Equivariant maps from invariant functions

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Abstract

In equivariant machine learning the idea is to restrict the learning to a hypothesis class where all the functions are equivariant with respect to some group action. Irreducible representations or invariant theory are typically used to parameterize the space of such functions. In this note, we explicate a general procedure, attributed to Malgrange, to express all polynomial maps between linear spaces that are equivariant with respect to the action of a group $G$, given a characterization of the invariant polynomials on a bigger space. The method also parametrizes smooth equivariant maps in the case that $G$ is a compact Lie group.

1 Introduction

Modern machine learning performs regression on classes of functions that are typically overparameterized, and where the optimization is non-convex. Therefore the model performance is highly dependent on how the class of functions is parameterized (see for instance [22] for an introductory discussion on the role of parameterization on linear models). The parameterization of the hypothesis class of functions is what in deep learning is typically referred to as the architecture. In the past years the most successful architectures have been the ones that took advantage of the compositional structure of the data to design the class of functions: convolutional neural networks, recurrent neural networks, graph neural networks, transformers, etc. The design of the architecture tries to answers one question: what is the correct inductive bias for this learning problem?

In cases where the learning problem comes from the physical sciences, there is a concrete set of rules that data must obey. Those rules are typically coming from coordinate freedoms and conservation laws. In order to do machine learning on those problems, researchers have designed models that are consistent with physical law; this is the case for physics-informed machine learning [24], neural ODEs and PDEs [5, 37], and equivariant machine learning [55, 8, 7, 31, 51].

Given data spaces $V, W$ and a group $G$ acting on both of them, a function $f : V \rightarrow W$ is equivariant if $f(g \cdot v) = g \cdot f(v)$ for all $g \in G$ and all $v \in V$. 

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Many physical problems are equivariant with respect to rotation, permutation or scaling. Equivariant machine learning restricts the hypothesis space to a class of equivariant functions. The philosophy is that every function that the machine learning model can express is equivariant, and therefore consistent with physical law.

Group equivariant machine learning was formally introduced by Cohen and Welling in [8], where they designed equivariant convolutional neural networks for images. Later work focused on the equivariant machine learning on particle systems [25, 14, 17], where classical representation theory is used to parameterize the space of equivariant functions. Graph neural networks can also be seen as equivariant functions that take a graph represented by its adjacency matrix $A \in \mathbb{R}^{n \times n}$ and output an embedding $f(A) \in \mathbb{R}^{n \times d}$ so that $f(\Pi A \Pi^T) = \Pi f(A)$ for all $\Pi \in \mathbb{R}^{n \times n}$ permutation matrices [10, 4, 19, 31, 6].

Recently, equivariant machine learning models have been extremely successful at predicting molecular structures and dynamics [1, 34, 42], protein folding [23], protein binding [41], and simulating turbulence and climate effects [54, 48, 49]. Theoretical developments have shown universality of certain equivariant models [11, 32, 3], generalization improvements of equivariant machine learning models over non-equivariant baselines [2, 12, 13, 33], and there has been some recent work studying the inductive bias of equivariant machine learning [28], and its relationship with data augmentation [50, 18].

Most equivariant machine learning models are implemented in terms of irreducible representations [25, 26, 27, 14, 45, 17]. In a nutshell, the idea is to parameterize the models as a feed-forward neural network (i.e. the composition of linear layers with non-linear activation functions), and restrict the linear layers to be linear equivariant functions (often on a tensor product of inputs to guarantee that the class of functions is expressive enough). To this end, the parameterization of the linear equivariant layers requires the decomposition of the tensor space into its irreducible representations, which is done in terms of the Clebsch-Gordan coefficients.

Recent works propose to use invariant polynomials to design machine learning models [21, 20, 46, 47, 53], which have been used in cosmology [43] and molecular dynamics [15]. This is also implicitly done in [38, 29]. In particular, the authors of this note and collaborators [46] show that for some physically relevant groups—the orthogonal group, the special orthogonal group, and the lorentz group—one can use classical invariant theory to design universally expressive equivariant machine learning models that are expressed in terms of the generators of the algebra of invariant polynomials. Following an idea attributed to B. Malgrange (that we learned from G. Schwarz), it is shown how to use the generators of the algebra of invariant polynomials to produce a parameterization of equivariant functions for a specific set of groups and actions.

To illustrate, let us focus on $O(d)$-equivariant functions, namely functions $f : (\mathbb{R}^d)^n \to \mathbb{R}^d$ such that $f(Qv_1, \ldots, Qv_n) = Qf(v_1, \ldots, v_n)$ for all $Q \in O(d)$ and all $v_1, \ldots, v_n \in \mathbb{R}^d$ (for instance, the prediction of the position and velocity of the center of mass of a particle system). The method of B. Malgrange (explicated
again below) leads to the conclusion that all such functions can be expressed as
\[ f(v_1, \ldots, v_n) = \sum_{s=1}^{n} f_s(v_1, \ldots, v_n)v_s \]  
(1)

where \( f_s : (\mathbb{R}^d)^n \to \mathbb{R} \) are \( O(d) \)-invariant functions. Classical invariant theory shows that \( f_s \) is \( O(d) \)-invariant if and only if it is a function of the pairwise inner products \( (v_i^T v_j)_{i,j=1}^n \). In other words, the pairwise inner products generate the algebra of invariant polynomials for this action, and every equivariant map is a linear combination of the vectors themselves with coefficients in this algebra.

In this note we explicate the method of B. Malgrange in full generality, showing how to convert knowledge of the algebra of invariant polynomials into a characterization of equivariant polynomial (or smooth) maps. We motivate the approach in Section 2 by working through the special case of \( O(d) \), discussed above. In Section 3 we explain the general philosophy of the method, and in Section 4 we give the precise algebraic formulation.

## 2 Example

Let \( V = (\mathbb{R}^d)^n \), \( W = \mathbb{R}^d \), and \( G = O(d) \) acting on copies of \( \mathbb{R}^d \) as
\[ Q(v_1, \ldots, v_n) = (Qv_1, \ldots, Qv_n) , \]
where \( Q \in O(d) \) is the standard matrix representation. The goal is to characterize all polynomial functions \( f : (\mathbb{R}^d)^n \to \mathbb{R}^d \) that are \( O(d) \)-equivariant. Given such an \( f \) we define the map:
\[ (\mathbb{R}^d)^n \times (\mathbb{R}^d)^* \to \mathbb{R} \]  
\[ (v_1, \ldots, v_n, \ell) \mapsto \ell(f(v_1, \ldots, v_n)) , \]  
(2)

where \( (\mathbb{R}^d)^* \) is the dual space of \( \mathbb{R}^d \), i.e., the space of linear maps \( \mathbb{R}^d \to \mathbb{R} \). The group \( O(d) \) acts on \( (\mathbb{R}^d)^* \) according to the dual representation (also called the contragredient representation), namely \( (Q\ell)(v) = \ell(Q^{-1}v) \) for all \( v \in \mathbb{R}^d \) and \( \ell \in (\mathbb{R}^d)^* \). A simple computation shows that (2) is an \( O(d) \)-invariant map.

By basic linear algebra (or the Riesz representation theorem) we know there exists \( v^* \) such that \( \ell(w) = w^T v^* \) for all \( w \in \mathbb{R}^d \). Using this identification of \( (\mathbb{R}^d)^* \) with \( \mathbb{R}^d \) we can express (2) as
\[ (\mathbb{R}^d)^n \times (\mathbb{R}^d) \to \mathbb{R} \]  
\[ (v_1, \ldots, v_n, v^*) \mapsto f(v_1, \ldots, v_n)^T v^* . \]  
(3)

Since the dual representation in \( (\mathbb{R}^d)^* \) corresponds with left multiplication by the inverse transpose, and for all \( Q \in O(d) \) we have \( (Q^{-1})^T = Q \), then \( O(d) \) acts in the same way on each of the \( n+1 \) copies of \( \mathbb{R}^d \). Therefore, the map (3) is invariant with respect to the action of \( O(d) \) in these \( n+1 \) copies. (For groups not contained in \( O(d) \), this will not be the case.)
The first fundamental theorem of invariant functions for $O(d)$ says that the algebra of invariant polynomials on $(v_1, \ldots, v_n, v^*) \in (\mathbb{R}^d)^{n+1}$ is generated by the inner products $(v_i^* v_j)_{i,j=1}^n \cup (v_i^* v^*)_{s=1}^n$.

Since the map in (3) is an invariant degree-1 homogeneous polynomial on $v^*$ we have

$$f(v_1, \ldots, v_n)^\top v^* = \sum_{s=1}^n p_s((v_i^* v_j)_{i,j=1}^n) v_s^* v^*,$$

(4)

for some $p_s$ polynomial functions. Since (4) holds for all $v^*$ we have

$$f(v_1, \ldots, v_n) = \sum_{s=1}^n p_s((v_i^* v_j)_{i,j=1}^n) v_s.$$

(5)

This is the proof of the polynomial version of Proposition 4 in [46]. The proof idea is due to Malgrange; we learned it from Gerald Schwarz.

**Proposition 2.1** (Proposition 4 in [46]). Let $f : (\mathbb{R}^d)^n \rightarrow \mathbb{R}^d$ a polynomial map. Then $f$ is $O(d)$-equivariant if and only if

$$f(v_1, \ldots, v_n) = \sum_{s=1}^n p_s((v_i^* v_j)_{i,j=1}^n) v_s,$$

(6)

where $p_s$ are arbitrary polynomials.

In this note we show how to use the approach above in general to derive characterizations of equivariant functions in terms of the invariants. We give a big picture idea in Section 3 and we present the method formally in Section 4.

### 3 Big picture

We are given a group $G$, and finite-dimensional linear $G$-representations $V$ and $W$ over a field $k$. (We can take $k = \mathbb{R}$ or $\mathbb{C}$.) We want to understand the equivariant polynomial maps $V \rightarrow W$. We assume we have a way to understand $G$-invariant polynomials on spaces related to $V$ and $W$, and the goal is to leverage that knowledge to understand the equivariant maps.

The following is a philosophical discussion, essentially to answer the question: why should it be possible to do this? It is not precise; its purpose is just to guide thinking. Below in Section 4 we show how to actually compute the equivariant polynomials $V \rightarrow W$ given an adequate knowledge of the invariants. That section is rigorous.

The first observation is that any reasonable family of maps $V \rightarrow W$ (for example: linear, polynomial, smooth, continuous, etc.) has a natural $G$-action induced from the actions on $V$ and $W$, and that the $G$-equivariant maps in such a family are precisely the fixed points of this action, as we now explain. This observation is a standard insight in representation and invariant theory.

Let Maps$(V, W)$ be the set of maps of whatever kind, and let $GL(V)$ (respectively $GL(W)$) be the group of linear invertible maps from $V$ (respectively
Given $f \in \text{Maps}(V, W)$ and $g \in G$ and $v \in V$, we define the map $gf$ by
\[
gf := \psi(g) \circ f \circ \phi(g^{-1}),
\] (7)
where $\phi : G \to GL(V)$ and $\psi : G \to GL(W)$ are the group homomorphisms defining the representations $V$ and $W$. The algebraic manipulation to verify that this is really a group action is routine and not that illuminating. A perhaps more transparent way to understand this definition of the action as “the right one” is that it is precisely the formula needed to make this square commute:

It follows from the definition of this action that the condition $gf = f$ is equivalent to the statement that $f$ is $G$-equivariant. The square above automatically commutes, so $gf = f$ is the same as saying that the below square commutes—

—an and this is what it means to be equivariant.

The second observation is that Maps($V,W$) can be identified with functions from a bigger space to the underlying field $k$ by “currying”, and this change in point of view preserves the group action. Again, this is a standard maneuver in algebra. Specifically, given any map $f \in \text{Maps}(V,W)$, we obtain a function $\tilde{f} : V \hat{\times} W^* \to k$, where $W^*$ is the linear dual of $W$, defined by the formula

Note that the function $\tilde{f}$ is linear homogeneous in $\ell \in W^*$. Conversely, given any function $f' : V \times W^* \to k$ that is linear homogeneous in the second coordinate, we can recover a map $f : V \to W$ such that $f' = \tilde{f}$, by taking $f(v)$ to be the element of $W$ identified along the canonical isomorphism $W \to W^{**}$ with the functional on $W^*$ that sends $\ell \in W^*$ to $f'(v, \ell)$—this functional is guaranteed to exist by the fact that $f'$ is linear homogeneous in the second coordinate. An observation we will exploit in the next section is that the desired functional is actually the total derivative of $f'(v, \ell)$ with respect to $\ell$.

This construction gives an identification of Maps($V,W$) with a subset of Maps($V \times W^*, k$). Furthermore, there is a natural action of $G$ on Maps($V \times W^*, k$), defined precisely by the above formula (7) with $V \times W^*$ in place of $V$, $k$
in place of \( W \), and trivial action on \( k \)\(^1\) and the identification described here preserves this action. Therefore, the fixed points for the \( G \)-action on \( \text{Maps}(V,W) \) correspond with fixed points for the \( G \)-action on \( \text{Maps}(V \times W^*, k) \), which are 

\textit{invariant functions} (since the action of \( G \) on \( k \) is trivial).

What has been achieved is the reinterpretation of equivariant maps \( f \in \text{Maps}(V,W) \) first as fixed points of a \( G \)-action, and then as invariant functions \( \tilde{f} \in \text{Maps}(V \times W^*, k) \). Thus, knowledge of invariant functions can be parlayed into knowledge of equivariant maps.

4 Equivariance from invariants

With the above imprecise philosophical discussion as a guide, Algorithm\(^1\) shows how in practice to get from a description of invariant polynomials on \( V \times W^* \), to equivariant polynomial (or smooth) maps \( V \to W \). The technique given here is attributed to B. Malgrange; see \([36, \text{Proposition 2.2}]\) where it is used to obtain the smooth equivariant maps, and \([40, \text{Proposition 6.8}]\) where it is used to obtain holomorphic equivariant maps. Variants on this method are used to compute equivariant maps in \([16, \text{Sections 2.1–2.2}], [35, \text{Section 3.12}], \) and \([9, \text{Section 4.2.3}]\).

The goal of the algorithm is to provide a parametrization of equivariant maps. That said, the proof of correctness is constructive: as an ancillary benefit, it furnishes a method for taking an arbitrary equivariant map given by explicit polynomial expressions for the coordinates, and expressing it in terms of this parametrization.

We now exposit in detail Algorithm\(^1\) and its proof of correctness, in the case where \( f \) is a polynomial map; for simplicity we take \( k = \mathbb{R} \). The argument is similar for smooth or holomorphic maps, except that one needs an additional theorem to arrive at the expression \((8)\) below. If \( G \) is a compact Lie group, the needed theorem is proven in \([39]\) for smooth maps, and in \([30]\) for holomorphic maps over \( \mathbb{C} \).

We begin with linear representations \( V \) and \( W \) of a group \( G \) over \( \mathbb{R} \). We take \( W^* \) to be the contragredient representation to \( W \), defined above. (If \( G \) is compact, we can work in a coordinate system in which the action of \( G \) on \( W \) is orthogonal, and then we may ignore the distinction between \( W \) and \( W^* \), as discussed above in the case of \( G = O(d) \).) We suppose we have an explicit set \( f_1, \ldots, f_m \) of polynomials that generate the algebra of invariant polynomials on the vector space \( V \times W^* \) (denoted as \( \mathbb{R}[V \times W^*]^G \))—in other words, they have the property that \textit{any} invariant polynomial can be written as a polynomial in these. We also assume they are \textit{bihomogeneous}, i.e., independently homogeneous in \( V \) and in \( W^* \). To reduce notational clutter we suppress the maps specifying the actions of \( G \) on \( V \) and \( W \) (which were called \( \varphi \) and \( \psi \) in the previous

\(^1\) The action of \( G \) on \( V \times W^* \) is defined by acting separately on each factor; the action on \( W^* \) is the contragredient representation defined in the previous section. As an aside, since \( W^* \) is the set of linear maps from \( W \) to \( k \), the contragredient representation, too, is defined by the formula \((7)\) with trivial action on \( k \).
Algorithm 1 Malgrange’s method for getting equivariant functions

**Input:** Bihomogeneous generators $f_1, \ldots, f_m$ for $\mathbb{R}[V \times W^*]^G$.

1. Order the generators so that $f_1, \ldots, f_r$ are of degree 0 and $f_{r+1}, \ldots, f_s$ are of degree 1 in $W^*$. Discard $f_{s+1}, \ldots, f_m$ (of higher degree in $W^*$).

2. Choose a basis $e_1, \ldots, e_n$ for $W$, and let $e_1^\top, \ldots, e_n^\top$ be the dual basis, so an arbitrary element $\ell \in W^*$ can be written

$$\ell = \sum_{i=1}^n \ell_i e_i^\top,$$

and $\ell(e_i) = \ell_i$.

3. For $j = r+1, \ldots, s$, and for $v \in V, \ell \in W^*$, let $F_j(v)$ be the total derivative of $f_j(v, \ell)$ with respect to $\ell \in W^*$, identified with an element of $W$ along the canonical isomorphism $W^{**} \cong W$: explicitly,

$$F_j(v) := \sum_{i=1}^n \left( \frac{\partial}{\partial \ell_i} f_j(v, \ell) \right) e_i.$$

Then each $F_j$ is a function $V \to W$.

**Output:** Equivariant functions $F_{r+1}, \ldots, F_s$ from $V$ to $W$ such that any equivariant $f : V \to W$ can be written as

$$f = \sum_{j=r+1}^s p_j(f_1, \ldots, f_r) F_j.$$
From the invariance of \( \tilde{f} \), and the fact that \( f_1, \ldots, f_m \) generate the algebra of invariant polynomials on \( V \times W^* \), we have an equality of the form

\[
\tilde{f}(v, \ell) = P(f_1(v), \ldots, f_m(v, \ell)),
\]

where \( P \in \mathbb{R}[X_1, \ldots, X_m] \) is a polynomial. Note that \( f_1, \ldots, f_r \) do not depend on \( \ell \), while \( f_{r+1}, \ldots, f_m \) do.

We now fix \( v \in V \) and take the total derivative \( D_\ell \) of both sides of (8) with respect to \( \ell \) viewed as an element of \( W^\ast \). Choosing dual bases \( e_1, \ldots, e_n \) for \( W \) and \( e_1^\top, \ldots, e_n^\top \) for \( W^* \), and writing \( \ell = \sum \ell_i e_i^\top \), we can express the operator \( D_\ell \) acting on a smooth function \( F : W^* \to \mathbb{R} \) explicitly by the formula

\[
D_\ell F = \sum_{i=1}^{n} \left( \frac{\partial}{\partial \ell_i} F \right) e_i.
\]

Applying \( D_\ell \) to the left side of (8), we get

\[
D_\ell \tilde{f}(v, \ell) = \sum_{i=1}^{n} \left( \frac{\partial}{\partial \ell_i} \ell(f(v)) \right) e_i = \sum_{i=1}^{n} \left( \frac{\partial}{\partial \ell_i} \left( \sum_{j=1}^{m} \ell_j e_j^\top f(v) \right) \right) e_i = \sum_{i=1}^{n} (e_i^\top f(v)) e_i = f(v),
\]

so \( D_\ell \) recovers \( f \) from \( \tilde{f} \). (Indeed, this was the point.) Meanwhile, applying \( D_\ell \) to the right side of (8), writing \( \partial_j P \) for the partial derivative of \( P \) with respect to its \( j \)th argument, and using the chain rule, we get

\[
D_\ell P(f_1, \ldots, f_m) = \sum_{j=1}^{m} \partial_j P(f_1, \ldots, f_m) D_\ell f_j.
\]

Combining these, we conclude

\[
f(v) = \sum_{j=1}^{m} \partial_j P(f_1(v), \ldots, f_m(v, \ell)) D_\ell f_j(v, \ell).
\]

Now we observe that \( D_\ell f_j(v) = 0 \) if \( j \leq r \), because in those cases \( f_j(v) \) is constant with respect to \( \ell \). But meanwhile, the left side of (9) does not depend on \( \ell \), and it follows the right side does not either; thus we can evaluate it at our favorite choice of \( \ell \); we take \( \ell = 0 \). Upon doing this, \( D_\ell f_j(v, \ell) \mid_{\ell=0} \) also becomes 0 for \( j > s \), because in these cases \( f(v, \ell) \) is homogeneous of degree at least 2 in

\footnote{In the background, we are using canonical isomorphisms to identify \( W^* \) with all its tangent spaces, and \( W^{**} \) with \( W \).}
\(\ell\), so its partial derivatives with respect to the \(\ell_i\) remain homogeneous degree at least 1 in \(\ell\), thus they vanish at \(\ell = 0\). Meanwhile, \(f_j(v, \ell)\) itself vanishes for \(j = r + 1, \ldots, m\), so that the \((r + 1)\)st to \(m\)th arguments of each \(\partial_j P\) vanish. Abbreviating

\[\partial_j P(f_1(v), \ldots, f_r(v), 0, \ldots, 0)\]

as \(p_j(f_1(v), \ldots, f_r(v))\), we may thus rewrite (9) as

\[f(v) = \sum_{j=r+1}^s p_j(f_1(v), \ldots, f_r(v))D_\ell f_j(v, \ell).\]

Finally, we observe that, \(f_j\) being linear homogeneous in \(\ell\) for \(j = r + 1, \ldots, s\), \(D_\ell f_j(v, \ell)\) is degree 0 in \(\ell\), i.e., it does not depend on \(\ell\). So we may call it \(F_j(v)\) as in the algorithm, and we have finally expressed \(f\) as the sum \(\sum_{j=r+1}^s p_j(f_1, \ldots, f_r)F_j\), as promised.

5 Discussion

This note shows how to parameterize equivariant maps \(V \to W\) given knowledge of the generators of the space of invariant polynomials on \(V \times W^*\). This is useful to design equivariant machine learning with respect to groups and actions where the invariants are known and are computationally tractable. This is not a panacea: sometimes the algebra of invariant polynomials is too large, or outright not known. Both these issues come up, for example, in the action of permutations on \(n \times n\) symmetric matrices by conjugation, the relevant one for graph neural networks. The invariant ring has not been fully described as of this writing, except for small \(n\), where the number of generators increases very rapidly with \(n\); see [44].

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