

Reducing Symmetry Increase in Equivariant Neural Networks

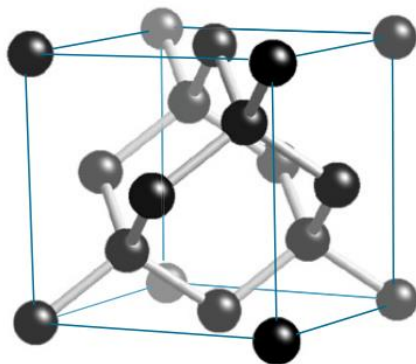
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Symmetry in Real World [1, 2]

3D Space



Diamond Crystal ($Fd\bar{3}m$)

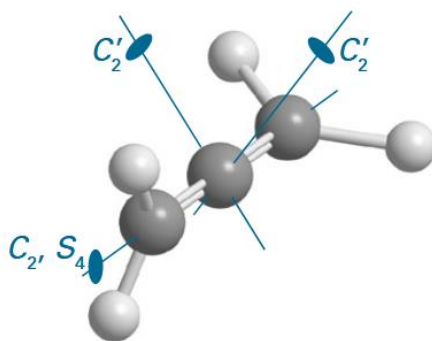
2D Space



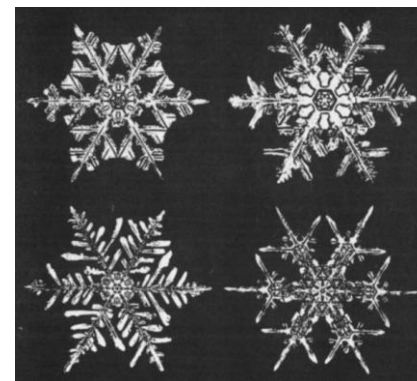
Egyptian Ornament ($p4g$)

Crystallographic Group

Point Group

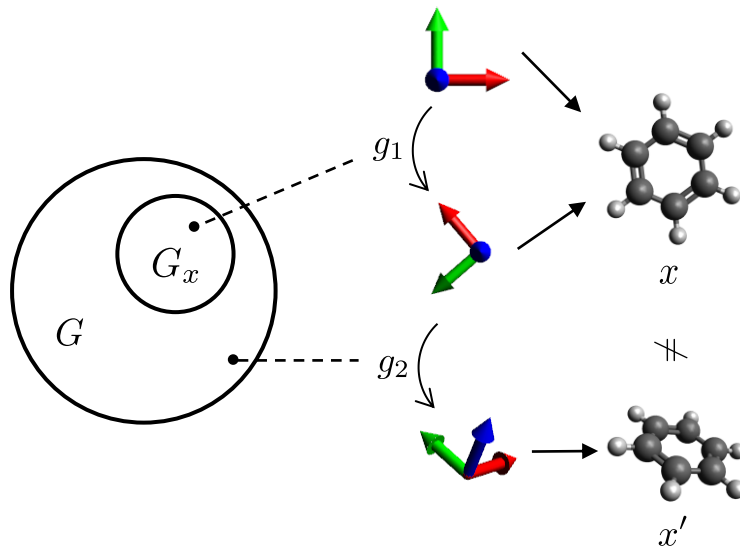


Propadiene molecule (D_{2d})



Snow Flakes (D_6)

Data Symmetry [3]



System (global) symmetry: Symmetry group describes the transformations between reference frames.

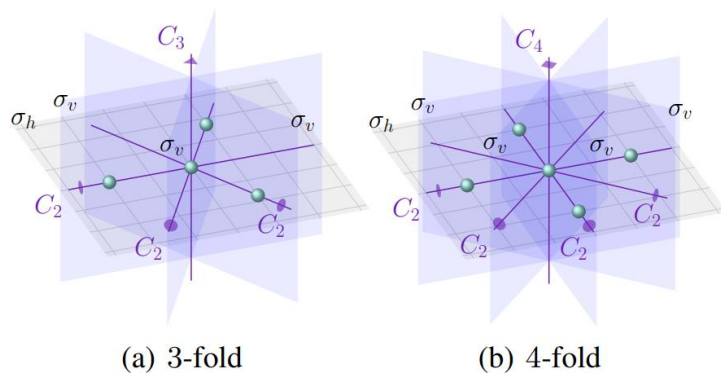
Data (local) symmetry: The set of transformations that leave data invariant, characterized by the isotropy subgroup

$$G_x := \{g \in G \mid g(x) = x\}$$

Case of 3D point cloud (k -fold, $k > 2$)

Global symmetry: $O(3) \times S_{k+1}$

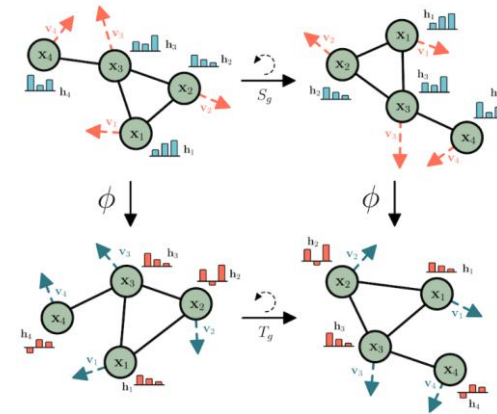
Local symmetry: geometric transformations (dihedral group with horizontal reflection D_{kh}) with the induced permutations.



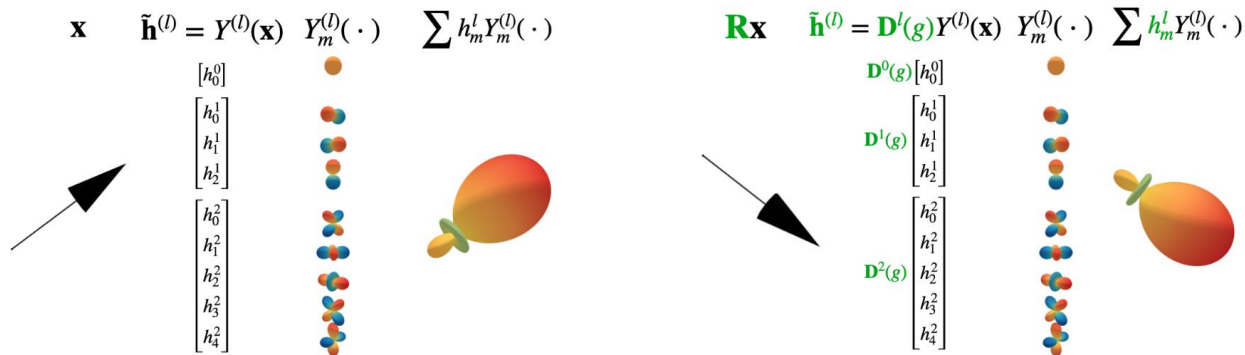
Equivariant Feature [3, 4]

Equivariant feature: In geometric deep learning, we seek features equivariant to frame transformations; in point cloud encoding, we enforce permutation invariance.

$$f : X \mapsto Y, f(\rho_X(g)(x)) = \rho_Y(g)(f(x))$$



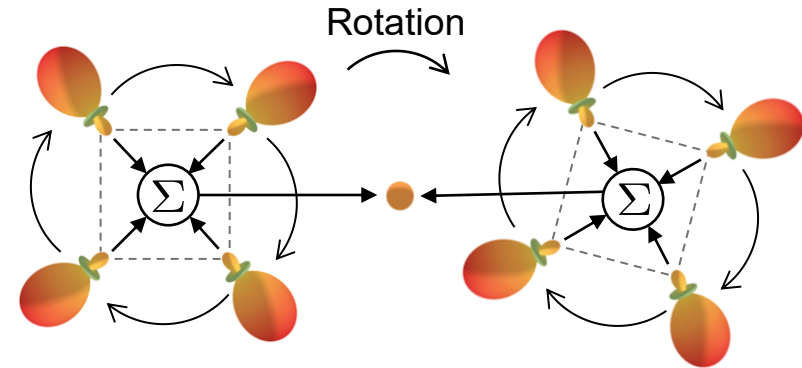
Spherical harmonics: Parity-matched $O(3)$ equivariant features can be characterized by spherical harmonics of different degrees; the spherical harmonic mapping is the simplest mapping from coordinates to equivariant features.



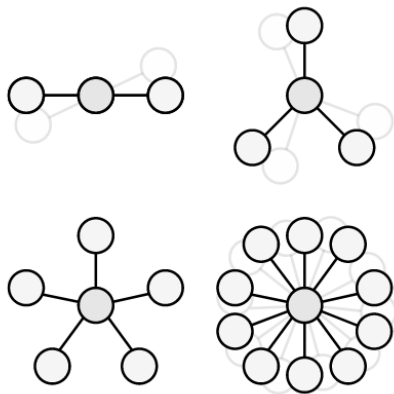
Equivariant Encoding of k -folds [4, 5]

First-order degeneracy: Averaging k -fold coordinates yields zero features, so k -fold and their rotations cannot be distinguished.

Spherical harmonics degeneracy: A similar indistinguishability is also observed in **spherical harmonic features** of different degrees.



General degeneracy: Joshi et al. (2023) experimentally showed restricting to **low-degree features** in equivariant networks induces **2D rotational collapse**.



		Rotational symmetry			
GNN Layer		2 fold	3 fold	5 fold	10 fold
Cart.	E-GNN _{L=1}	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0
	GVP-GNN _{L=1}	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0
Spherical	TFN/MACE _{L=1}	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0
	TFN/MACE _{L=2}	100.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0
	TFN/MACE _{L=3}	100.0 ± 0.0	100.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0
	TFN/MACE _{L=5}	100.0 ± 0.0	100.0 ± 0.0	100.0 ± 0.0	50.0 ± 0.0
	TFN/MACE _{L=10}	100.0 ± 0.0	100.0 ± 0.0	100.0 ± 0.0	100.0 ± 0.0

Collapse-to-zero Model [6]

Full degeneracy: Cen et al. (2024)

attribute feature indistinguishability to feature annihilation.

Degree-wise modeling: The annihilated degrees are characterized using trace properties of Wigner matrices

Notation	Data for Wigner-D matrix traces $D^{(l)}(H)$
C_i	$(2l + 1) \cdot \delta_{l \bmod 2,0}$
C_n	$2 \lfloor l/n \rfloor + 1$
D_n	$\lfloor l/n \rfloor + \delta_{l \bmod 2,0}$
T	$r = 6$ $b = 100110$
O	$r = 12$ $b = 100010101110$
I	$r = 30$ $b = 10000010001010011010111011110$

Full degeneracy

$$f(x) \equiv 0$$



Average trace Collapse-to-zero

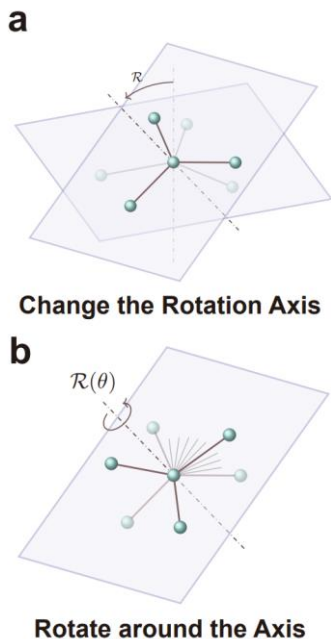
$$\frac{1}{|G_x|} \sum_{g \in G_x} \text{tr}(\rho_Y(g)) = 0$$

		Rotational symmetry			
GNN Layer		2 fold	3 fold	5 fold	10 fold
Cart.	E-GNN $_{l=1}$	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0
	GVP-GNN $_{l=1}$	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0
Single Type Spherical	HEGNN $_{l=1}$	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0
	HEGNN $_{l=2}$	95.0 ± 15.0	95.0 ± 15.0	95.0 ± 15.0	95.0 ± 15.0
	HEGNN $_{l=3}$	50.0 ± 0.0	75.0 ± 40.31	50.0 ± 0.0	50.0 ± 0.0
	HEGNN $_{l=4}$	100.0 ± 0.0	95.0 ± 15.0	95.0 ± 15.0	95.0 ± 15.0
	HEGNN $_{l=5}$	50.0 ± 0.0	100.0 ± 0.0	100.0 ± 0.0	50.0 ± 0.0
	HEGNN $_{l=6}$	100.0 ± 0.0	95.0 ± 15.0	100.0 ± 0.0	95.0 ± 15.0
	HEGNN $_{l=7}$	50.0 ± 0.0	95.0 ± 15.0	90.0 ± 30.0	50.0 ± 0.0
	HEGNN $_{l=8}$	100.0 ± 0.0	90.0 ± 30.0	85.0 ± 32.02	85.0 ± 32.02
	HEGNN $_{l=9}$	50.0 ± 0.0	100.0 ± 0.0	100.0 ± 0.0	50.0 ± 0.0
	HEGNN $_{l=10}$	100.0 ± 0.0	100.0 ± 0.0	100.0 ± 0.0	100.0 ± 0.0
	HEGNN $_{l=11}$	50.0 ± 0.0	100.0 ± 0.0	95.0 ± 15.0	50.0 ± 0.0
Sph.	HEGNN/TFN/MACE $_{l \leq 1}$	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0	50.0 ± 0.0
	HEGNN/TFN/MACE $_{l \leq 2}$	100.0 ± 0.0	100.0 ± 0.0	100.0 ± 0.0	100.0 ± 0.0

Equivariant Feature Visualization

3D rotations:

- Randomly sample the rotation axes
- Uniformly select **res** rotation angles

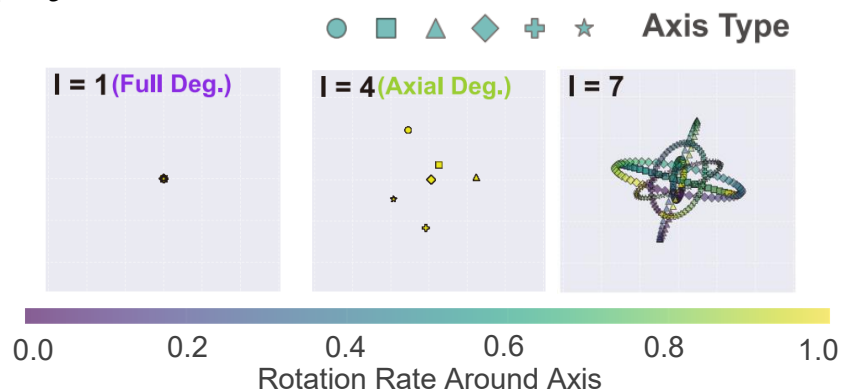


Classification: Degree-wise k -fold experiments reveal finer degeneracy:

- **Half Deg.** π / k rotation around z -axis
- **Axial Deg.** any rotation around z -axis
- **Full Deg.** any rotation around any axis

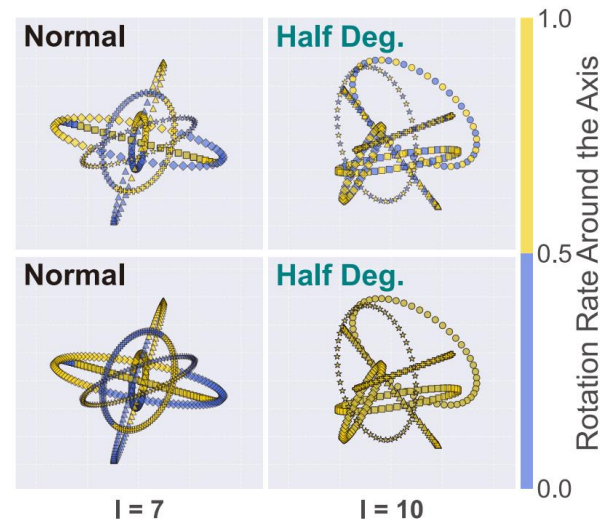
Collapse-to-zero model is not enough!

Visualization: Embedded and projected into 2D



res = 49

res = 98



Symmetry Increase of Full Degeneracy [6, 7]

Fact 1 (trace and fixed subspace dimension): The averaged trace computed by [Cen et al. \(2024\)](#) is exactly the dimension of the fixed subspace of the isotropy group.

$$\dim Y^{G_x} = \frac{1}{|G_x|} \sum_{g \in G_x} \text{tr}(\rho_Y(g))$$

Fact 2 (equivariant map does not decrease symmetry): [Kaba et al. \(2023\)](#) showed that equivariant features belong to the fixed-point subspace.

Theorem (Curie's principle). *Let $f : X \rightarrow Y$ be a G -equivariant map. For $x \in X$, the isotropy subgroup of x is contained in that of its image $f(x)$, i.e.,*

$$G_x \subseteq G_{f(x)}.$$

When the fixed-point subspace vanishes, equivariant features exhibit global symmetry, and thus cannot distinguish any rotations!

Key Questions

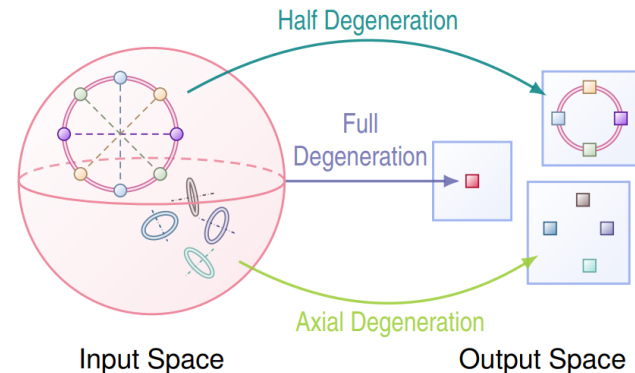
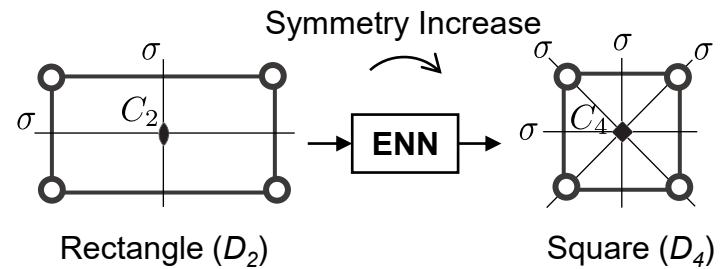
Symmetry increase reduces expressivity:

Transformations in the larger isotropy group can map distinct data and its transformed versions to the same output.

$$f(\rho_X(g)(x)) = \rho_Y(g)(f(x)) = f(x)$$

To understand symmetry increase and mitigate its adverse effects, we address the following **key questions**:

- **Symmetry Infimum:** For a given data point, does its representation under an equivariant map admit a **unique minimal level of symmetry**? When does this minimal symmetry match that of the input?
- **Learning guarantee:** If the minimal symmetry matches the input symmetry, do there **exist** equivariant maps that preserve it? Are such maps common (**generic**) among all equivariant mappings?
- **Computation:** How can this minimal symmetry be **computed**?



Symmetry Infimum

Orbit type: As isotropy subgroups transform by conjugation, orbit types (conjugacy classes) provide a group-invariant characterization of symmetry.

$$(G_x) = \{gG_xg^{-1} | g \in G\}, \mathcal{O}_G(X) = \{(G_x) | x \in X\}$$

Order of symmetry:

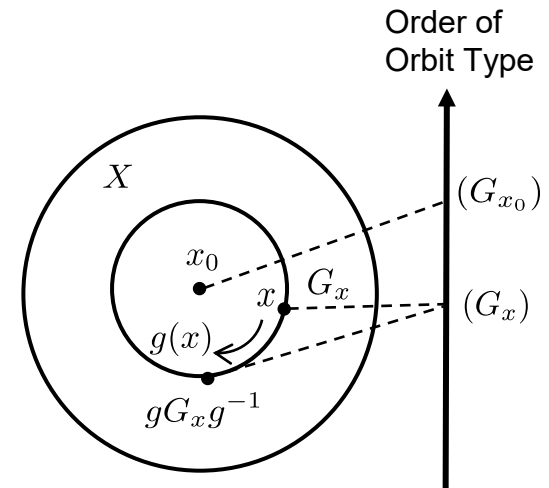
$$(H_1) > (H_2) \iff \exists g \in G, gH_2g^{-1} \subset H_1$$

Uniqueness of minimal type:

Theorem. *Let X be a representation of a compact Lie group G . For any closed subgroup $H \subseteq G$, a unique minimal orbit type exists among the points in the fixed-point subspace X^H , denoted as $I_G(X, H)$*

Answers:

- Q: For a given data point, does its representation under an equivariant map admit a unique minimal level of symmetry?
- A: **Yes.**
- Q: When does this minimal symmetry match that of the input?
- A: **When the symmetry infimum matches the input orbit type.**

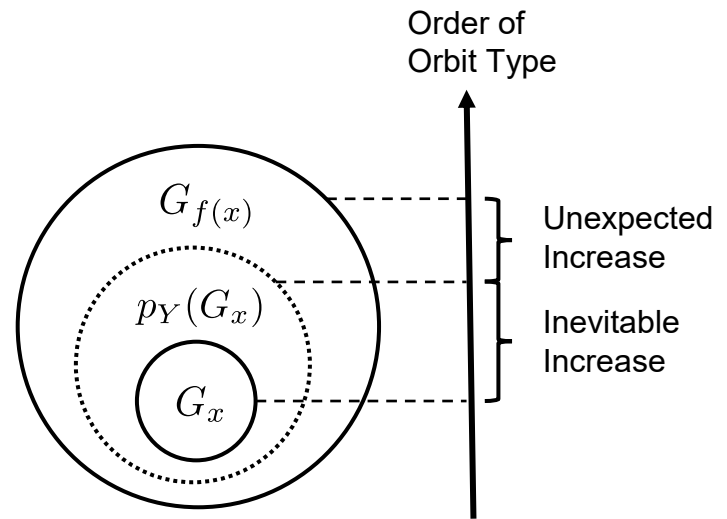


(Relatively) Isovariant Maps

Isovariant map: Isovariant mappings describe symmetry-preserving equivariant maps.

Representation kernel: The kernel consists of group elements that leave all data unchanged. Task-required invariances enforce the kernel to include specific elements.

$$\ker \rho_X := \{g \in G \mid g(x) = x, \forall x \in X\}$$



Relatively isovariant map : Task-required invariances can induce symmetry increase, motivating a relaxation of isovariance.

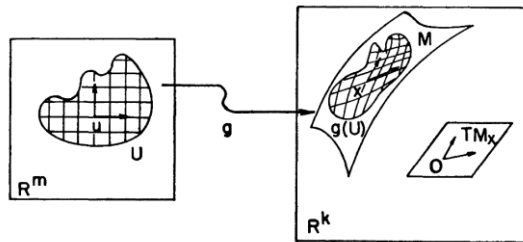
$$\pi_Y : G \mapsto G/\ker \rho_Y, p_Y(G_x) := \pi_Y^{-1}(\pi_Y(G_x)) = G_{f(x)}$$

Necessary condition for relative isovariance:

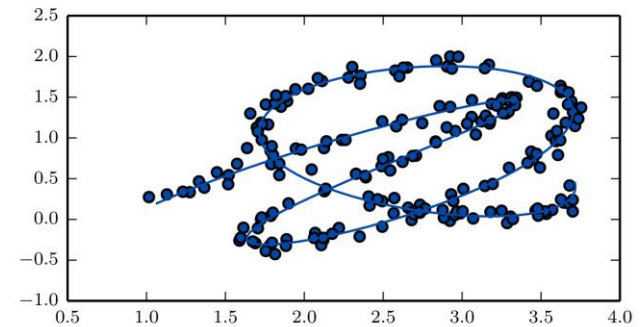
Theorem. *A necessary condition for the existence of an isovariant map relative to Y from a representation X to a representation Y is that $I_G(Y, H) = (p_Y(H))$ for all $(H) \in \mathcal{O}_G(X)$.*

Data Assumption [8, 9]

Union of Manifold Assumption: The data is a **finite union** of compact, connected, **smooth**, and invariant submanifolds of input space



Counterexample: The necessary condition of orbit type inclusion is **not sufficient** for isovariance



Proposition. For a compact Lie group G , consider a representation \tilde{Y} with no trivial component, i.e. $\tilde{Y}^G = \{0\}$. Let $Y = \tilde{Y}^{\oplus r}$ and $X = Y^{\oplus (n_0+1)}$ for some $r, n_0 > \dim G$. We have $\mathcal{O}_G(X) = \mathcal{O}_G(Y)$, yet no isovariant map exists from the unit sphere in X to Y for a sufficiently large integer n_0 .

Almost (relatively) isovariant maps: Equivariant maps that are (relatively) isovariant almost within each orbit type, except on a set of Hausdorff **measure zero**.

Density of (Almost) Isovariant Mappings

Sufficient condition for relative isovariance (density theorem):

Theorem. *Let \mathcal{F} be a equivariant parametrization with C^∞ approximation capability. If for every $(H) \in \mathcal{O}_G(M)$ we have $(p_Y(H)) \in \mathcal{O}_G(Y)$, then for any finite union of compact, smooth G -submanifolds $M \subset X$, any $f \in C_G^\infty(X, Y)$, any integer $r \geq 0$, and any $\epsilon > 0$, there exists a map $g \in \mathcal{F}$ such that*

$$\max_{x \in M} \|D^k f(x) - D^k g(x)\| < \epsilon, k \leq r,$$

and $g|_M$ is almost isovariant relative to Y . Furthermore, if Y contains a representation $\tilde{Y}^{\oplus r}$ for an integer $r > \max_j \{\dim M_j\}$, where \tilde{Y} itself satisfies $(p_{\tilde{Y}}(H)) \in \mathcal{O}_G(\tilde{Y})$, then $g|_M$ can be chosen to be isovariant relative to Y .

Answer:

- Q: If the minimal symmetry matches the input symmetry, do there exist equivariant maps that preserve it?
- **A: No; but yes under almost isovariant mappings.**
- Q: Are such maps common (generic) among all equivariant mappings?
- **A: No; however, almost isovariance is generic. Moreover, under sufficient multiplicity, full isovariance is also generic.**

Symmetry Infimum Calculation ^[10]

Orbit type criterion: To **high-multiplicity representations** for representation learning, we extend **Michel criterion** of Michel (1980)

Theorem. *In a G -representation V , a closed subgroup H is an isotropy subgroup only if for any adjacent $H \subsetneq H'$,*

$$\dim V^{H'} < \dim V^H.$$

If $V = V_0^{\oplus r}$ with $r > \dim G$, this condition is sufficient.

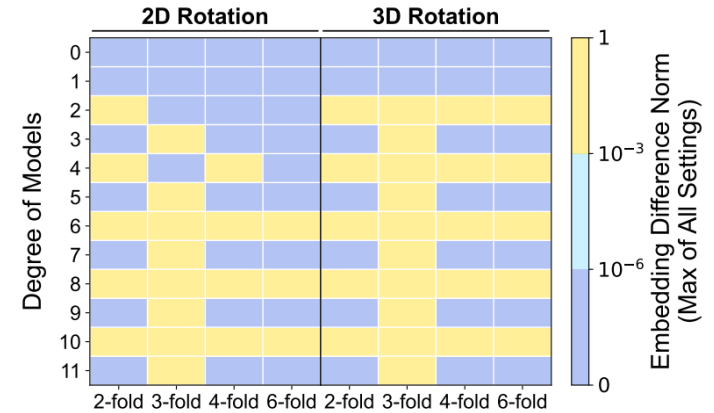
Answer:

- Q: For a given data point, does its representation under an equivariant map admit a unique minimal level of symmetry?
- **A: For high-multiplicity representations, the symmetry infimum can be computed via a procedure**
 - ❖ Enumerate all closed supergroups
 - ❖ Retain those whose conjugacy classes are valid orbit types by criterion
 - ❖ Return the minimal one

Results for k -folds

Degree-wise finer degeneracy explanation:

- **No Deg.** $I_{O(3)}(V_{l=l_0}, D_{kh}) = (D_{kh})$
- **Half Deg.** $I_{O(3)}(V_{l=l_0}, D_{kh}) = (D_{2kh})$
- **Axial Deg.** $I_{O(3)}(V_{l=l_0}, D_{kh}) = (D_{\infty h})$
- **Full Deg.** $I_{O(3)}(V_{l=l_0}, D_{kh}) = (O(3))$



Experiment (k -folds rotation detection): Compare the distance between equivariant features before and after random rotations.

Guideline for orientation-dependent tasks: Avoid non-trivial symmetry increase; select components that maximally preserve the input orbit type.

	$l_0 < k$		$k \leq l_0 < 2k$		$l_0 \geq 2k$	
	l_0 is even	l_0 is odd	l_0 is even	l_0 is odd	l_0 is even	l_0 is odd
k is even	$(D_{\infty h})$	$(O(3))$	(D_{kh})	$(O(3))$	(D_{kh})	$(O(3))$
k is odd	$(D_{\infty h})$	$(O(3))$	$(D_{\infty h})$	(D_{kh})	(D_{2kh})	(D_{kh})

Results for Point Groups

Table of point groups: Symmetry infimum for axial subgroups of $O(3)$

- **No (Relative) Deg.** No symmetry increase (or predictable increase)
- **Discrete Deg.** Increase to a same-dimensional supergroup
- **Continuous Deg.** Increase to a higher-dimensional supergroup
- **Full Deg.** Increase to the full group

Subgroup		$0 < l_0 < k$		$k \leq l_0 < 2k$		$l_0 \geq 2k$	
		l_0 even	l_0 odd	l_0 even	l_0 odd	l_0 even	l_0 odd
C_k		D_∞	$C_{\infty v}$	C_k	C_k	C_k	C_k
S_{2k}	k even	K_h	K_h	S_{2k}	S_{2k}	S_{2k}	S_{2k}
	k odd	K_h	K_h	K_h	K_h	K_h	K_h
C_{kh}	k even	K_h	K_h	K_h	K_h	K_h	K_h
	k odd	K_h	K_h	C_{kh}	C_{kh}	C_{kh}	C_{kh}
$C_{kv}(k > 2)$	k even	K_h	$C_{\infty v}$	D_{kd}	C_{kv}	C_{kv}	C_{kv}
	k odd	K_h	$C_{\infty v}$	D_{kh}	C_{kv}	C_{kv}	C_{kv}
$D_k(k > 2)$	k even	D_∞	K_h	D_k	D_{kd}	D_k	D_k
	k odd	D_∞	K_h	D_k	D_{kh}	D_k	D_k
$D_{kh}(k > 2)$	k even	K_h	K_h	K_h	K_h	K_h	K_h
	k odd	K_h	K_h	D_{kh}	D_{kh}	D_{kh}	D_{kh}
$D_{kd}(k > 2)$	k even	K_h	K_h	D_{kd}	D_{kd}	D_{kd}	D_{kd}
	k odd	K_h	K_h	K_h	K_h	K_h	K_h

Subgroup		$0 < l_0 < k$		$k \leq l_0 < 2k$		$l_0 \geq 2k$	
		l_0 even	l_0 odd	l_0 even	l_0 odd	l_0 even	l_0 odd
C_k	k even	$D_{\infty h}$	$C_{\infty h}$	C_{kh}	C_{kh}	C_{kh}	C_{kh}
	k odd	$D_{\infty h}$	$C_{\infty h}$	S_{2k}	S_{2k}	S_{2k}	S_{2k}
S_{2k}	k even	$D_{\infty h}$	$C_{\infty h}$	$D_{\infty h}$	$C_{\infty h}$	C_{2kh}	C_{2kh}
	k odd	$D_{\infty h}$	$C_{\infty h}$	S_{2k}	S_{2k}	S_{2k}	S_{2k}
C_{kh}	k even	$D_{\infty h}$	$C_{\infty h}$	C_{kh}	C_{kh}	C_{kh}	C_{kh}
	k odd	$D_{\infty h}$	$C_{\infty h}$	$D_{\infty h}$	$C_{\infty h}$	C_{2kh}	C_{2kh}
$C_{kv}(k > 2)$	k even	$D_{\infty h}$	K_h	D_{kh}	D_{kh}	D_{kh}	D_{kh}
	k odd	$D_{\infty h}$	K_h	D_{kd}	D_{kd}	D_{kd}	D_{kd}
$D_k(k > 2)$	k even	$D_{\infty h}$	K_h	D_{kh}	D_{kh}	D_{kh}	D_{kh}
	k odd	$D_{\infty h}$	K_h	D_{kd}	D_{kd}	D_{kd}	D_{kd}
$D_{kh}(k > 2)$	k even	$D_{\infty h}$	K_h	D_{kh}	D_{kh}	D_{kh}	D_{kh}
	k odd	$D_{\infty h}$	K_h	$D_{\infty h}$	K_h	D_{2kh}	D_{2kh}
$D_{kd}(k > 2)$	k even	$D_{\infty h}$	K_h	$D_{\infty h}$	K_h	D_{2kh}	D_{2kh}
	k odd	$D_{\infty h}$	K_h	D_{kd}	D_{kd}	D_{kd}	D_{kd}

Results for QM9 Molecules

Table of molecular symmetry: Symmetry infimum for symmetry groups of molecules in QM9

	0	1	2	3	4	5	6	7	8	9	10	11
C_1	K	C_1	C_s	C_1	C_s	C_1	C_s	C_1	C_s	C_1	C_s	C_1
C_s	K_h	C_s	C_{2h}	C_s	C_{2h}	C_s	C_{2h}	C_s	C_{2h}	C_s	C_{2h}	C_s
C_2	K	$C_{\infty v}$	C_{2h}	C_2	C_{2h}	C_2	C_{2h}	C_2	C_{2h}	C_2	C_{2h}	C_2
C_{2v}	K_h	$C_{\infty v}$	D_{2h}	C_{2v}	D_{2h}	C_{2v}	D_{2h}	C_{2v}	D_{2h}	C_{2v}	D_{2h}	C_{2v}
C_{3v}	K_h	$D_{\infty h}$	$C_{\infty v}$	C_{3v}	D_{3d}	C_{3v}	D_{3d}	C_{3v}	D_{3d}	C_{3v}	D_{3d}	C_{3v}
C_{2h}	K_h	K_h	C_{2h}	K_h	C_{2h}	K_h	C_{2h}	K_h	C_{2h}	K_h	C_{2h}	K_h
$C_i = S_2$	K_h	K_h	C_i	K_h	C_i	K_h	C_i	K_h	C_i	K_h	C_i	K_h
D_{3h}	K_h	K_h	$D_{\infty h}$	D_{3h}	$D_{\infty h}$	D_{3h}	D_{6h}	D_{3h}	D_{6h}	D_{3h}	D_{6h}	D_{3h}
D_{2d}	K_h	K_h	$D_{\infty h}$	T_d	D_{4h}	D_{2d}	D_{4h}	D_{2d}	D_{4h}	D_{2d}	D_{4h}	D_{2d}
C_3	K	$C_{\infty v}$	$D_{\infty h}$	C_3	C_{3h}	C_3	C_{3h}	C_3	C_{3h}	C_3	C_{3h}	C_3
$D_{\infty h}$	K_h	K_h	$D_{\infty h}$	K_h	$D_{\infty h}$	K_h	$D_{\infty h}$	K_h	$D_{\infty h}$	K_h	$D_{\infty h}$	K_h
$C_{\infty v}$	K_h	$C_{\infty v}$	$D_{\infty h}$	$C_{\infty v}$	$D_{\infty h}$	$C_{\infty v}$	$D_{\infty h}$	$C_{\infty v}$	$D_{\infty h}$	$C_{\infty v}$	$D_{\infty h}$	$C_{\infty v}$
D_{3d}	K_h	K_h	$D_{\infty h}$	K_h	D_{3d}	K_h	D_{3d}	K_h	D_{3d}	K_h	D_{3d}	K_h
D_{2h}	K_h	K_h	D_{2h}	K_h	D_{2h}	K_h	D_{2h}	K_h	D_{2h}	K_h	D_{2h}	K_h
T_d	K_h	K_h	K_h	T_d	O_h	K_h	O_h	T_d	O_h	T_d	O_h	T_d
C_{3h}	K_h	K_h	$D_{\infty h}$	C_{3h}	$D_{\infty h}$	C_{3h}	C_{6h}	C_{3h}	C_{6h}	C_{3h}	C_{6h}	C_{3h}

Symmetry Infimum of QM9 Molecules [2]

Experiment (property prediction): Finetune with pretrained equivariant feature

Group

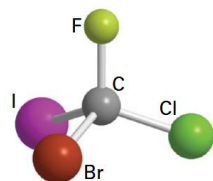
C_1

C_{2h}

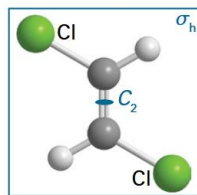
C_{3h}

T_d

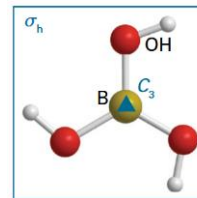
Example



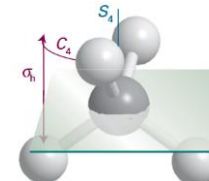
CBrClFI



trans-CHCl=CHCl

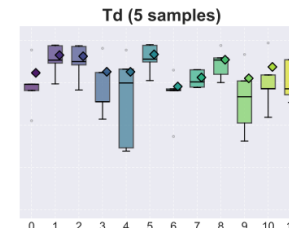
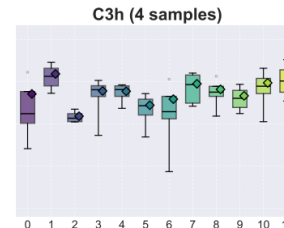
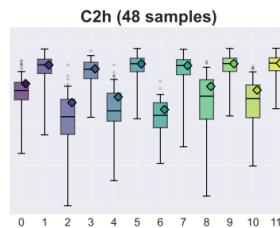
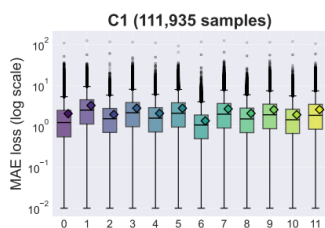


B(OH)₃

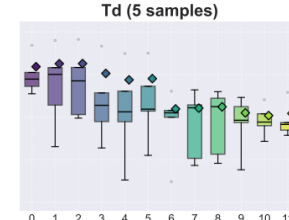
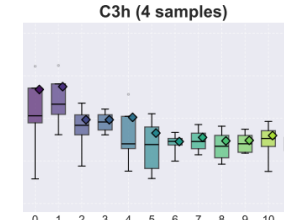
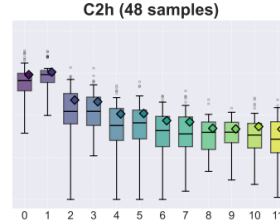
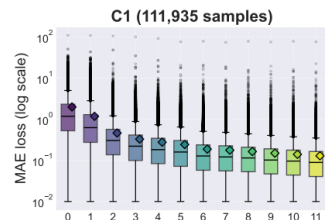


CH₄

With feature degree $l = l_0$



With feature degree $l \leq l_0$



Guideline for general tasks: Avoid symmetry increases that overly compress the fixed-point subspace, especially those leading to **full degeneracy**.

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