Why Equivariant Networks Lose Information: Invariant Rings and the Role of Aggregation

Anonymous authors
Paper under double-blind review

Abstract

Equivariant neural networks exhibit fundamental expressivity limitations: rotation-equivariant networks collapse directional information to radial features, and matrix-equivariant networks show rank degeneracy. We explain these phenomena using classical invariant theory and prehomogeneous vector space (PVS) theory. For SO(3) on $\mathbb{R}^3$, the First Fundamental Theorem forces equivariant maps to be radial scalings; for $\mathrm{GL}(n) \times \mathrm{GL}(n)$ on matrices, PVS theory shows the invariant ring contains only constants. Our central finding is that aggregation, not depth, escapes these constraints: product representations V^n have richer invariant rings with cross-invariants (e.g., dot products encoding angles) inaccessible to single-fiber processing. We connect this theory to modern architectures—SchNet, PaiNN, DimeNet, MACE—showing their body-order corresponds to which V^n they access. Experiments confirm that SO(3)- versus O(3)-invariant networks exhibit categorically different expressivity on pseudoscalar targets ($R^2 = 1.00$ vs. $R^2 < 0$), and that cross-invariants enable learning angles while norm-only features cannot. These results provide design guidance: prioritize multi-body interactions over depth when expressivity is limited.

1 Introduction

1.1 Equivariant Neural Networks and Their Importance

Many problems in science and engineering involve data with inherent symmetries. Molecules look the same regardless of how we orient them in space; the laws of physics do not depend on our choice of coordinate system; and the properties of a crystal are unchanged by the symmetries of its lattice. When building neural networks to learn from such data, it is natural to ask that the network respect these symmetries: if the input is rotated, the output should transform accordingly.

This requirement defines equivariant neural networks. Formally, given a group G acting on input space V and output space W, a function $\Phi : V \to W$ is G-equivariant if $\Phi(g \cdot v) = g \cdot \Phi(v)$ for all group elements g and inputs v. When the output is a scalar (unchanged by the group action), the function is called G-invariant.

Equivariant architectures have proven highly successful in practice. In computational chemistry and materials science, machine-learned interatomic potentials based on rotation-equivariant networks (Thomas et al., 2018; Schütt et al., 2018; Batzner et al., 2022) can predict molecular properties with near quantum-mechanical accuracy at a fraction of the computational cost. These potentials now enable molecular dynamics simulations that were previously intractable, with applications ranging from drug discovery to catalyst design. In computer vision, translation-equivariant convolutional networks (Cohen and Welling, 2016) remain the foundation of image recognition. In physics simulation, equivariant graph networks (Sanchez-Gonzalez et al., 2020) learn to predict the dynamics of complex systems. By building symmetry into the architecture, we reduce the hypothesis space, improve sample efficiency, and guarantee physically sensible predictions.

1.2 The Problem: Expressivity Limitations

Equivariance constraints impose fundamental limitations on what functions a network can represent. These limitations take several forms:

Scalar collapse. Rotation-equivariant networks processing single 3D vectors are algebraically constrained to collapse directional information to radial features. An SO(3)-equivariant map $\Phi : \mathbb{R}^3 \to \mathbb{R}^3$ must have the form $\Phi(v) = p(|v|^2) \cdot v$ (Weyl, 1946; Blum-Smith and Villar, 2023), where p is a scalar function of the squared norm. The direction of v is preserved but cannot be discriminated—two vectors pointing in different directions but with the same length produce proportional outputs.

Rank collapse. Networks equivariant to matrix transformations exhibit degeneracy at low rank. When $\mathrm{GL}(n) \times \mathrm{GL}(n)$ acts on $n \times n$ matrices by $(A, B) \cdot M = AMB^{-1}$, the action is transitive on invertible matrices, making this a prehomogeneous vector space. The invariant ring is just constants ($k[\mathrm{Mat}_n]^G = k$), so invariant scalar features carry no information. The geometry is governed by the relative invariant $\det(M)$, which defines the singular set, and the rank stratification of that set.

Orbit limitations. More generally, equivariant networks cannot distinguish inputs that lie on the same group orbit. This is a fundamental constraint, but the practical severity depends on the orbit structure: when most inputs lie in a single large orbit, the network loses discriminating power.

These constraints have motivated theoretical analyses of equivariant network expressivity (Joshi et al., 2023; Pacini et al., 2024; Villar et al., 2021) and various architectural innovations to circumvent them. The question we address is: why do these limitations arise algebraically, and what determines their severity?

1.3 The Knowledge Gap

Two largely independent lines of research address equivariant network expressivity, but neither provides an algebraic explanation of why certain representations lead to expressivity limitations.

The machine learning community has developed sophisticated tools for analyzing what networks can do. The Weisfeiler-Leman hierarchy (Xu et al., 2019; Morris et al., 2019) characterizes the discriminating power of graph neural networks. Joshi et al. (2023) extend this to geometric graphs with their Geometric Weisfeiler-Leman (GWL) test, which assigns colors to geometric neighborhoods via an idealized "I-HASH" function assumed to be orbit-injective; GWL determines what geometric GNNs can and cannot distinguish—for instance, that invariant layers cannot distinguish 1-hop identical graphs. Universality results address a different question: Maron et al. (2019c) and Dym and Maron (2020) establish conditions under which equivariant networks can approximate any equivariant function; Villar et al. (2021) showed that scalar features suffice for universal approximation; Kondor (2025) provides a comprehensive treatment of equivariant architectures for physics. These results answer whether networks can represent certain function classes, but do not explain why particular representations impose particular constraints. In the GWL framework, I-HASH is treated as a black box—the theory does not specify which invariants it actually computes.

Classical invariant theory, recently made accessible to machine learning by Blum-Smith and Villar (2023), provides tools for parameterizing equivariant maps. Given a group action, Malgrange's method constructs explicit bases for equivariant polynomial maps in terms of generating invariants (Weyl, 1946; Kraft and Procesi, 2000). Puny et al. (2023) enumerated equivariant polynomial bases for specific groups. This work answers how to build equivariant networks, but the connection between invariant ring structure and practical expressivity limitations—why some representations are severely constrained while others are not—has not been systematically developed.

The gap we address is the question of constraints and impossibilities: which invariants are available to a network, which are not, and what algebraic structure explains the difference? For the GWL framework, we provide the algebraic content of I-HASH: the First Fundamental Theorem specifies exactly which invariants are computable (e.g., norms and dot products for O(3)), explaining why the discrimination limits that Joshi et al. identify arise. More broadly, prehomogeneous vector space theory (Sato and Kimura, 1977; Kimura, 2003), which classifies representations with open orbits and characterizes their relative invariants, provides precisely the tools needed for this analysis. To our knowledge, this paper is the first to apply PVS theory to machine learning expressivity.

1.4 Our Approach and Contributions

We analyze expressivity limitations through two classical mathematical theories:

Classical invariant theory, particularly the First Fundamental Theorems (FFTs) that characterize the generators of invariant rings for classical groups. For SO(3) acting on $\mathbb{R}^3$, the FFT states that all invariants are generated by the squared norm $|v|^2$, and all equivariant maps $\mathbb{R}^3 \to \mathbb{R}^3$ are generated by the identity map $v \mapsto v$ with coefficients in this invariant ring. This immediately explains scalar collapse.

Prehomogeneous vector space (PVS) theory, developed by Sato and Kimura (1977), which classifies representations (G, V) where the group has an open dense orbit. For such representations, there exists a unique (up to character) relative invariant whose zero set is the complement of the open orbit. When (G, V) is a PVS, equivariant maps on the generic orbit are severely constrained.

A key contribution of this paper is clarifying when each theory applies. The commonly studied representation $(\mathrm{SO}(3), \mathbb{R}^3)$ is not a PVS—its orbits are spheres of codimension 1, not an open dense set. Scalar collapse follows from the FFT, not from prehomogeneity. In contrast, $(\mathrm{GL}(n) \times \mathrm{GL}(n), \mathrm{Mat}_n)$ is a PVS, and the Sato-Kimura theory genuinely illuminates its structure.

Expressivity limitations of equivariant networks are empirically known. Our contribution is explaining why they arise and when different mathematical tools apply. We clarify a common conflation: the representation $(\mathrm{SO}(3), \mathbb{R}^3)$ is not a prehomogeneous vector space (Proposition 3.1), so PVS theory does not apply—scalar collapse follows from the First Fundamental Theorem instead. This distinction matters: PVS theory governs matrix-equivariant networks (Section 4), where the determinant is a relative invariant, not an invariant. Misapplying one theory to the other's domain leads to incorrect predictions.

Our central theoretical finding concerns how these constraints can be escaped. We show that aggregation—moving from a single fiber V to product representations V^n—enriches the invariant ring and enables discrimination of geometric relationships that single-fiber processing cannot access. For SO(3) on $(\mathbb{R}^3)^n$, the invariant ring is generated by all pairwise dot products and norms, providing access to angular information. This explains why message-passing architectures, which aggregate information from multiple neighbors, succeed where per-edge processing fails.

We also clarify the role of depth. Contrary to what one might hope, increasing network depth does not expand the class of representable functions for single-fiber inputs—it only improves approximation quality within that class. Depth helps approximate complex functions of the available invariants, but cannot create new invariants.

2 Mathematical Background

We work over a field k, typically $\mathbb{R}$ or $\mathbb{C}$. Let G be a linear algebraic group acting rationally on a finite-dimensional vector space V. We write $k[V]$ for the ring of polynomial functions on V.

2.1 Invariants and Relative Invariants

The distinction between invariants and relative invariants is central to this paper and has been a source of confusion.

Definition 2.1 (Invariant)**.** A polynomial $f \in k[V]$ is a G-invariant if $f(g \cdot v) = f(v)$ for all $g \in G$ and $v \in V$. The ring of all G-invariants is denoted $k[V]^G$.

Definition 2.2 (Relative Invariant)**.** A polynomial $f \in k[V]$ is a G-relative invariant (or semi-invariant) if there exists a character $\chi : G \to k^*$ (a group homomorphism to the nonzero scalars) such that

$$f(g \cdot v) = \chi(g) f(v) \quad \text{for all } g \in G,\ v \in V.$$

An invariant is a relative invariant with trivial character $\chi \equiv 1$. But a relative invariant with non-trivial character is not an invariant.

Example 2.3. Let $G = \mathrm{SO}(3) \times \mathbb{R}^*$ act on $V = \mathbb{R}^3$ by $(g, \lambda) \cdot v = \lambda \cdot gv$. The function $f(v) = |v|^2$ satisfies $f((g, \lambda) \cdot v) = \lambda^2 |v|^2 = \chi(g, \lambda) f(v)$ where $\chi(g, \lambda) = \lambda^2$. Thus f is a relative invariant. It is not an invariant: $f(2v) = 4f(v) \neq f(v)$.

For this group, the invariant ring is $\mathbb{R}[V]^G = \mathbb{R}$ (constants only), since any polynomial invariant must satisfy $p(\lambda v) = p(v)$ for all $\lambda \neq 0$, forcing p constant.

2.2 Covariants and Equivariant Maps

Definition 2.4 (Covariant)**.** Let W be another G-representation. A polynomial map $\Phi : V \to W$ is a G-covariant (or equivariant polynomial) if $\Phi(g \cdot v) = g \cdot \Phi(v)$ for all $g \in G$, $v \in V$.

The set of all covariants $V \to W$, denoted $\mathrm{Cov}_G(V, W)$, forms a module over the invariant ring $k[V]^G$ (meaning covariants can be multiplied by invariant polynomials to get new covariants). When G is reductive (as are all groups considered here), this module is finitely generated: every covariant can be written as a linear combination of finitely many "basic" covariants with coefficients in $k[V]^G$. This is Malgrange's theorem.

2.3 Prehomogeneous Vector Spaces

Definition 2.5. A representation (G, V) is a prehomogeneous vector space (PVS) if V contains an open G-orbit Ω (a single orbit that is "almost all" of V, with complement defined by polynomial equations).

The complement $S = V \setminus \Omega$ is the singular set. For "regular" PVS with reductive G, the singular set is a hypersurface defined by a relative invariant.

Theorem 2.6 (Sato-Kimura Structure Theorem (Sato and Kimura, 1977))**.** *Let (G, V) be an irreducible regular PVS with G reductive. Then:*

(i) The singular set S is either empty or a hypersurface defined by a single irreducible polynomial f, unique up to scalar.

(ii) This f is a relative invariant. All relative invariants with the same character are scalar multiples of powers of f.

Remark 2.7 (Invariant Ring for PVS)**.** The invariant ring $k[V]^G$ (polynomials fixed by G, not just transforming by a character) depends on the structure of G. When G contains scaling transformations $v \mapsto \lambda v$ for $\lambda \in k^*$—as in most PVS relevant to machine learning—the invariant ring is typically $k[V]^G = k$ (constants only). This is because any polynomial satisfying $p(\lambda v) = p(v)$ for all $\lambda \neq 0$ must be constant.

Some sources incorrectly state "$k[V]^G = k[f]$" for a PVS with relative invariant f. This is false in general: the relative invariant f generates relative invariants (up to character), not invariants. For most PVS, invariants are just constants.

3 Analysis of $\mathrm{SO}(3)$ on Vectors

We begin with the representation most common in geometric deep learning: SO(3) acting on $\mathbb{R}^3$. This analysis establishes the appropriate tools and corrects a potential misconception.

3.1 $\mathrm{SO}(3)$ on $\mathbb{R}^3$ is Not a PVS

Proposition 3.1. *The representation $(\mathrm{SO}(3), \mathbb{R}^3)$ is not a prehomogeneous vector space.*

Proof. The orbits of SO(3) on $\mathbb{R}^3$ are spheres $S_r^2 = \{v : |v| = r\}$ for $r > 0$, plus the origin. Each sphere has dimension 2, hence codimension 1 in $\mathbb{R}^3$. There is no orbit of codimension 0, so $(\mathrm{SO}(3), \mathbb{R}^3)$ is not prehomogeneous. □

This observation is important: PVS theory does not apply to this representation. We must use classical invariant theory instead.

3.2 The First Fundamental Theorem for $\mathrm{SO}(3)$

Classical invariant theory provides the First Fundamental Theorem (FFT) for orthogonal groups, which completely characterizes the invariant ring and the module of covariants.

Theorem 3.2 (FFT for SO(3) on $\mathbb{R}^3$)**.** *Let* $\mathrm{SO}(3)$ *act on* $V = \mathbb{R}^3$ *by rotations.*

(i) The invariant ring is $\mathbb{R}[V]^{\mathrm{SO}(3)} = \mathbb{R}[\rho]$ *where* $\rho = |v|^2$*.*

(ii) The module of covariants $\mathrm{Cov}_{\mathrm{SO}(3)}(\mathbb{R}^3, \mathbb{R}^3)$ *is free of rank 1 over* $\mathbb{R}[\rho]$*, generated by the identity map* $\iota : v \mapsto v$*.*

This theorem, due to Weyl (1946), has an immediate consequence:

Corollary 3.3 (Scalar Collapse)**.** *Any* $\mathrm{SO}(3)$*-equivariant polynomial map* $\Phi : \mathbb{R}^3 \to \mathbb{R}^3$ *has the form*

$$\Phi(v) = p(|v|^2) \cdot v$$

for some polynomial p*.*

This is the algebraic origin of scalar collapse: an SO(3)-equivariant network processing a single vector can only modulate the output by functions of the squared norm. The direction of v is preserved (the output is parallel to v), but the network cannot discriminate between different directions at the same norm.

Remark 3.4 (Polynomial vs. Smooth/Continuous Maps)**.** Theorem 3.2 and Corollary 3.3 concern polynomial maps. For $v \neq 0$, the stabilizer $\mathrm{Stab}(v) \cong \mathrm{SO}(2)$ fixes exactly the line $\mathbb{R}v$, so equivariance forces $\Phi(v) \in \mathbb{R}v$ and hence $\Phi(v) = f(v) \cdot v$ for some scalar function f. Equivariance implies $f(gv) = f(v)$, so f is SO(3)-invariant.

For continuous invariants on $\mathbb{R}^3$, invariance means $f(v)$ depends only on the orbit parameter $|v|$ (equivalently $|v|^2$), so $\Phi(v) = h(|v|^2) \cdot v$ for a continuous h. For smooth invariants, Schwarz's theorem (Schwarz, 1975) implies f factors smoothly through the polynomial generator $|v|^2$. The polynomial setting captures the essential algebraic structure.

3.3 Connection to PVS via Scaling

If we extend SO(3) to $G = \mathrm{SO}(3) \times \mathbb{R}^*$ acting by $(g, \lambda) \cdot v = \lambda g v$, then $(G, \mathbb{R}^3)$ is a PVS with open orbit $\mathbb{R}^3 \setminus \{0\}$. The function $|v|^2$ becomes a relative invariant (not an invariant), and the invariant ring collapses to constants. This connection explains why PVS ideas are "morally" relevant, but for practical machine learning with pure rotations, the FFT is the correct tool.

4 $\mathrm{GL}(n) \times \mathrm{GL}(n)$ on Matrices: A Genuine PVS

We now analyze a representation where PVS theory is genuinely essential.

The term "rank collapse" requires explanation. Unlike scalar collapse—where vector information collapses to scalar (length) information—rank collapse refers to the collapse of discriminating power. The key insight is simple: any invertible matrix can be transformed into any other invertible matrix by left and right multiplication. Concretely, given invertible M and M', we have $M' = (M'M^{-1}) \cdot M \cdot I$. This transitivity has a severe consequence: any function that is invariant under the group action must take the same value on all invertible matrices, because they all lie in a single orbit. Therefore, invariant scalar outputs are constant on the entire open orbit—they carry no information about which invertible matrix we have. The situation worsens at lower-rank matrices: powers like M^2 cannot be used to build richer features because $(AMB^{-1})^2 \neq AM^2B^{-1}$ in general. The only remaining geometric structure is which rank stratum the matrix lies in.

4.1 Prehomogeneous Structure

Consider $G = \mathrm{GL}(n) \times \mathrm{GL}(n)$ acting on $V = \mathrm{Mat}_n(k)$ by $(A, B) \cdot M = AMB^{-1}$.

Theorem 4.1. *The representation* $(\mathrm{GL}(n) \times \mathrm{GL}(n), \mathrm{Mat}_n)$ *is a prehomogeneous vector space with open orbit* $\Omega = \mathrm{GL}(n)$ *(invertible matrices) and singular set* $S = \{M : \det(M) = 0\}$.

Proof. For transitivity on $\mathrm{GL}(n)$: given invertible M, M', we have $M' = (M'M^{-1}, I) \cdot M$. The set $\mathrm{GL}(n)$ is open in Mat_n (its complement, the singular matrices, is defined by $\det = 0$), so it is the open orbit. □

4.2 The Determinant as Relative Invariant

Theorem 4.2. *For* $(\mathrm{GL}(n) \times \mathrm{GL}(n), \mathrm{Mat}_n)$*:*

(i) The relative invariant is $f(M) = \det(M)$*, with character* $\chi(A, B) = \det(A)/\det(B)$.

(ii) The invariant ring is $k[\mathrm{Mat}_n]^G = k$ *(constants only).*

Proof. For (i): $\det(AMB^{-1}) = \det(A)\det(M)\det(B)^{-1} = \chi(A, B)\det(M)$.

For (ii): Any invariant satisfies $p(\lambda M) = p(M)$ for all λ (take $A = \lambda I$, $B = I$), forcing p constant. □

The determinant is a relative invariant, not an invariant. This distinction, emphasized by the Sato-Kimura theory, is essential.

4.3 Rank Stratification

The singular set carries a natural stratification by rank.

Theorem 4.3 (Rank Stratification)**.** *The singular set decomposes as* $S = \bigsqcup_{r=0}^{n-1} \Sigma_r$ *where* $\Sigma_r = \{M : \mathrm{rank}(M) = r\}$*. Each* Σ_r *is a single* G*-orbit with* $\mathrm{codim}(\Sigma_r) = (n - r)^2$.

Proof sketch. Any rank-r matrix can be transformed via row and column operations (i.e., left and right multiplication by invertible matrices) to the canonical form $\mathrm{diag}(1, \ldots, 1, 0, \ldots, 0)$ with r ones. Hence $G = \mathrm{GL}(n) \times \mathrm{GL}(n)$ acts transitively on Σ_r. For the codimension: the variety of matrices of rank at most r has dimension $2nr - r^2$ (view rank-r matrices as products XY^T with $X, Y \in \mathrm{Mat}_{n\times r}$, then quotient by the $\mathrm{GL}(r)$ action). Hence $\mathrm{codim}(\Sigma_r) = n^2 - (2nr - r^2) = (n - r)^2$. □

This stratification, predicted by PVS theory, illuminates rank collapse. We first establish a key lemma.

Lemma 4.4 (Polynomial equivariants for the left–right action are linear)**.** *Let* $G = \mathrm{GL}(n) \times \mathrm{GL}(n)$ *act on* Mat_n *by* $(A, B) \cdot M = AMB^{-1}$*. If* $\Phi : \mathrm{Mat}_n \to \mathrm{Mat}_n$ *is a polynomial* G*-equivariant map (with the same action on the output), then* Φ *is linear.*

Proof. Equivariance with $(A, B) = (\lambda I, I)$ implies $\Phi(\lambda M) = \lambda\Phi(M)$ for all $\lambda \in k^*$. Writing $\Phi = \sum_{d\geq 0} \Phi_d$ as a sum of homogeneous polynomial maps of degree d, we get $\sum_d \lambda^d \Phi_d(M) = \lambda \sum_d \Phi_d(M)$ for all λ. Comparing coefficients of λ^d forces $\Phi_d = 0$ for $d \neq 1$. Hence Φ is homogeneous of degree 1, i.e., linear. □

The key distinctions for rank collapse are:

- Invariant scalars: The invariant ring is $k[\mathrm{Mat}_n]^G = k$ (constants only). An invariant scalar head extracts no information from the input.
- Relative invariants: The determinant $\det(M)$ is a relative invariant defining the singular set. It transforms by a character, so it is not available to invariant computations.

- Covariants: Polynomial G-equivariant maps $\Phi : \mathrm{Mat}_n \to \mathrm{Mat}_n$ (with the same left–right action on the output) are extremely limited. The maps $M \mapsto I$ and $M \mapsto M^k$ for $k \geq 2$ are not equivariant: for instance, $(AMB^{-1})^2 = AM(B^{-1}A)MB^{-1} \neq AM^2B^{-1}$ in general. By Lemma 4.4, any polynomial equivariant self-map is linear. Working over $\mathbb{C}$ (or complexifying if starting over $\mathbb{R}$), Schur's lemma (which states that the only linear maps commuting with an irreducible group action are scalar multiples of the identity) gives $\Phi(M) = cM$ for some $c \in k$.

The severity of rank collapse is now clear: not only does the invariant ring contain no information, but equivariant self-maps are trivial. The only geometric structure is the rank stratification of the singular set.

Remark 4.5 (Depth for Matrix-Equivariant Networks)**.** This makes depth even less useful for matrix-equivariant networks than for rotation-equivariant networks. For SO(3) on $\mathbb{R}^3$, the invariant ring $\mathbb{R}[|v|^2]$ is nontrivial, so depth helps approximate complex functions of $|v|^2$. For matrices under $\mathrm{GL}(n) \times \mathrm{GL}(n)$, the invariant ring is just constants, and equivariant layers can only scale: $M \mapsto cM$. Composing such layers yields $M \mapsto c_1c_2 \cdots c_kM$—still just scaling. There are no nontrivial invariants to build complex functions of, and no nontrivial equivariant transformations to compose.

5 Aggregation Escapes the Constraints

Having characterized the limitations of single-fiber processing, we now show how aggregation escapes them.

5.1 Product Representations Have Richer Invariants

Let G act on V, and consider the product representation (G, V^n) with diagonal action: $g \cdot (v_1, \ldots, v_n) = (g \cdot v_1, \ldots, g \cdot v_n)$.

The invariant ring $k[V^n]^G$ contains not only "fiber invariants" $p(v_i)$ for $p \in k[V]^G$, but also "cross-invariants" depending on multiple v_i. When G acts nontrivially, these cross-invariants typically enrich the invariant structure. The following classical result makes this precise for orthogonal groups.

Theorem 5.1 (O(3) on Multiple Vectors)**.** *For* O(3) *acting diagonally on* $(\mathbb{R}^3)^n$*:*

$$\mathbb{R}[(\mathbb{R}^3)^n]^{\mathrm{O}(3)} = \mathbb{R}\left[\{|v_i|^2\}_{i=1}^n \cup \{v_i \cdot v_j\}_{1 \leq i < j \leq n}\right].$$

Remark 5.2 (Generators vs. Algebraic Independence)**.** For $n \leq 3$, the $\frac{n(n+1)}{2}$ generators (norms and dot products) are algebraically independent, so the invariant ring is a polynomial ring. For $n > 3$, these generators satisfy algebraic relations: the Gram matrix $(v_i \cdot v_j)$ has rank at most 3 (since the vectors lie in $\mathbb{R}^3$), so all 4×4 Gram determinants vanish. The invariant ring is still generated by these dot products, but is not a polynomial ring in $\frac{n(n+1)}{2}$ independent variables.

Remark 5.3 (SO(3) vs. O(3))**.** For SO(3) rather than O(3), the invariant ring also includes scalar triple products $[v_i, v_j, v_k] := \det(v_i, v_j, v_k)$ when $n \geq 3$. These are preserved by rotations but change sign under reflections. The main point—that aggregation enriches the invariant structure—holds for both groups.

Corollary 5.4 (Angles are Accessible)**.** *For two vectors, the angle* θ *satisfies* $\cos\theta = v_1 \cdot v_2/(|v_1||v_2|)$*, which is an orthogonal-group invariant. Networks on pairs of vectors can learn angular relationships.*

Example 5.5 (Aggregation for Matrices)**.** The same principle applies to the PVS case. For $(\mathrm{GL}(n) \times \mathrm{GL}(n), \mathrm{Mat}_n^k)$ with $k \geq 2$ matrices under diagonal action $(A, B) \cdot (M_1, \ldots, M_k) = (AM_1B^{-1}, \ldots, AM_kB^{-1})$, new invariants appear. On the open orbit where all matrices are invertible, we have rational invariants (regular functions on $\mathrm{GL}(n)^k$, not polynomials on Mat_n^k):

$$\mathrm{tr}(M_iM_j^{-1}) \quad \text{for } i \neq j.$$

To verify: $\mathrm{tr}(AM_iB^{-1} \cdot (AM_jB^{-1})^{-1}) = \mathrm{tr}(AM_iB^{-1} \cdot BM_j^{-1}A^{-1}) = \mathrm{tr}(AM_iM_j^{-1}A^{-1}) = \mathrm{tr}(M_iM_j^{-1})$. These "cross-invariants" are unavailable for single matrices, where even rational invariants on $\mathrm{GL}(n)$ are constant. Aggregation escapes PVS constraints just as it escapes FFT constraints.

This explains why message-passing architectures succeed: they aggregate from multiple neighbors, moving from (G, V) to (G, V^n) where richer invariants become accessible.

5.2 Implications for Modern Equivariant Architectures

The algebraic theory developed above—particularly the transition from $k[V]^G$ to $k[V^n]^G$—directly explains design choices in modern equivariant neural networks. We introduce the concept of body-order to formalize this connection.

Definition 5.6 (Body-Order)**.** An architecture has body-order ν at a given layer if its scalar features can be expressed as functions of invariants from $k[V^\nu]^G$—that is, invariants depending jointly on ν local geometric inputs rather than fiber-wise invariants alone.

For SO(3)-equivariant networks on atomic systems, body-order determines which geometric information is accessible:

- $\nu = 1$: Only individual distances $|v_i|$ (fiber-wise invariants from $\prod_i k[V]^G$)
- $\nu = 2$: Distances and angles via $v_i \cdot v_j$ (cross-invariants from $k[V^2]^G$)
- $\nu = 3$: Distances, angles, and dihedral-like correlations (from $k[V^3]^G$)

We analyze four prominent architectures through this lens:

Table 1: Architecture comparison through invariant ring theory. "Irreps" indicates which SO(3) representations are used ($l = 0$ is scalar, $l = 1$ is vector). "Body-order/layer" is ν achieved per message-passing layer. "Parity" indicates whether parity-odd (pseudoscalar/pseudovector) features are accessible.

Architecture	**Irreps**	**Body-order/layer**	**Parity**	**Mechanism**
SchNet	$l = 0$ only	$\nu = 1$	even only	RBF of distances
PaiNN	$l = 0, 1$	$\nu = 2$	even only	$\langle \vec{v}, \vec{v} \rangle$
DimeNet	$l = 0$ only	$\nu = 2$	even only	explicit triplet angles
MACE	$l = 0, \ldots, l_{\max}$	ν (tunable)	tunable	tensor products

SchNet (Schütt et al., 2018) uses only scalar features ($l = 0$) with radial basis functions of pairwise distances. In our framework, SchNet operates in $\prod_i k[|v_i|^2]$—the product of fiber-wise invariant rings. Cross-invariants like $v_i \cdot v_j$ are not directly computed. To access angular information, SchNet must implicitly learn the law of cosines $\cos\theta = (d_{ij}^2 + d_{ik}^2 - d_{jk}^2)/(2d_{ij}d_{ik})$ through network depth, requiring at least 2 layers for a central atom to "see" distances between its neighbors.

PaiNN (Schütt et al., 2021) augments scalars with vector features ($l = 1$). The key operation is the vector inner product in the update block: accumulated vectors $\vec{v}_i = \sum_j w_{ij}\hat{r}_{ij}$ satisfy

$$\langle \vec{v}_i, \vec{v}_i \rangle = \sum_{j,k} w_{ij} w_{ik} (\hat{r}_{ij} \cdot \hat{r}_{ik}) = \sum_{j,k} w_{ij} w_{ik} \cos\theta_{jik}.$$

This directly computes the cross-invariant $v_j \cdot v_k$ from Theorem 5.1, achieving body-order $\nu = 2$ in a single layer. PaiNN's design choice—adding vectors and taking their inner product—is precisely the mechanism that accesses $k[V^2]^G$.

DimeNet (Klicpera et al., 2020) takes an alternative route to body-order 2: explicit enumeration of atom triplets (k, j, i) with direct computation of bond angles θ_{kji}. While DimeNet uses only scalar features, its triplet message-passing accesses $k[V^2]^G$ by construction. The trade-off is computational: DimeNet's complexity scales as $O(|\mathcal{E}| \cdot \bar{k})$ where $\bar{k}$ is average degree, versus $O(|\mathcal{E}|)$ for PaiNN.

MACE (Batatia et al., 2022) achieves higher body-order through systematic tensor products. The key construction is:

$$A_i^{(\nu)} = A_i^{(1)} \otimes A_i^{(1)} \otimes \cdots \otimes A_i^{(1)} \quad (\nu \text{ factors})$$

where $A_i^{(1)} = \sum_j R(d_{ij}) Y(\hat{r}_{ij})$ aggregates radial functions times spherical harmonics over neighbors. In our framework, these tensor products create equivariant tensors that encode ν-body correlations; invariant scalar

features arise after projecting to $l = 0$ components via Clebsch-Gordan decomposition. The resulting scalars can access ν-body cross-invariants from $k[V^\nu]^G$. The body-order parameter ν is architecturally tunable, allowing MACE to directly access dihedral-like correlations ($\nu = 3$) or higher without requiring network depth.

Remark 5.7 (Parity and Chirality)**.** The invariant rings $k[V^n]^{\mathrm{O}(3)}$ and $k[V^n]^{\mathrm{SO}(3)}$ differ: the latter includes pseudoscalars like $\det(v_1, v_2, v_3)$. Architectures restricted to parity-even scalar features—effectively O(3)-invariant readouts—provably cannot represent pseudoscalars and therefore cannot detect chirality. Architectures that include parity-odd (pseudo) channels, such as MACE configured with parity tracking through Clebsch-Gordan decompositions, can access the full SO(3) invariant ring and detect chirality. This is a direct consequence of which invariant ring the architecture can access, not a limitation of specific named models per se (implementations vary in whether they include parity-odd features).

Remark 5.8 (Depth vs. Body-Order)**.** Our analysis clarifies when depth helps and when it cannot. The typical scaling is as follows: for SchNet ($\nu = 1$ per layer), L layers can access up to L-body correlations, since each layer propagates distance information one hop further. For PaiNN/DimeNet ($\nu = 2$ per layer), depth can provide up to $(L + 1)$-body correlations. For MACE with tunable ν, depth can provide up to $L \cdot \nu$-body correlations. These are upper bounds; the precise body-order achieved depends on the specific operations and how information combines across layers. However, if a target function requires invariants outside the architecture's accessible ring (e.g., chirality for parity-even networks), no amount of depth suffices.

The practical implication is that architecture choice should match task requirements: angle-dependent properties require $\nu \geq 2$ (ruling out shallow SchNet), dihedral-dependent properties benefit from $\nu \geq 3$ (favoring MACE over PaiNN/DimeNet at equivalent depth), and chiral properties require parity-odd features (ruling out any parity-even-only configuration).

6 The Role of Depth

A natural question is whether depth can compensate for single-fiber limitations. It cannot.

Theorem 6.1 (Depth Does Not Add Invariants)**.** *Consider a G-equivariant neural network with equivariant linear layers, pointwise nonlinearities applied only to scalar (invariant) channels, tensor products, and an input layer that extracts generating invariants of $k[V]^G$. For invariant scalar outputs:*

(a) Points on the same G-orbit cannot be separated, regardless of depth.

(b) The network output is a function of the generating invariants of $k[V]^G$. For polynomial activations, this is a polynomial in the generators; for continuous activations, a continuous function of them.

(c) Depth allows approximating more complex functions of these generating invariants, but does not create new algebraically independent invariant features.

Proof. (a) If $v' = g \cdot v$ for some $g \in G$, then for any G-invariant function ϕ we have $\phi(v') = \phi(g \cdot v) = \phi(v)$ by definition. Since the network computes a G-invariant output (by equivariance of intermediate layers and invariance of the final scalar), it cannot distinguish v from v'.

(b) We proceed by induction on layers. By assumption, the input layer extracts the generating invariants of $k[V]^G$ as scalar features. At each subsequent layer: (i) equivariant linear maps preserve the property that scalar channels contain invariants; (ii) tensor products followed by Clebsch-Gordan (CG) decomposition (the standard method to decompose tensor products into irreducible representations) produce new channels, but the scalar components remain invariants; (iii) pointwise nonlinearities σ applied to scalar channels produce $\sigma(p_1, \ldots, p_k)$ where p_i are functions of the generating invariants—this remains a function of those generators. By induction, the final output is a function (polynomial or continuous, depending on σ) of the generating invariants.

(c) For polynomial networks: the invariant ring $k[V]^G$ has a fixed transcendence degree (the number of algebraically independent generators) over k, determined by representation theory. Polynomial composition

cannot increase transcendence degree, so depth cannot create new algebraically independent invariants. For continuous networks: MLPs with continuous activations can approximate arbitrary continuous functions of their inputs (universal approximation), but the inputs to the MLP are still only the fixed set of generating invariants. Depth improves approximation quality within the class of continuous functions of these generators. □

7 Experimental Validation

We test two non-trivial predictions of the theory: (1) networks with different symmetry groups but the same architecture template exhibit qualitatively different expressivity, and (2) aggregation enables learning that per-fiber processing cannot achieve. Code is provided as supplementary.

7.1 Setup

All networks are MLPs with two hidden layers of 64 units and ReLU activations, operating on hand-computed invariant features. Training uses Adam with learning rate 10^{-3} for 1000 epochs on 10,000 samples, with evaluation on 2,000 held-out samples. We report R^2 scores; $R^2 = 1$ indicates perfect prediction, $R^2 = 0$ indicates prediction of the mean, and $R^2 < 0$ indicates worse-than-mean predictions.

We sample vectors from an isotropic distribution: directions are uniform on S^2, and radii are drawn independently from a distribution bounded away from zero. For Experiment 1, we additionally ensure reflection symmetry by including both each triple (v_1, v_2, v_3) and its reflection, so parity-even features are unchanged while the triple product flips sign. These distributional choices make the "impossibility" claims that follow mathematically precise rather than heuristic.

7.2 Experiment 1: SO(3) vs O(3) on the Triple Product

Motivation. The triple product $\det(v_1, v_2, v_3) = v_1 \cdot (v_2 \times v_3)$ is a pseudoscalar: it is SO(3)-invariant but changes sign under reflection, so it is not O(3)-invariant. The invariant rings have different generators: $\mathbb{R}[(\mathbb{R}^3)^3]^{\mathrm{O}(3)}$ is generated by norms $|v_i|^2$ and dot products $v_i \cdot v_j$, while $\mathbb{R}[(\mathbb{R}^3)^3]^{\mathrm{SO}(3)}$ is generated by norms, dot products, and the triple product (subject to algebraic relations, e.g., $\det(\mathrm{Gram}(v_1, v_2, v_3)) = \det(v_1, v_2, v_3)^2$). This provides a clean test: both networks process three vectors with identical MLP architectures, differing only in which invariants they compute.

Architectures. The SO(3)-invariant network computes 7 features: three squared norms $|v_i|^2$, three dot products $v_i \cdot v_j$, and the triple product $\det(v_1, v_2, v_3)$. The O(3)-invariant network computes only the 6 parity-even features, excluding the triple product.

Target. $f(v_1, v_2, v_3) = \det(v_1, v_2, v_3) = v_1 \cdot (v_2 \times v_3)$.

Results.

Network	Test MSE	R^2
SO(3)-invariant (7 features)	4×10^{-6}	1.000
O(3)-invariant (6 features)	1.76	-0.308

Interpretation. The SO(3) network learns the target perfectly because the triple product is in its feature set. The O(3) network achieves $R^2 < 0$, performing worse than predicting zero. Under our reflection-symmetric sampling, any function of parity-even invariants has zero correlation with the parity-odd target: $\mathbb{E}[\det(v_1, v_2, v_3) \mid \text{parity-even features}] = 0$. Thus the Bayes-optimal predictor given only parity-even features is the constant 0, and the fundamental limit is $R^2 = 0$. The negative R^2 is a finite-sample optimization artifact where the network fits spurious correlations that fail to generalize. This is not a failure of architecture or optimization but a mathematical impossibility: no function of parity-even invariants can correlate with a parity-odd target under reflection-symmetric data.

7.3 Experiment 2: Aggregation Escapes Scalar Collapse

Motivation. Theorem 5.1 predicts that the invariant ring $\mathbb{R}[(\mathbb{R}^3)^2]^{\mathrm{O}(3)}$ contains cross-invariants $v_1 \cdot v_2$ that are unavailable to per-fiber processing. (For $n = 2$, the SO(3) and O(3) invariants coincide since there is no triple product.) We test whether this algebraic difference translates to a learning difference.

Architectures. The norm-only network processes each vector independently: it computes $|v_1|^2$ and $|v_2|^2$, passes each through a shared MLP, then combines the outputs. This simulates a network without message-passing. The cross-invariant network computes all three invariants $|v_1|^2$, $|v_2|^2$, $v_1 \cdot v_2$ jointly.

Target. $f(v_1, v_2) = \cos\theta = (v_1 \cdot v_2)/(|v_1||v_2|)$, defined on $\{v_1 \neq 0, v_2 \neq 0\}$; we sample vectors with norms bounded away from zero. This is a continuous invariant (involving division), not a polynomial, but continuous invariants on $\mathbb{R}^3$ depend only on the orbit parameters and hence are functions of the polynomial generators.

Results.

Network	Test MSE	R^2
Norm-only (no cross-invariants)	0.342	-0.023
Cross-invariant (has $v_1 \cdot v_2$)	2.1×10^{-5}	0.9999

Interpretation. The norm-only network cannot learn angles because angular information is discarded before combination—this is scalar collapse at the per-fiber level. Under isotropic sampling, $\mathbb{E}[\cos\theta \mid |v_1|, |v_2|] = 0$, so no function of $(|v_1|^2, |v_2|^2)$ can predict $\cos\theta$ better than a constant baseline. The cross-invariant network succeeds because $v_1 \cdot v_2$ is directly available. The gap is not gradual: it is perfect learning versus complete failure, matching the algebraic prediction that angles are functions of cross-invariants but not of fiber-wise norms alone.

Both experiments confirm sharp, qualitative predictions of the theory: different symmetry groups yield different invariant rings, causing identical architectures to exhibit categorically different expressivity (SO(3) vs O(3)), and aggregation enriches the invariant ring, enabling learning that per-fiber processing provably cannot achieve. These results go beyond "invariant networks cannot learn non-invariant targets" (which is true by construction) to demonstrate that the specific structure of invariant rings—which invariants are present, not just that some exist—determines what can be learned.

8 Discussion

8.1 When Different Tools Apply

Our analysis clarifies when different mathematical frameworks are appropriate:

Classical invariant theory (FFT) applies to non-prehomogeneous representations like SO(3) on $\mathbb{R}^3$. The invariant ring is computed by classical methods, and expressivity follows from covariant module structure.

PVS theory applies to prehomogeneous representations like $\mathrm{GL}(n) \times \mathrm{GL}(n)$ on matrices. The Sato-Kimura classification identifies the relative invariant, and the discriminant stratification provides geometric insight.

General invariant theory governs aggregation: moving from V to V^n enriches invariants regardless of PVS status.

8.2 Connection to Universality and Separation Results

Our algebraic framework complements and clarifies several lines of work on neural network expressivity.

Universal approximation. Keriven and Peyré (2019) and Yarotsky (2022) establish that sufficiently expressive equivariant architectures can approximate any continuous equivariant function. Our results are consistent: Theorem 6.1 shows that networks can approximate arbitrary functions of the generating invariants. For the specific case of SO(3) on $\mathbb{R}^3$, the orbit space is one-dimensional (parameterized by $|v|$), so continuous invariants are automatically functions of $|v|^2$; for smooth invariants of compact Lie groups more generally,

Schwarz's theorem (Schwarz, 1975) guarantees they factor through polynomial generators. The limitation is not approximation power but the input features: if the invariant ring is k (constants), there is nothing to approximate.

Separation and discrimination. Maron et al. (2019a) and Xu et al. (2019) characterize when graph neural networks can distinguish non-isomorphic graphs, connecting to the Weisfeiler-Leman hierarchy. Our Theorem 6.1(a) provides the algebraic version: points on the same G-orbit cannot be separated by invariant outputs, regardless of architecture details. This is not a limitation of specific networks but a fundamental constraint from representation theory.

Higher-order methods. The success of higher-order graph networks (Maron et al., 2019b; Morris et al., 2019) and k-WL methods parallels our aggregation results: moving from single-node to k-tuple processing enriches the invariant structure, just as $(G, V) \to (G, V^n)$ enriches $k[V]^G$ to $k[V^n]^G$ with cross-invariants.

Geometric deep learning. Bronstein et al. (2021) provide a unified framework viewing many architectures through the lens of symmetry. Our contribution is the explicit computation of which symmetries lead to which expressivity constraints, via classical invariant theory. The FFT and PVS theory provide the algebraic tools to make these constraints precise.

8.3 Limitations

Our analysis concerns polynomial maps; extending to smooth or continuous maps requires additional tools such as Schwarz's theorem. Finite groups like S_n are better handled by the Weisfeiler-Leman framework than by classical invariant theory. We have characterized which functions are representable but not how gradient descent navigates the space of equivariant functions—learning dynamics remain to be studied.

9 Conclusion

We asked why certain group representations lead to expressivity limitations in equivariant neural networks, and found that the answer lies in the algebraic structure of invariant rings.

The case of $\mathrm{SO}(3)$ acting on $\mathbb{R}^3$ illustrates the mechanism. This representation is not prehomogeneous—its orbits are spheres, not an open dense set—so the First Fundamental Theorem rather than PVS theory applies. The theorem tells us that the invariant ring is generated by $|v|^2$ alone, and consequently every equivariant map $\mathbb{R}^3 \to \mathbb{R}^3$ has the form $v \mapsto p(|v|^2) \cdot v$. Directional information is not suppressed by accident or poor architecture; it is algebraically inaccessible. The case of $\mathrm{GL}(n) \times \mathrm{GL}(n)$ on matrices is more severe: here the representation is genuinely prehomogeneous, the invariant ring contains only constants, and equivariant self-maps reduce to scalar multiples of the identity. The rank stratification predicted by PVS theory is all the geometric structure that remains.

The escape from these constraints comes not from depth but from aggregation. When we pass from a single fiber V to the product V^n, the invariant ring acquires cross-invariants that encode relationships between fibers. For orthogonal groups, these are the dot products $v_i \cdot v_j$ that give access to angles; for $n \geq 3$, the triple products $\det(v_i, v_j, v_k)$ give access to chirality. This algebraic fact explains why message-passing architectures succeed where per-edge processing fails, and why body-order—the number of geometric inputs combined before extracting invariants—is the relevant architectural parameter for expressivity.

For practitioners, the implication is concrete: when performance plateaus, check the invariant ring before adding layers. Depth improves approximation of functions that are already representable; it cannot conjure invariants that the algebra forbids.

References

Ilyes Batatia, Dávid Péter Kovács, Gregor N. C. Simm, Christoph Ortner, and Gábor Csányi. MACE: Higher order equivariant message passing neural networks for fast and accurate force fields. In *Advances in Neural Information Processing Systems (NeurIPS)*, volume 35, pages 11423–11436, 2022.

Simon Batzner, Albert Musaelian, Lixin Sun, Mario Geiger, Jonathan P. Mailoa, Mordechai Kornbluth, Nicola Molinari, Tess E. Smidt, and Boris Kozinsky. E(3)-equivariant graph neural networks for data-efficient and accurate interatomic potentials. *Nature Communications*, 13:2453, 2022.

Ben Blum-Smith and Soledad Villar. Machine learning and invariant theory. *Notices of the American Mathematical Society*, 70(8):1205–1213, 2023. doi: 10.1090/noti2760.

Michael M. Bronstein, Joan Bruna, Taco Cohen, and Petar Veličković. Geometric deep learning: Grids, groups, graphs, geodesics, and gauges. *arXiv:2104.13478*, 2021.

Taco Cohen and Max Welling. Group equivariant convolutional networks. In *International Conference on Machine Learning (ICML)*, 2016.

Nadav Dym and Haggai Maron. On the universality of rotation equivariant point cloud networks. In *International Conference on Learning Representations (ICLR)*, 2020.

Chaitanya K. Joshi, Cristian Bodnar, Simon V. Mathis, Taco Cohen, and Pietro Liò. On the expressive power of geometric graph neural networks. In *International Conference on Machine Learning (ICML)*, 2023.

Nicolas Keriven and Gabriel Peyré. Universal invariant and equivariant graph neural networks. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2019.

Tatsuo Kimura. *Introduction to Prehomogeneous Vector Spaces*, volume 215 of *Translations of Mathematical Monographs*. American Mathematical Society, 2003.

Johannes Klicpera, Janek Groß, and Stephan Günnemann. Directional message passing for molecular graphs. In *International Conference on Learning Representations (ICLR)*, 2020.

Risi Kondor. The principles behind equivariant neural networks for physics and chemistry. *Proceedings of the National Academy of Sciences*, 122(41):e2415656122, 2025. doi: 10.1073/pnas.2415656122.

Hanspeter Kraft and Claudio Procesi. Classical invariant theory: A primer. Lecture notes, University of Basel, 2000.

Haggai Maron, Heli Ben-Hamu, Hadar Serviansky, and Yaron Lipman. Provably powerful graph networks. In *Advances in Neural Information Processing Systems (NeurIPS)*, 2019a.

Haggai Maron, Heli Ben-Hamu, Nadav Shamir, and Yaron Lipman. Invariant and equivariant graph networks. In *International Conference on Learning Representations (ICLR)*, 2019b.

Haggai Maron, Ethan Fetaya, Nimrod Segol, and Yaron Lipman. On the universality of invariant networks. In *International Conference on Machine Learning (ICML)*, 2019c.

Christopher Morris, Martin Ritzert, Matthias Fey, William L. Hamilton, Jan Eric Lenssen, Gaurav Rattan, and Martin Grohe. Weisfeiler and Leman go neural: Higher-order graph neural networks. In *AAAI Conference on Artificial Intelligence*, 2019.

Marco Pacini, Gabriele Santin, Xiaowen Dong, and Bruno Lepri. Separation power of equivariant neural networks. *arXiv:2406.08966*, 2024.

Omri Puny, Derek Lim, Bobak T. Kiani, Haggai Maron, and Yaron Lipman. Equivariant polynomials for graph neural networks. In *International Conference on Machine Learning (ICML)*, 2023.

Alvaro Sanchez-Gonzalez, Jonathan Godwin, Tobias Pfaff, Rex Ying, Jure Leskovec, and Peter Battaglia. Learning to simulate complex physics with graph networks. In *International Conference on Machine Learning (ICML)*, 2020.

Mikio Sato and Tatsuo Kimura. A classification of irreducible prehomogeneous vector spaces and their relative invariants. *Nagoya Mathematical Journal*, 65:1–155, 1977. doi: 10.1017/s0027763000017633.

Kristof T. Schütt, Huziel E. Sauceda, Pieter-Jan Kindermans, Alexandre Tkatchenko, and Klaus-Robert Müller. SchNet – a deep learning architecture for molecules and materials. *Journal of Chemical Physics*, 148:241722, 2018.

Kristof T. Schütt, Oliver T. Unke, and Michael Gastegger. Equivariant message passing for the prediction of tensorial properties and molecular spectra. In *International Conference on Machine Learning (ICML)*, pages 9377–9388, 2021.

Gerald W. Schwarz. Smooth functions invariant under the action of a compact Lie group. *Topology*, 14: 63–68, 1975.

Nathaniel Thomas, Tess Smidt, Steven Kearnes, Lusann Yang, Li Li, Kai Kohlhoff, and Patrick Riley. Tensor field networks: Rotation- and translation-equivariant neural networks for 3D point clouds. *arXiv:1802.08219*, 2018.

Soledad Villar, David W. Hogg, Kate Storey-Fisher, Weichi Yao, and Ben Blum-Smith. Scalars are universal: Equivariant machine learning, structured like classical physics. *Advances in Neural Information Processing Systems (NeurIPS)*, 34:28848–28863, 2021.

Hermann Weyl. *The Classical Groups: Their Invariants and Representations*. Princeton University Press, 1946.

Keyulu Xu, Weihua Hu, Jure Leskovec, and Stefanie Jegelka. How powerful are graph neural networks? In *International Conference on Learning Representations (ICLR)*, 2019.

Dmitry Yarotsky. Universal approximations of invariant maps by neural networks. *Constructive Approximation*, 55:407–474, 2022.