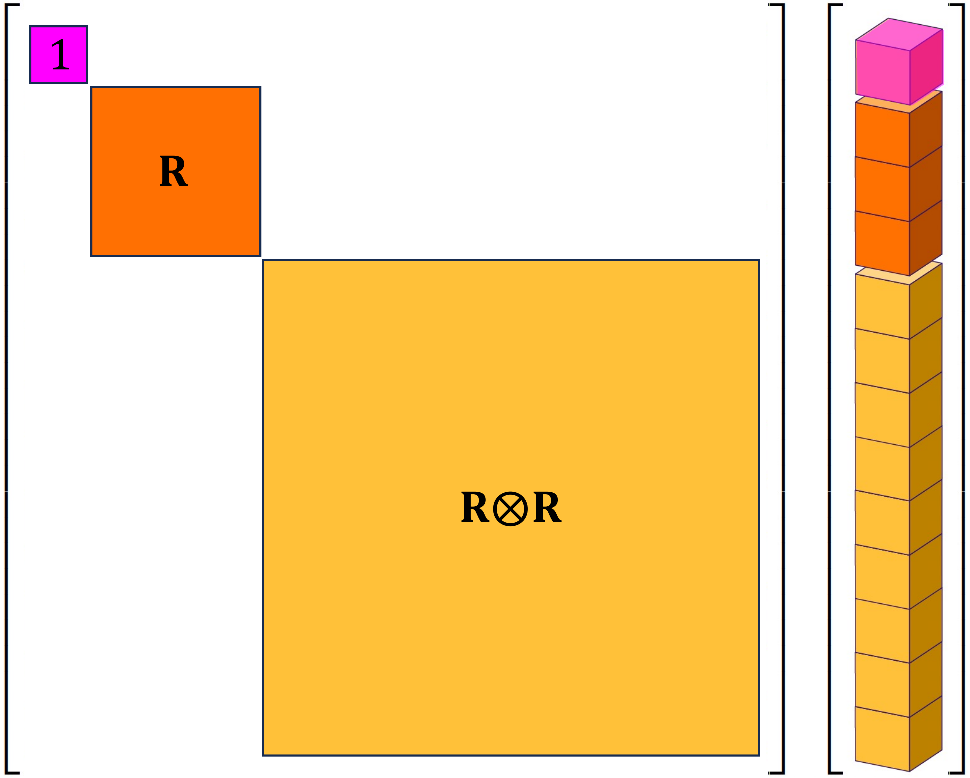


Figure: S. Mathis (from Duval et al. 2023)

IRREDUCIBLE REPRESENTATIONS

Reminder: Group Representations

- A (**linear**) **representation** of group G on a vector space X is group homomorphism
$$\rho\colon G \to \mathrm{GL}(X)$$
- Given representations ρ_X and ρ_Y of G on vector spaces X and Y, respectively, we can construct another representation $(\rho_X \oplus \rho_Y)\colon G \to \mathrm{GL}(X \oplus Y)$. In the finite dimensional case, the representation is a *block-diagonal matrix*
$$g \longmapsto \begin{pmatrix} \rho_X(g) & \\ & \rho_Y(g) \end{pmatrix}$$

Reminder: A **direct sum** of two vector spaces $V \oplus W$ is defined as their Cartesian product with operations carried out coordinate-wise, $(v_1, w_1) + (v_2, w_2) = (v_1 + v_2, w_1 + w_2)$. Roughly, direct sum is a "*concatenation*" of vectors.

Irreducible Representations

- Let $\rho: G \rightarrow \mathrm{GL}(X)$ be a representation of G let $Y \subset X$ be a vector subspace. If for all $g \in G$ and $\mathbf{y} \in Y$ we have $\rho(g)\mathbf{y} \in Y$, we say that Y is an **invariant** (or **stable**) **subspace**.

Note I: In general, $\rho(g)\mathbf{y} \neq \mathbf{y}$. Invariance in this case implies that the action of the group on the subspace remains in the same subspace (hence the term "stable" is more correct).

Note II: For any group, $Y = X$ and $Y = \{0\}$ are **trivial invariant subspaces**.

- A representation with a non-trivial invariant subspace is **reducible**, and one without such a subspace is **irreducible** (also called "**irrep**" for short).

Irreducible Representations

- Given a reducible finite-dimensional representation $\rho: G \to \mathrm{GL}(X)$ with an invariant subspace $Y \subset X$, we can find a change of basis $\mathbf{A}$ to make it upper-triangular:

$$\tilde{\rho}(g) = \mathbf{A}\rho(g)\mathbf{A}^{-1} \longmapsto \begin{pmatrix} \tilde{\rho}_{11}(g) & \tilde{\rho}_{12}(g) \\ & \tilde{\rho}_{22}(g) \end{pmatrix}$$

- A vector of the form $\tilde{\mathbf{y}} = (\mathbf{y} \quad 0)^{\mathrm{T}}$ will remain of this form: $\tilde{\rho}(g)\tilde{\mathbf{y}} = (\tilde{\rho}_{11}(g)\mathbf{y} \quad 0)^{\mathrm{T}}$, i.e., $\tilde{\rho}Y \subseteq Y$.
- If we can make $\tilde{\rho}_{12}(g) = 0$ by a change of basis (i.e., $\rho = \tilde{\rho}_{11} \oplus \tilde{\rho}_{22}$ direct product or a block-diagonal matrix), ρ is **decomposable**, and **indecomposable** otherwise.

Note III: Irreducible representations are always indecomposable, but the converse is not always true. However, with additional assumptions that hold in many important cases (e.g. finite groups with representations over the complex field), the two notions are equivalent.

Diaconis 1988

Some facts about Irreducible Representations

- Irreducible representations are the “Lego block” of Representation Theory: any representation of a group can be written as a direct sum (“block diagonal matrix”) of the group’s irreducible representations.
- The irreducible representations of the groups of interest to use are well-known.
- Any 1-dimensional representation is irreducible.
- Any group has a 1-dimensional irreducible trivial representation.
- Abelian (commutative) groups have 1-dimensional (complex) irreducible representations.

Diaconis 1988

Example: Irreducible Representations of Permutations S_n

- *Trivial representation*: identity $\rho(\pi) = 1$ (1D)
- *Alternating representation*: the sign of the permutation $\rho(\pi) = \text{sign}(\pi)$ (1D)
- S_3 has *2D irreducible representations* (shared with dihedral group $D_3 \cong S_3$):

$$\rho(I) = \begin{bmatrix} 1 & \\ & 1 \end{bmatrix} \qquad \rho(R) = \begin{bmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{bmatrix} \qquad \rho(R^2) = \begin{bmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{bmatrix}$$

$$\rho(F) = \begin{bmatrix} -1 & \\ & 1 \end{bmatrix} \qquad \rho(FR) = \begin{bmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{bmatrix} \qquad \rho(FR^2) = \begin{bmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{bmatrix}$$

Note: Our usual representation of $n{\times}n$ permutation matrices is *reducible*. To see this, recall that permutation matrices are bi-stochastic ($\mathbf{P1} = \mathbf{1}$), i.e., the subspace of vectors with constant elements is invariant.

Diaconis 1988

Example: Irreducible Representations of Z_n

- Z_n is an abelian group, hence all irreducible representations are 1-dimensional
- Any ρ is determined by the image of 1 (unit shift):

$$\rho(k) = \rho(1)^k$$
$$\rho(1)^n = 1$$

  implying that $\rho(1)$ must be an nth root of unity: $e^{\mathrm{i}\frac{2\pi}{n}j}$

- Irreducible representations are $\rho_j(k) = e^{\mathrm{i}\frac{2\pi}{n}jk}$. We already know them from the previous lecture on **Discrete Fourier Transforms**!

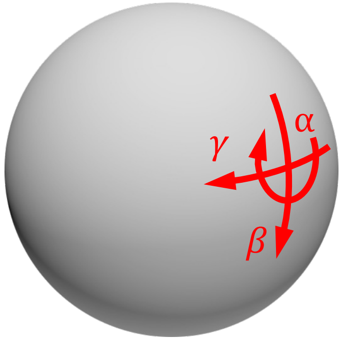
Diaconis 1988

Example: Irreducible Representations of $\mathrm{SO}(3)$

- *Trivial representation*: identity $\rho = 1$
- 3×3 *rotation matrices*

$$\mathbf{R}_{\alpha\beta\gamma} = \begin{bmatrix} \cos\alpha\cos\gamma - \sin\alpha\cos\beta\sin\gamma & \sin\beta\sin\gamma & \cos\alpha\cos\beta\sin\gamma + \sin\alpha\cos\gamma \\ \sin\alpha\sin\beta & \cos\beta & -\cos\alpha\sin\beta \\ -\sin\alpha\cos\beta\cos\gamma - \cos\alpha\sin\gamma & \sin\beta\cos\gamma & \cos\alpha\cos\beta\cos\gamma - \sin\alpha\sin\gamma \end{bmatrix}$$

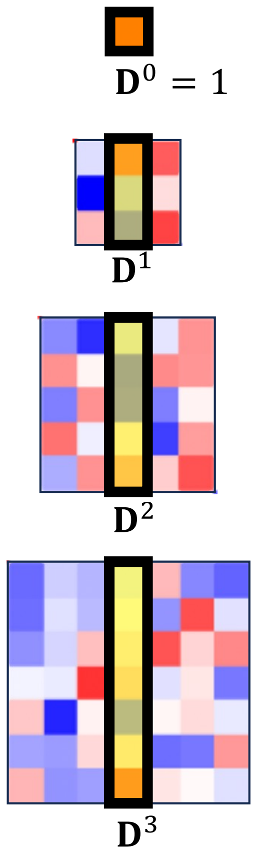
parameterised through *Euler angles* α, β, γ



$S^2 \cong \mathrm{SO}(3)/\mathrm{SO}(2)$

Example: Irreducible Representations of SO(3)

- *Trivial representation*: identity $\rho = 1$
- 3×3 *rotation matrices*
- General case: $(2l+1)\times(2l+1)$ *Wigner D-matrices* $\mathbf{D}^l$ of degree l
  - Elements $\mathbf{D}^l_{mn}$ indexed on $m, n = -l, \ldots, +l$
  - Functions $\mathbf{D}^l_{mn}\colon \mathrm{SO}(3) \to \mathbb{C}$ ("*Wigner D-functions*") form an *orthonormal basis* for $L_2(\mathrm{SO}(3))$
  - Central columns $\mathbf{D}^l_{m0}$ are invariant to rotations around a chosen axis ($\mathbf{D}^l_{m0}(\mathbf{R}\mathbf{R}_\alpha) = \mathbf{D}^l_{m0}(\mathbf{R})$) and can be thought of functions on the sphere $S^2 \cong \mathrm{SO}(3)/\mathrm{SO}(2)$ called **spherical harmonics** $Y^l_m\colon S^2 \to \mathbb{C}$ and forming an *orthonormal basis* for $L_2(S^2)$.



Wigner "*Darstellung*" ("representation") matrices

Wigner 1927; D-matrices image: E. Bekkers

FOURIER ANALYSIS ON GROUPS

Convolution on Finite Groups

- Let G be a finite group and $f, \varphi: G \to \mathbb{C}$ functions on the group.
- **Convolution** of f with φ (not necessarily symmetric!)

$$(f \star \varphi)(g) = \sum_{h \in G} f(gh^{-1})\varphi(h)$$

Diaconis 1988

Fourier Transform on Finite Groups

- Let G be a finite group with a d-dimensional representation $\rho: G \to \mathrm{GL}(X)$ on X. Let $f: G \to \mathbb{C}$ a function on the group.

- **Fourier transform** of f (*at the representation* ρ):

$$\hat{f}(\rho) = \sum_{g \in G} f(g)\rho(g)$$

$d \times d$ matrix (not necessarily invertible!)

Diaconis 1988

Fourier Transform on Finite Groups

- Let G be a finite group with a d-dimensional representation $\rho: G \to \mathrm{GL}(X)$ on X. Let $f: G \to \mathbb{C}$ a function on the group.

- **Fourier transform** of f (*at the representation* ρ):

$$\hat{f}(\rho) = \sum_{g \in G} f(g)\rho(g)$$

Convolution Theorem: $(\widehat{f \star \varphi})(\rho) = \hat{f}(\rho)\hat{\varphi}(\rho)$

Exercise: Prove.

Diaconis 1988

Fourier Transform on Finite Groups

- Let G be a finite group with irreducible representations $\rho_1, \ldots, \rho_k$ on $X_1, \ldots, X_k$. Let $f: G \to \mathbb{C}$ a function on the group.

- **Fourier transform** of f (*at the representation* ρ_j):

$$\hat{f}(\rho_j) = \sum_{g \in G} f(g)\rho_j(g)$$

- **Inverse Fourier transform**:

$$f(g) = \frac{1}{|G|}\sum_{j=1}^{k} \dim(X_j)\,\mathrm{tr}\left(\rho_j(g^{-1})\hat{f}(\rho_j)\right)$$

Diaconis 1988

Fourier Transform on Finite Abelian Groups

- Let G be a finite abelian group with 1-dimensional irreducible representations $\rho_1, \dots, \rho_k$. Let $f: G \to \mathbb{C}$ a function on the group.
- **Fourier transform** of f (*at the representation* ρ_j):

$$\hat{f}(\rho_j) = \sum_{g \in G} f(g)\rho_j(g)$$

- **Inverse Fourier transform**:

$$f(g) = \frac{1}{|G|}\sum_{j=1}^{k} \rho_j(g^{-1})\hat{f}(\rho_j)$$

Diaconis 1988

Fourier Transform on Z_n: the "classical" DFT

- Let $G = Z_n$ (integers mod n). It is an abelian group with irreducible representations $\rho_j(k) = \mathrm{e}^{\mathrm{i}\frac{2\pi}{n}jk}$ for $j, k = 0, \dots, n-1$. Let $f: Z_n \to \mathbb{C}$ a function on the group.
- **Fourier transform** of f:

$$\hat{f}(\rho_j) = \sum_{k=0}^{n-1} f(k)\mathrm{e}^{\mathrm{i}\frac{2\pi}{n}jk}$$

- **Inverse Fourier transform**:

$$f(k) = \frac{1}{n}\sum_{j=0}^{n-1} \mathrm{e}^{-\mathrm{i}\frac{2\pi}{n}jk}\hat{f}(\rho_j)$$

Diaconis 1988

Fourier Transform on $\mathrm{SO}(3)$*: Wigner D-functions*

- Let $G = \mathrm{SO}(3)$. Its irreducible representations are the Wigner D-matrices $\rho_l(\mathbf{R}) = \mathbf{D}^l(\mathbf{R})$. Let $f: \mathrm{SO}(3) \to \mathbb{C}$ a function on the group. Then, we can express it as

$$f(\mathbf{R}) = \sum_l \mathrm{tr}\left(\mathbf{D}^l(\mathbf{R}^{-1})\hat{f}(\rho_l)\right)$$

Note: $\mathrm{SO}(3)$ is a *continuous* group and the definitions of the Fourier transform are different from the finite case (e.g. sum has to be replaced by the integral $\hat{f}(\rho_l) = \int_{\mathrm{SO}(3)} f(g)\rho_l(g)\mathrm{d}g$ w.r.t. Haar measure). We are not going into the full details here.

Diaconis 1988

Fourier Transform on $\mathrm{SO}(3)$*: Wigner D-functions*

- Let $G = \mathrm{SO}(3)$. Its irreducible representations are the Wigner D-matrices $\rho_l(\mathbf{R}) = \mathbf{D}^l(\mathbf{R})$. Let $f: \mathrm{SO}(3) \rightarrow \mathbb{C}$ a function on the group. Then, we can express it w.r.t. the orthogonal (Fourier) basis of the Wigner D-functions $\mathbf{D}^l_{mn}$

$$f(\mathbf{R}) = \sum_{l} \sum_{m,n=-l}^{+l} \mathbf{D}^l_{mn}(\mathbf{R}) \hat{f}^l_{mn}$$

Note: $\mathrm{SO}(3)$ is a *continuous* group and the definitions of the Fourier transform are different from the finite case (e.g. sum has to be replaced by the integral $\hat{f}(\rho_l) = \int_{\mathrm{SO}(3)} f(g)\rho_l(g)\mathrm{d}g$ w.r.t. Haar measure). We are not going into the full details here.

Diaconis 1988

“SPHERICAL” EQUIVARIANT GEOMETRIC GNNs

Dichotomy of Geometric GNNs

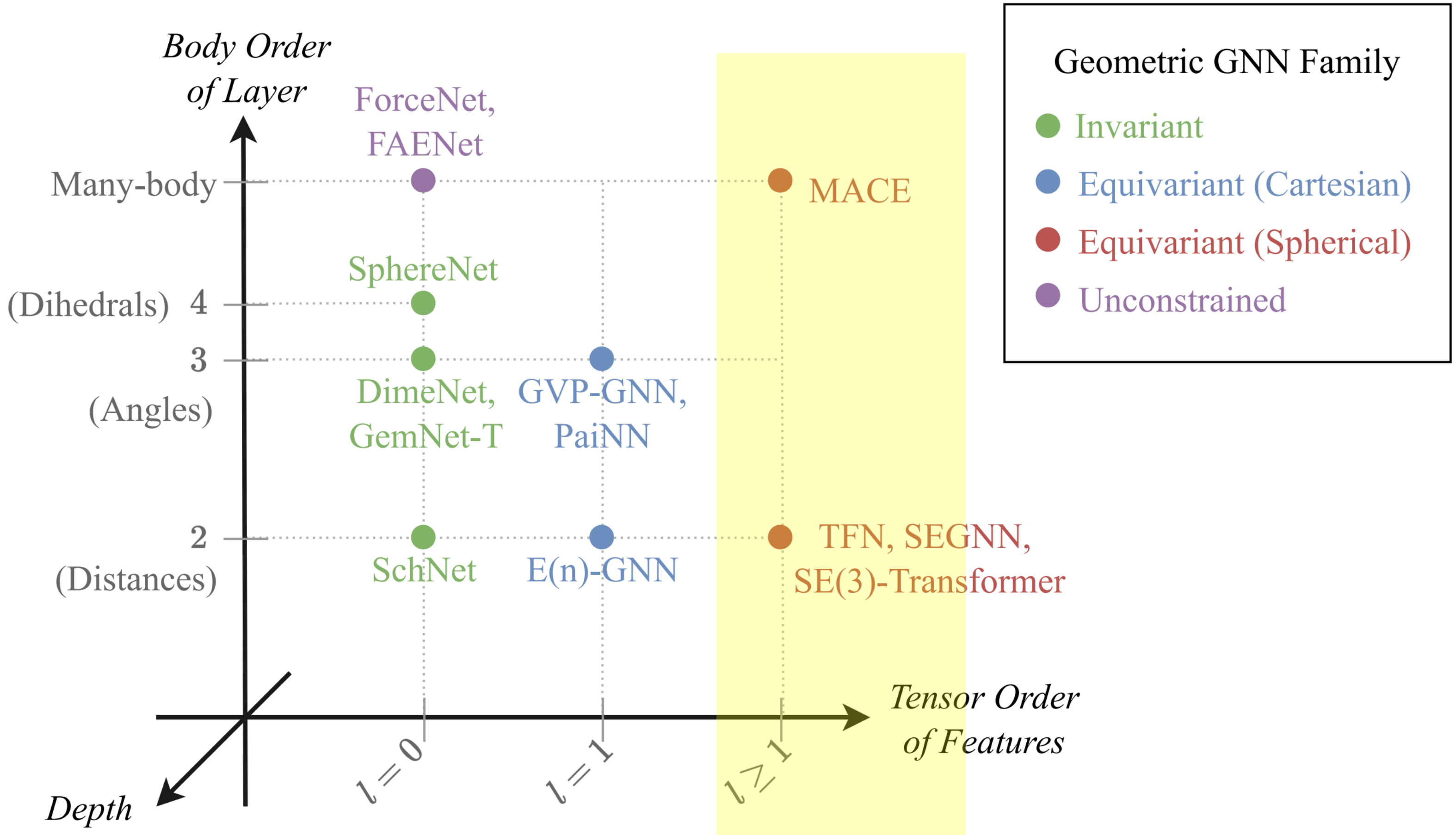


Figure: Duval et al. 2023

From Cartesian to Spherical Tensors

$$\vec{M} = \begin{bmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{bmatrix}$$

$$= m_{11}\begin{bmatrix} 1 & & \\ & & \\ & & \end{bmatrix} + m_{12}\begin{bmatrix} & 1 & \\ & & \\ & & \end{bmatrix} + m_{13}\begin{bmatrix} & & 1 \\ & & \\ & & \end{bmatrix} + \ \dots + m_{33}\begin{bmatrix} & & \\ & & \\ & & 1 \end{bmatrix}$$

Duval et al. 2023

From Cartesian to Spherical Tensors

$$\vec{M} = \begin{bmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{bmatrix}$$

$$= \frac{m_{11} + m_{22} + m_{33}}{3} \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix}$$

$$+ \frac{m_{23} - m_{32}}{2} \begin{bmatrix} & & \\ & & 1 \\ & -1 & \end{bmatrix} + \frac{m_{13} - m_{31}}{2} \begin{bmatrix} & & 1 \\ & & \\ -1 & & \end{bmatrix} + \frac{m_{12} - m_{21}}{2} \begin{bmatrix} & 1 & \\ -1 & & \\ & & \end{bmatrix}$$

$$+ \frac{2m_{11} - m_{22} - m_{33}}{3} \begin{bmatrix} 1 & & \\ & -1 & \\ & & \end{bmatrix} + \frac{m_{12} + m_{21}}{2} \begin{bmatrix} & 1 & \\ 1 & & \\ & & \end{bmatrix} + \frac{m_{13} + m_{31}}{2} \begin{bmatrix} & & 1 \\ & & \\ 1 & & \end{bmatrix}$$

$$+ \frac{m_{23} + m_{32}}{2} \begin{bmatrix} & & \\ & & 1 \\ & 1 & \end{bmatrix} + \frac{2m_{33} - m_{11} - m_{22}}{3} \begin{bmatrix} & & \\ & -1 & \\ & & 1 \end{bmatrix}$$

Duval et al. 2023

From Cartesian to Spherical Tensors

$$\vec{M} = \begin{bmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{bmatrix}$$

$$= \mu_1 \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix}$$

$$+\mu_2 \begin{bmatrix} & & \\ & & 1 \\ & -1 & \end{bmatrix} + \mu_3 \begin{bmatrix} & & 1 \\ & & \\ -1 & & \end{bmatrix} + \mu_4 \begin{bmatrix} & 1 & \\ -1 & & \\ & & \end{bmatrix}$$

$$+\mu_5 \begin{bmatrix} 1 & & \\ & -1 & \\ & & \end{bmatrix} + \mu_6 \begin{bmatrix} & 1 & \\ 1 & & \\ & & \end{bmatrix} + \mu_7 \begin{bmatrix} & & 1 \\ & & \\ 1 & & \end{bmatrix} + \mu_8 \begin{bmatrix} & & \\ & & 1 \\ & 1 & \end{bmatrix} + \mu_9 \begin{bmatrix} & & \\ & -1 & \\ & & 1 \end{bmatrix}$$

Duval et al. 2023

From Cartesian to Spherical Tensors

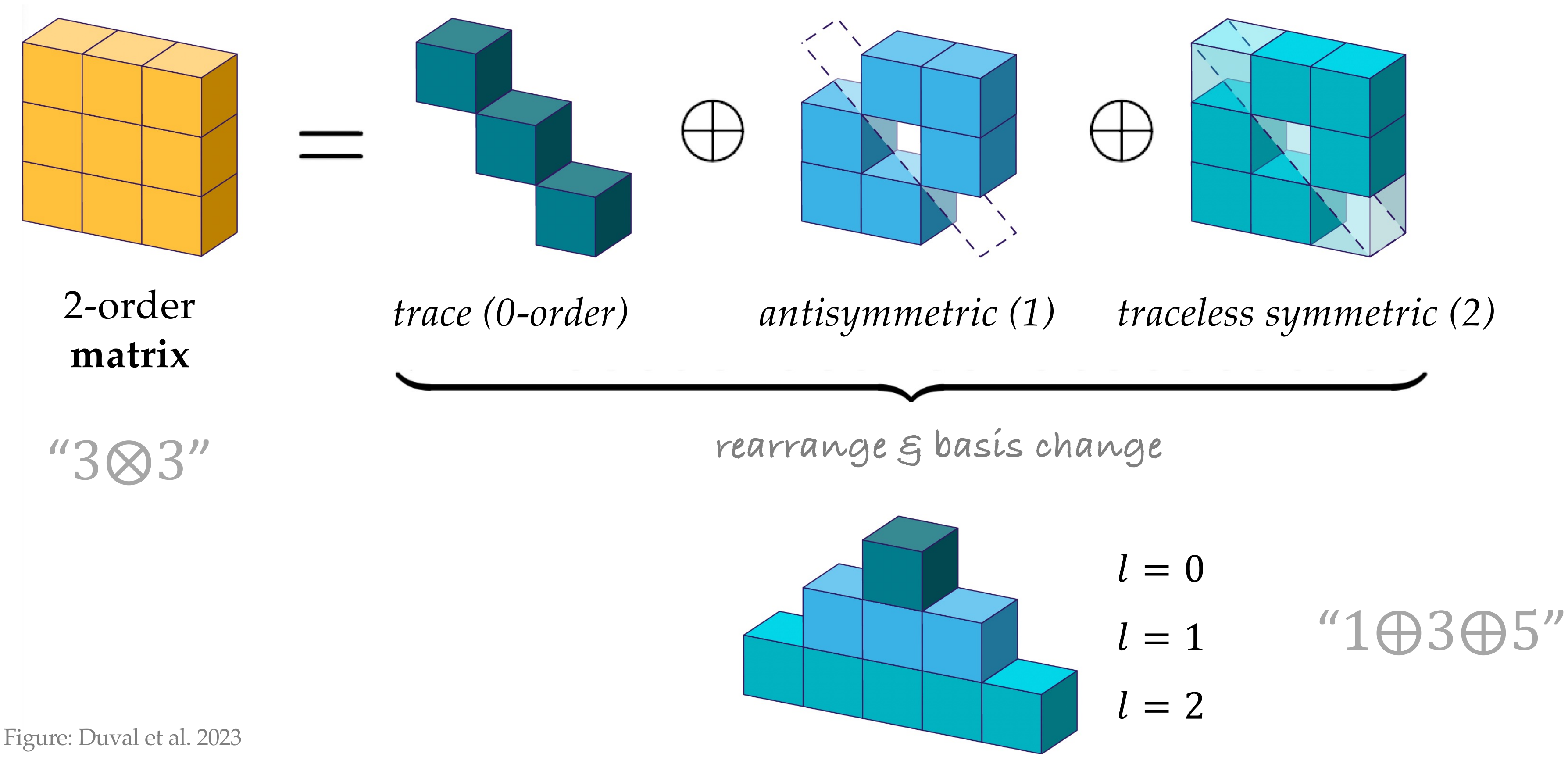
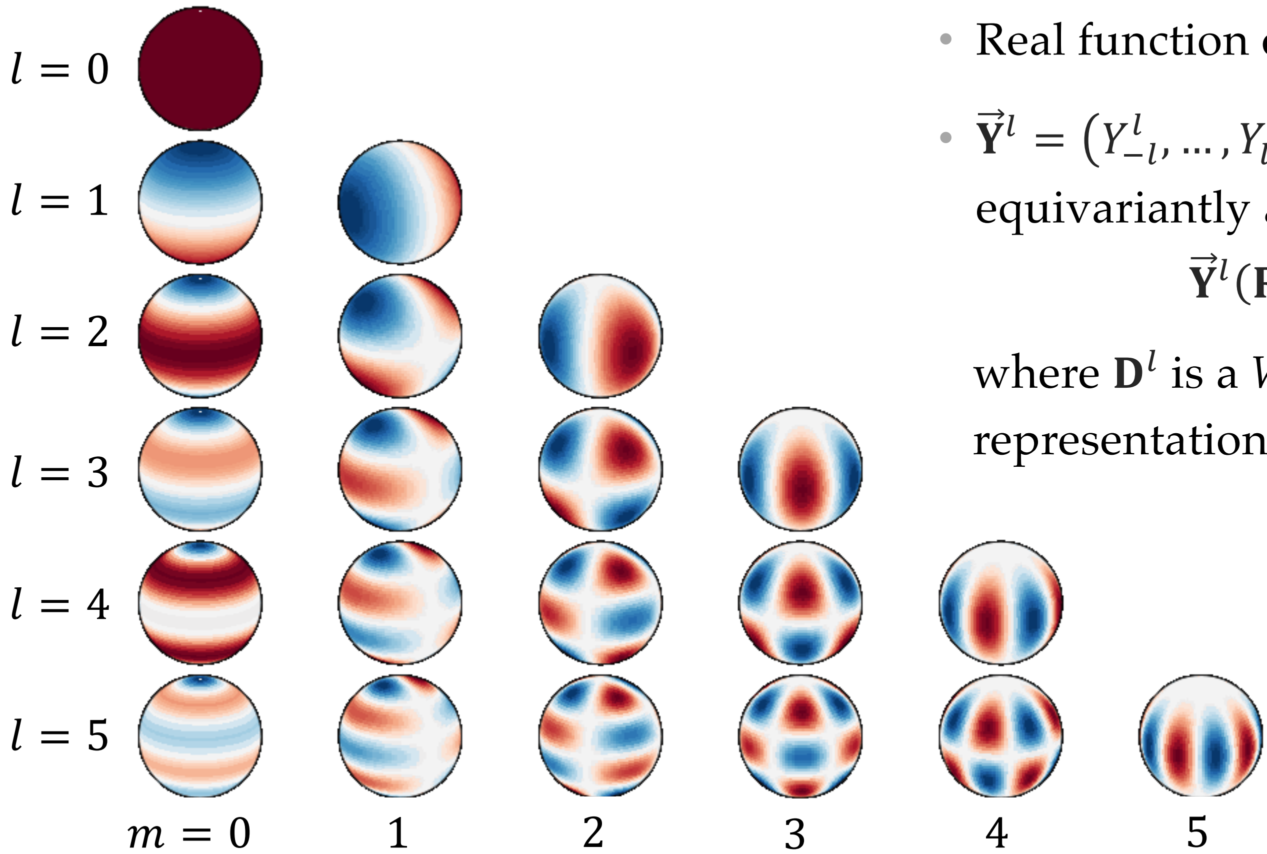


Figure: Duval et al. 2023

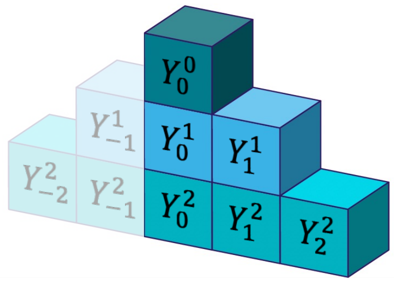
Spherical Harmonics



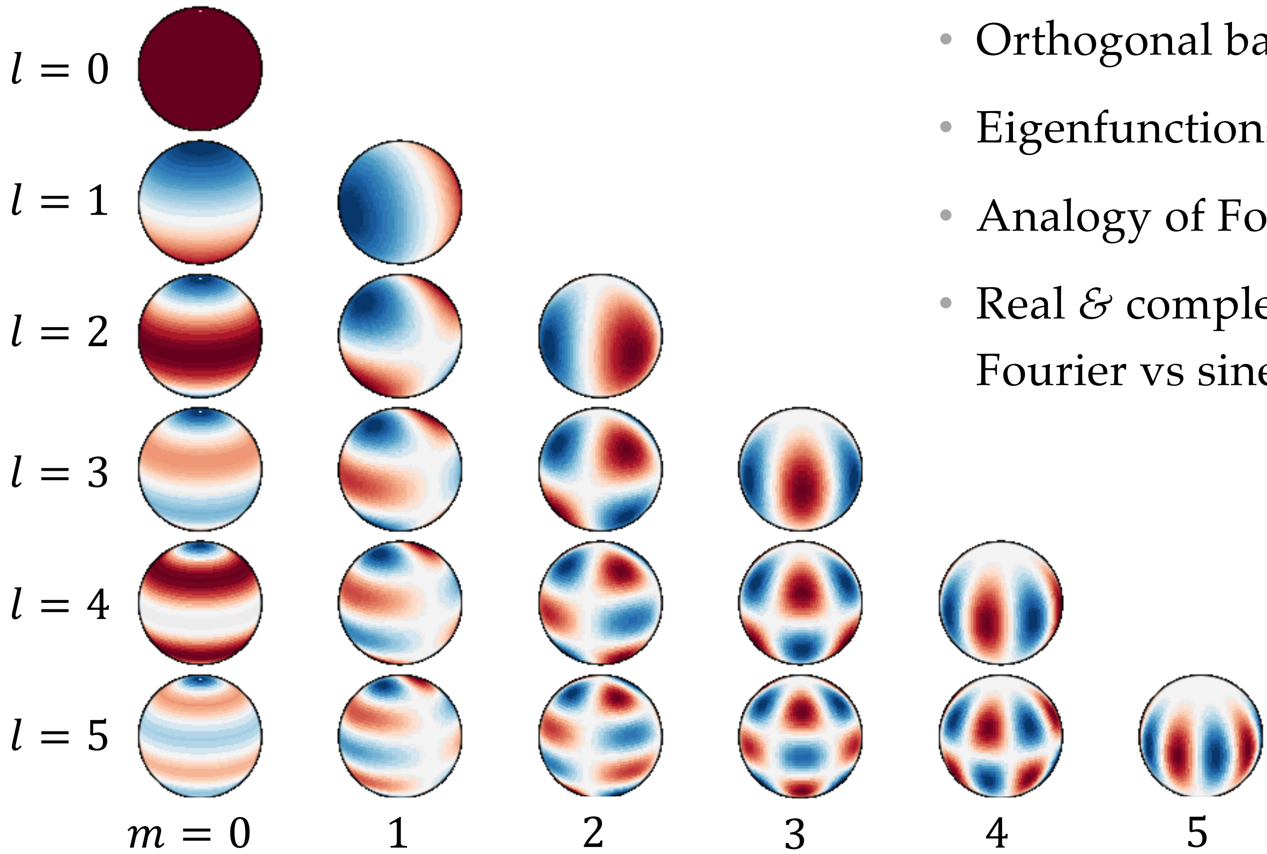
- Real function on the sphere $Y_m^l : S^2 \to \mathbb{R}$
- $\vec{\mathbf{Y}}^l = \left(Y_{-l}^l, \dots, Y_l^l\right) : S^2 \to \mathbb{R}^{2l+1}$ transforms equivariantly as

$$\vec{\mathbf{Y}}^l(\mathbf{R}\hat{\mathbf{v}}) = \mathbf{D}^l(\mathbf{R})\vec{\mathbf{Y}}(\hat{\mathbf{v}})$$

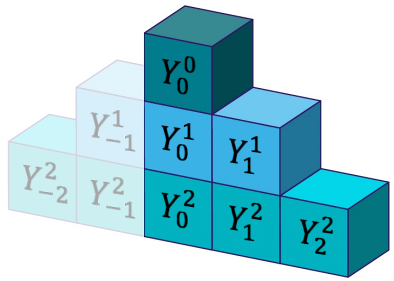
  where $\mathbf{D}^l$ is a *Wigner D-matrix*, irreducible representation of the group $\mathrm{SO}(3)$



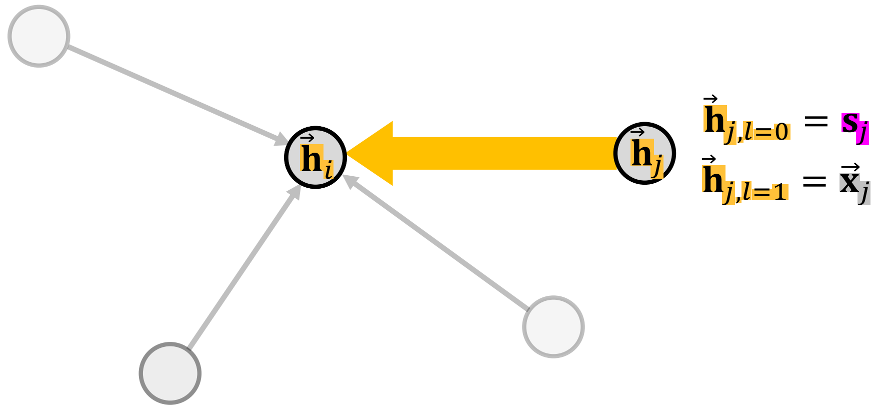
Spherical Harmonics



- Orthogonal basis on the sphere S^2
- Eigenfunctions of the spherical Laplacian
- Analogy of Fourier transform
- Real & complex versions (compare to Fourier vs sine / cosine transforms)



Tensor Field Networks

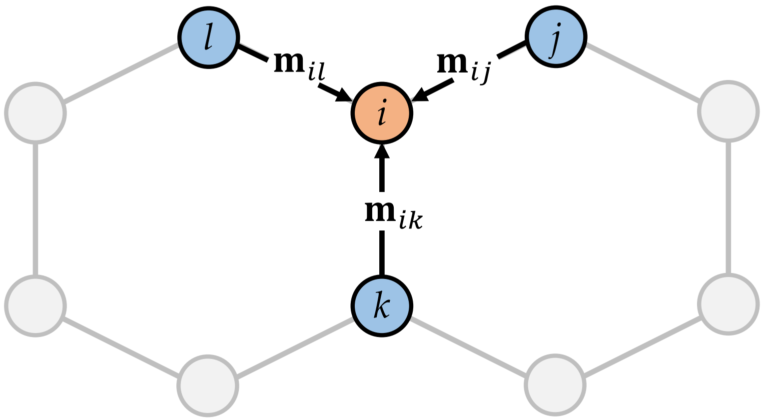


$$\vec{\mathbf{h}}_i \leftarrow \vec{\mathbf{h}}_i + \sum_{j \in \mathcal{N}_i} \vec{Y}\left(\frac{\vec{\mathbf{x}}_j - \vec{\mathbf{x}}_i}{\|\vec{\mathbf{x}}_j - \vec{\mathbf{x}}_i\|}\right) \otimes_{\mathbf{w}} \vec{\mathbf{h}}_j \qquad \mathbf{w} = \phi\left(\mathbf{s}_j, \|\vec{\mathbf{x}}_i - \vec{\mathbf{x}}_j\|\right)$$

- Use higher-order tensors as node features
- Update via tensor products of neighbours & SH expansion of displacement

Thomas et al. 2018 (TFN); also Brandstetter et al. 2022 (SEGNN); Batatia et al. 2022 (MACE); Geiger & Smidt 2022 (E3NN)

Multi-Atomic Cluster Expansion (MACE)

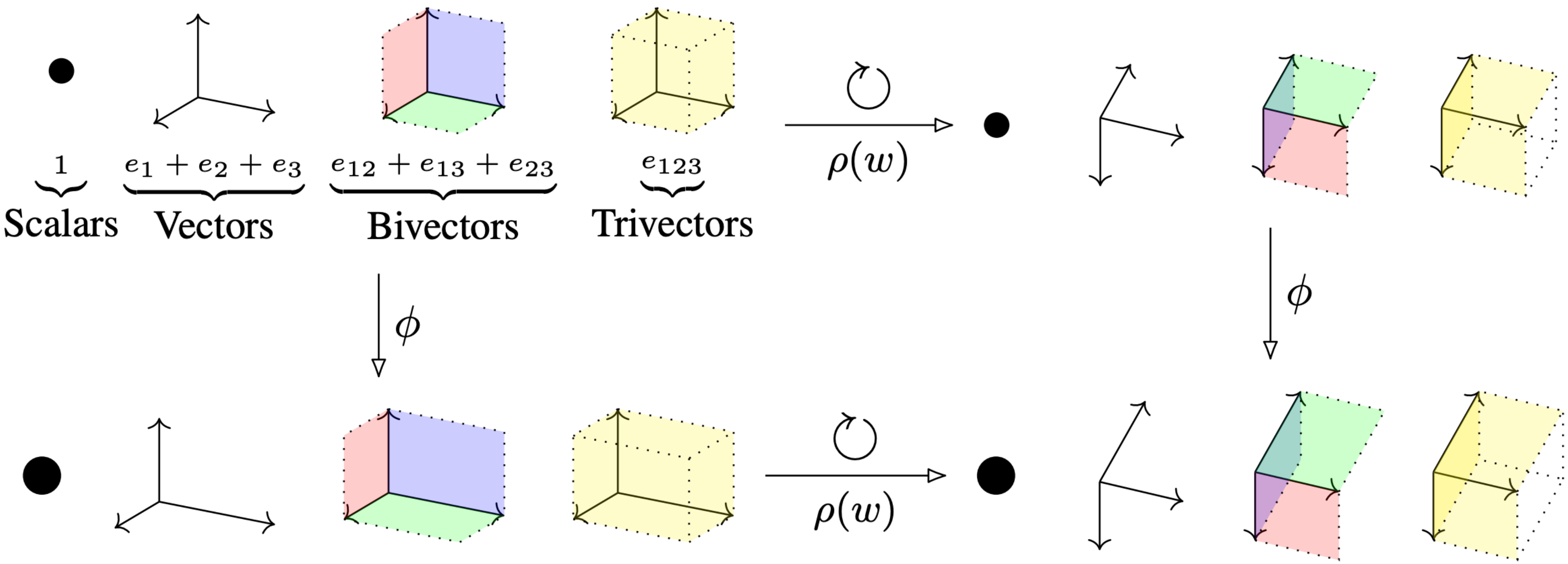


$$\mathbf{m}_i = \sum_{p \in \mathcal{N}_i} \mathbf{m}_{ip} \qquad \mathbf{m}_i^2 = \mathbf{m}_{ij}^2 + \mathbf{m}_{ik}^2 + \mathbf{m}_{il}^2 + 2\underbrace{\left(\mathbf{m}_{ij}\mathbf{m}_{ik} + \mathbf{m}_{ij}\mathbf{m}_{il} + \mathbf{m}_{il}\mathbf{m}_{ik}\right)}_{\text{implicit 3-body terms}}$$

- Take tensors products of aggregated message with itself to obtain many-body features

Batatia et al. 2022 (MACE)

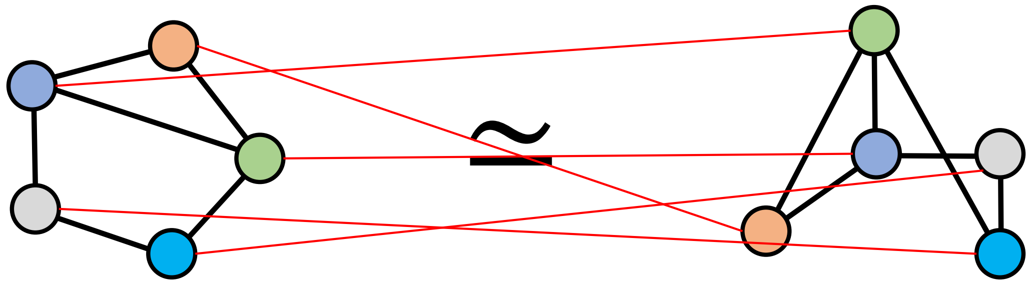
Clifford Group Equivariant GNNs



Ruhe et al. 2023

EXPRESSIVE POWER OF GEOMETRIC GNNs

Graph Isomorphism

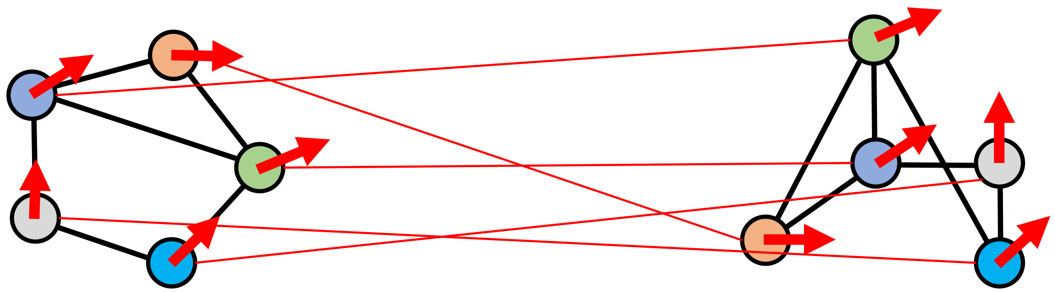


$\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{S})$ $\simeq$ $\mathcal{G}' = (\mathcal{V}', \mathcal{E}', \mathbf{S}')$

- Two graphs with scalar node attributes $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{S})$ and $\mathcal{G}' = (\mathcal{V}', \mathcal{E}', \mathbf{S}')$ are **isomorphic** ($\mathcal{G} \simeq \mathcal{G}'$) if there exists a *bijection* $\varphi: \mathcal{V} \to \mathcal{V}'$ s.t.
- *Structure preservation:* $u{\sim}v$ in $\mathcal{G}$ iff $\varphi(u){\sim}\varphi(v)$ in $\mathcal{G}'$
- *Scalar feature preservation:* $\mathbf{s}_{\boldsymbol{u}} = \mathbf{s}'_{\varphi(\boldsymbol{u})}$

WL test is a necessary condition for isomorphism

Geometric Graph Isomorphism



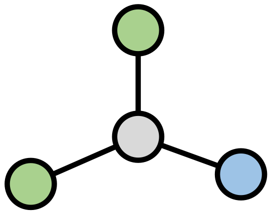
$\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{S}, \vec{\mathbf{X}}, \vec{\mathbf{V}})$ $\qquad\qquad$ $\mathcal{G}' = (\mathcal{V}', \mathcal{E}', \mathbf{S}', \vec{\mathbf{X}}', \vec{\mathbf{V}}')$

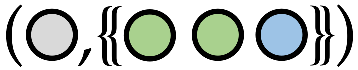
- Two graphs with scalar, positional, and geometric node attributes $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{S}, \vec{\mathbf{X}}, \vec{\mathbf{V}})$ and $\mathcal{G}' = (\mathcal{V}', \mathcal{E}', \mathbf{S}', \vec{\mathbf{X}}', \vec{\mathbf{V}}')$ are **geometrically isomorphic** if there exists a *bijection* $\varphi: \mathcal{V} \to \mathcal{V}'$ s.t.
- *Structure preservation:* $u \sim v$ in $\mathcal{G}$ iff $\varphi(u) \sim \varphi(v)$ in $\mathcal{G}'$
- *Scalar feature preservation:* $\mathbf{s}_{\boldsymbol{u}} = \mathbf{s}'_{\varphi(\boldsymbol{u})}$
- *Pos & geometric feature preservation:* $\vec{\mathbf{x}}_{\boldsymbol{u}} = \mathbf{R}\vec{\mathbf{x}}'_{\varphi(\boldsymbol{u})} + \mathbf{t}$ and $\vec{\mathbf{v}}_{\boldsymbol{u}} = \mathbf{R}\vec{\mathbf{v}}'_{\varphi(\boldsymbol{u})}$ up to some $\mathbf{R}, \mathbf{t}$

Joshi et al. 2023

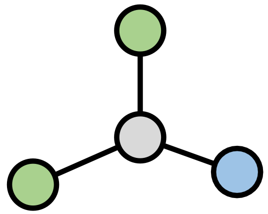
Extending Weisfeiler-Lehman to Geometric Graphs

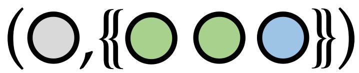
Standard WL



- **Neighbourhood:** set of *invariant* scalar features
- **Node colouring:** unique for every neighbourhood type 

Geometric WL

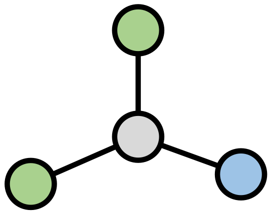


- **Neighbourhood:** set of *invariant* scalar + *equivariant* positional & geometric features
- **Node colouring:** unique for every neighbourhood type 
- **Geometric information:** relative neighbourhood orientation

Joshi et al. 2023

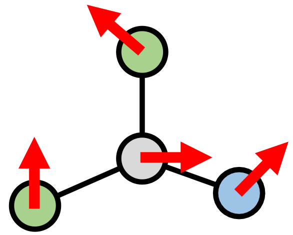
Extending Weisfeiler-Lehman to Geometric Graphs

Standard WL



- **Neighbourhood:** set of *invariant* scalar features
- **Node colouring:** unique for every neighbourhood type $(\bigcirc, \{\{\bigcirc\ \bigcirc\ \bigcirc\}\})$

Geometric WL



- **Neighbourhood:** set of *invariant* scalar + *equivariant* positional *&* geometric features
- **Node colouring:** unique for every neighbourhood type $(\bigcirc, \{\{\bigcirc\ \bigcirc\ \bigcirc\}\})$
- **Geometric information:** relative neighbourhood orientation

Joshi et al. 2023

Takeways

- Geometric Graphs are embedded in the Euclidean space and acted upon by (subgroups of) the Euclidean group
- Different types of features (scalars, vectors, tensors) transform differently under rotation and must be treated differently in message passing
- Geometric GNNs
  - Invariant: limited expressivity
  - Equivariant: distinguish larger classes of graphs, propagate geometric information beyond the local neighbourhood
- Spherical Harmonics are a spherical version of the Fourier Transform and an irreducible representation of the group $SO(3)$

Key Concepts

- Geometric Graphs
- Geometric Vectors & Tensors
- Irreducible Representations
- Convolution & Fourier Transform on a group
- Spherical Harmonics & Wigner D-matrices

Main References

- A. Duval et al., A Hitchhiker's guide to Geometric GNNs for 3D atomic systems, arXiv:2312.07511, 2021. Survey on Geometric GNNs and their mathematical foundations
- P. Diaconis, Group Representation in Probability and Statistics, 1988. Textbook on representation theory