

On the Generalization of Equivariance and Convolution in Neural Networks to the Action of Compact Groups

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Abstract

Convolutional neural networks have been extremely successful in the image recognition domain because they ensure equivariance to translations. There have been many recent attempts to generalize this framework to other domains, including graphs and data lying on manifolds. In this paper we give a rigorous, theoretical treatment of convolution and equivariance in neural networks with respect to not just translations, but the action of any compact group. Our main result is to prove that (given some natural constraints) convolutional structure is not just a sufficient, but also a necessary condition for equivariance to the action of a compact group. Our exposition makes use of concepts from representation theory and noncommutative harmonic analysis and derives new generalized convolution formulae.

1. Introduction

One of the most successful neural network architectures is convolutional neural networks (CNNs) (LeCun et al., 1989). In the image recognition domain, where CNNs were originally conceived, convolution plays two crucial roles. First, it ensures that in any given layer, exactly the same filters are applied to each part of the image. Consequently, if the input image is translated, the activations of the network in each layer will translate the same way. This property is called *equivariance* (Cohen & Welling, 2016). Second, in conjunction with pooling, convolution ensures that each neuron’s effective receptive field is a spatially contiguous domain. As we move higher in the network, these domains generally get larger, allowing the CNN to capture structure in images at *multiple different scales*.

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Recently, there has been considerable interest in extending neural networks to more exotic types of data, such as graphs or functions on manifolds (Niepert et al., 2016; Defferrard et al., 2016; Duvenaud et al., 2015; Li et al., 2016; Cohen et al., 2018; Monti et al., 2017; Masci et al., 2015). In these domains, equivariance and multiscale structure are just as important as for images, but finding the right notion of convolution is not obvious.

On the other hand, mathematics does offer a sweeping generalization of convolution tied in deeply with some fundamental ideas of abstract algebra: if G is a compact group and f and g are two functions $G \rightarrow \mathbb{C}$, then the convolution of f with g is defined

$$(f * g)(u) = \int_G f(uv^{-1}) g(v) d\mu(v). \quad (1)$$

Note the striking similarity of this formula to the ordinary notion of convolution, except that in the argument of f , $u - v$ has been replaced by the group operation uv^{-1} , and integration is with respect to the Haar measure, μ .

The goal of this paper is to relate (1) to the various looser notions of convolution used in the neural networks literature, and show that several practical neural networks implicitly already take advantage of the above group theoretic concept of convolution. In particular, we prove the following theorem (paraphrased here for simplicity).

Theorem 1. *A feed forward neural network \mathcal{N} is equivariant to the action of a compact group G on its inputs if and only if each layer of \mathcal{N} implements a generalized form of convolution derived from (1).*

To the best of our knowledge, this is the first time that the connection between equivariance and convolution in neural networks has been stated at this level of generality. One of the technical challenges in proving our theorem is that the activations in each layer of a neural net correspond to functions on a sequence of spaces *acted on* by G (called *homogeneous spaces* or *quotient spaces*) rather than functions on G itself. This necessitates a discussion of group convolution that is rather more thoroughgoing than is customary in pure algebra.

This paper does not present any new algorithms or neural

network architectures. Rather, its goal is to provide the language for thinking about generalized notions of equivariance and convolution in neural networks, and thereby facilitate the development of future architectures for data with non-trivial symmetries. To avoid interruptions in the flow of our exposition, we first present the theory in its abstract form, and then illustrate it with examples in Section 6. For better understanding, the reader might choose to skip back and forth between these sections. One work that is close in spirit to the present paper but only considers discrete groups is (Ravanbakhsh et al., 2017).

2. Notation

In the following $[a]$ will denote the set $\{1, 2, \dots, a\}$. Given a set \mathcal{X} and a vector space V , $L_V(\mathcal{X})$ will denote the space of functions $\{f: \mathcal{X} \rightarrow V\}$.

3. Equivariance in neural networks

A feed-forward neural network consists of some number of “neurons” arranged in $L + 1$ distinct layers. Layer $\ell = 0$ is the input layer, where data is presented to the network, while layer $\ell = L$ is where the output is read out. Each neuron n_x^ℓ (denoting neuron number x in layer ℓ) has an *activation* f_x^ℓ . For the input layer, the activations come directly from the data, whereas in higher layers they are computed via a simple function of the activations of the previous layer, such as

$$f_x^\ell = \sigma(b_x^\ell + \sum_y w_{x,y}^\ell f_y^{\ell-1}). \quad (2)$$

Here, the $\{b_x^\ell\}$ bias terms and the $\{w_{x,y}^\ell\}$ weights are the network’s learnable parameters, while σ is a fixed nonlinear function, such as the ReLU function $\sigma(z) = \max(0, z)$. In the simplest case, each f_x^ℓ is a scalar, but, in the second half of the paper we consider neural networks with more general, vector or tensor valued activations.

For the purposes of the following discussion it is actually helpful to take a slightly more abstract view, and, instead of focusing on the individual activations, consider the activations in any given layer collectively as a function $f^\ell: \mathcal{X}_\ell \rightarrow V_\ell$, where \mathcal{X}_ℓ is a set indexing the neurons and V_ℓ is a vector space. Omitting the bias terms in (2) for simplicity, each layer $\ell = 1, 2, \dots, L$ can then just be thought of as implementing a linear transformation $\phi_\ell: L_{V_{\ell-1}}(\mathcal{X}_{\ell-1}) \rightarrow L_{V_\ell}(\mathcal{X}_\ell)$ followed by the pointwise nonlinearity σ . Our operational definition of neural networks for the rest of this paper will be as follows.

Definition 1. Let $\mathcal{X}_0, \dots, \mathcal{X}_L$ be a sequence of index sets, V_0, \dots, V_L vector spaces, ϕ_1, \dots, ϕ_L linear maps

$$\phi_\ell: L_{V_{\ell-1}}(\mathcal{X}_{\ell-1}) \longrightarrow L_{V_\ell}(\mathcal{X}_\ell),$$

and $\sigma_\ell: V_\ell \rightarrow V_\ell$ appropriate pointwise nonlinearities, such as the ReLU operator. The corresponding **multi-layer feed-forward neural network (MFF-NN)** is then a

sequence of maps $f_0 \mapsto f_1 \mapsto f_2 \mapsto \dots \mapsto f_L$, where $f_\ell(x) = \sigma_\ell(\phi_\ell(f_{\ell-1}(x)))$.

If we are interested in constructing a neural net for recognizing $m \times m$ pixel images, it is tempting to take $\mathcal{X}_0 = [m] \times [m]$ and define $\mathcal{X}_1, \dots, \mathcal{X}_L$ similarly. However, again for notational simplicity, we extend each of these index sets to the entire integer plane \mathbb{Z}^2 , and simply assume that outside of the square region $[m] \times [m]$, $f^0(x_1, x_2) = 0$. A traditional *convolutional neural network (CNN)* is a network of this type where the ϕ_ℓ functions are constrained to have the special form

$$\phi_\ell(f_{\ell-1})(x_1, x_2) = \sum_{u_1=1}^w \sum_{u_2=1}^w f_{\ell-1}(x_1 - u_1, x_2 - u_2) \chi_\ell(u_1, u_2). \quad (3)$$

The above function is known as the *discrete convolution* of $f^{\ell-1}$ with the *filter* χ , and is usually denoted $f_{\ell-1} * \chi_\ell$. In most CNNs the width w of the filters is quite small, on the order of $3 \sim 10$, while the number of layers can be as small as 3 or as large as a few dozen.

Some of the key features of CNNs are immediately apparent from the convolution formula (3):

1. The number of parameters in CNNs is much smaller than in general (fully connected) feed-forward networks, since we only have to learn the w^2 numbers defining the χ_ℓ filters rather than $O((m^2)^2)$ weights.
2. (3) applies the same filter to every part of the image. Therefore, if the networks learns to recognize a certain feature, e.g., eyes, in one part of the image, then it will be able to do so in any other part as well.
3. Equivalently to the above, if the input image is translated by any vector (t_1, t_2) (i.e., $f^{0'}(x_1, x_2) = f^0(x_1 - t_1, x_2 - t_2)$), then all higher layers will translate in exactly the same way. This property is called **equivariance** (sometimes *covariance*) to translations.

The goal of the present paper is to understand the mathematical generalization of the above properties to other domains, such as graphs, manifolds, and so on.

3.1. Group actions

The jumping off point to our analysis is the observation that the above is a special case of the following scenario.

1. We have a set \mathcal{X} and a function $f: \mathcal{X} \rightarrow \mathbb{C}$.
2. We have a group G acting on \mathcal{X} . This means that each $g \in G$ has a corresponding transformation $T_g: \mathcal{X} \rightarrow \mathcal{X}$, and for any $g_1, g_2 \in G$, $T_{g_2 g_1} = T_{g_2} \circ T_{g_1}$.
3. The action of G on \mathcal{X} extends to functions on \mathcal{X} by

$$\mathbb{T}_g: f \mapsto f' \quad f'(T_g(x)) = f(x).$$

In the case of translation invariant image recognition, $\mathcal{X} = \mathbb{Z}^2$, G is the group of integer translations, which is isomorphic to \mathbb{Z}^2 (note that this is a very special case, in general

\mathcal{X} and G are different objects), the action is

$$T_{(t_1, t_2)}(x_1, x_2) = (x_1 + t_1, x_2 + t_2) \quad (t_1, t_2) \in \mathbb{Z}^2,$$

and the corresponding (induced) action on functions is

$$\mathbb{T}: f \mapsto f' \quad f'(x_1, x_2) = f(x_1 - t_1, x_2 - t_2).$$

We give several other (more interesting) examples of group actions in Section 6, but for now continue with our abstract development. Also note that to simplify notation, in the following, where this does not cause confusion, we will simply write group actions as $x \mapsto g(x)$ rather than the more cumbersome $x \mapsto T_g(x)$.

Most of the actions considered in this paper have the property that taking any $x_0 \in \mathcal{X}$, any other $x \in \mathcal{X}$ can be reached by the action of some $g \in G$, i.e., $x = g(x_0)$. This property is called **transitivity**, and if the action of G on \mathcal{X} is transitive, we say that \mathcal{X} is a **homogeneous space** of G .

3.2. Equivariance

Equivariance is a concept that applies very broadly, whenever we have a group acting on a pair of spaces and there is a map from functions on one to functions on the other.

Definition 2. Let G be a group and $\mathcal{X}_1, \mathcal{X}_2$ be two sets with corresponding G -actions

$$T_g: \mathcal{X}_1 \rightarrow \mathcal{X}_1, \quad T'_g: \mathcal{X}_2 \rightarrow \mathcal{X}_2.$$

Let V_1 and V_2 be vector spaces, and \mathbb{T} and \mathbb{T}' be the induced actions of G on $L_{V_1}(\mathcal{X}_1)$ and $L_{V_2}(\mathcal{X}_2)$. We say that a (linear or non-linear) map $\phi: L_{V_1}(\mathcal{X}_1) \rightarrow L_{V_2}(\mathcal{X}_2)$ is **equivariant** with the action of G (or **G -equivariant** for short) if

$$\phi(\mathbb{T}_g(f)) = \mathbb{T}'_g(\phi(f)) \quad \forall f \in L_{V_1}(\mathcal{X}_1)$$

for any group element $g \in G$.

Equivariance is represented graphically by a so-called commutative diagram, in our case

$$\begin{array}{ccc} L_{V_1}(\mathcal{X}_1) & \xrightarrow{\mathbb{T}_g} & L_{V_1}(\mathcal{X}_1) \\ \downarrow \phi & & \downarrow \phi \\ L_{V_2}(\mathcal{X}_2) & \xrightarrow{\mathbb{T}'_g} & L_{V_2}(\mathcal{X}_2) \end{array}$$

We are finally in a position to define the objects that we study in this paper, namely generalized equivariant neural networks.

Definition 3. Let \mathcal{N} be a feed-forward neural network as defined in Definition 1, and G be a group that acts on each index space $\mathcal{X}_0, \dots, \mathcal{X}_L$. Let $\mathbb{T}^0, \mathbb{T}^1, \dots, \mathbb{T}^L$ be the corresponding actions on $L_{V_0}(\mathcal{X}_0), \dots, L_{V_L}(\mathcal{X}_L)$. We say that \mathcal{N} is a **G -equivariant feed-forward network** if, when the inputs are transformed $f_0 \mapsto \mathbb{T}_g^0(f_0)$ (for any $g \in G$), the activations of the other layers correspondingly transform as $f_\ell \mapsto \mathbb{T}_g^\ell(f_\ell)$.

It is important to note how general the above framework is. In particular, we have not said whether G and $\mathcal{X}_0, \dots, \mathcal{X}_L$ are discrete or continuous. In any actual implementation of a neural network, the index sets would of course be finite. However, it has been observed before that in certain cases, specifically when \mathcal{X}_0 is an object such as the sphere or other manifold which does not have a discretization that fully takes into account its symmetries, it is easier to describe the situation in terms of abstract “continuous” neural networks than seemingly simpler discrete ones (Cohen et al., 2018).

Note also that invariance is a special case of equivariance, where $T_g = \text{id}$ for all g . In fact, this is another major reason why equivariant architectures are so prevalent in the literature: any equivariant network can be turned into a G -invariant network simply by tacking on an extra layer that is equivariant in this degenerate sense (in practice, this often means either averaging or creating a histogram of the activations of the last layer). Nowhere is this more important than in graph learning, where it is a hard constraint that whatever representation is learnt by a neural network, it must be invariant to reordering the vertices. Today’s state of the art solution to this problem are message passing networks (Gilmer et al., 2017), whose invariance behavior we discuss in section 6. Another architecture that achieves invariance by stacking equivariant layers followed by a final invariant one is that of scattering networks (Mallat, 2012).

4. Convolution on groups and quotient spaces

According to its usual definition in signal processing, the **convolution** of two functions $f, g: \mathbb{R} \rightarrow \mathbb{R}$ is

$$(f * g)(x) = \int f(x - y) g(y) dy. \quad (4)$$

Intuitively, we can think of f as a template and g as a modulating function (or the other way round, since convolution on \mathbb{R} is commutative): we get $f * g$ by placing a “copy” of f at each point on the x axis, but scaled by the value of g at that point, and superimposing the results. The discrete variant of (4) for $f, g: \mathbb{Z} \rightarrow \mathbb{R}$ is of course

$$(f * g)(x) = \sum_{y \in \mathbb{Z}} f(x - y) g(y), \quad (5)$$

and both the above formulae have natural generalizations to higher dimensions. In particular, (3) is just the two dimensional version of (5) with a limited width filter.

What we are interested in for this paper, however, is the much broader generalization of convolution to the case when f and g are functions on a compact group G . As mentioned in the Introduction, this takes the form

$$(f * g)(u) = \int_G f(uv^{-1}) g(v) d\mu(v). \quad (6)$$

Note that (6) only differs from (4) in that $x-y$ is replaced by the group operation uv^{-1} , which is not surprising, since the group operation on \mathbb{R} in fact is exactly $(x, y) \mapsto x + y$, and the “inverse” of y in the group sense is $-y$. Furthermore, the Haar measure μ makes an appearance. At this point, the main reason that we restrict ourselves to compact groups is because this guarantees that μ is essentially unique¹. The discrete counterpart of (6) for countable (including finite) groups is

$$(f * g)(u) = \sum_{v \in G} f(uv^{-1}) g(v). \quad (7)$$

All these definitions are standard and have deep connections to the algebraic properties of groups. In contrast, the various extensions of convolution to homogeneous spaces that we derive below are not often discussed in pure algebra.

4.1. Convolution on quotient spaces

The major complication in neural networks is that $\mathcal{X}_0, \dots, \mathcal{X}_L$ (which are the spaces that the f_0, \dots, f_L activations are defined on) are homogeneous spaces of G , rather than being G itself. Fortunately, the strong connection between the structure of groups and their homogeneous spaces (see boxed text) allows generalizing convolution to this case as well. Note that from now on, to keep the exposition as simple as possible, we present our results assuming that G is countable (or finite). The generalization to continuous groups is straightforward. We also allow all our functions to be complex valued, because representation theory itself, which is the workhorse behind our results, is easiest to formulate over \mathbb{C} .

Definition 4. Let G be a finite or countable group, \mathcal{X} and \mathcal{Y} be (left or right) quotient spaces of G , $f: \mathcal{X} \rightarrow \mathbb{C}$, and $g: \mathcal{Y} \rightarrow \mathbb{C}$. We then define the **convolution** of f with g as

$$(f * g)(u) = \sum_{v \in G} f \uparrow^G(uv^{-1}) g \uparrow^G(v), \quad u \in G. \quad (8)$$

¹Non-compact groups would also cause trouble because their representation theory is much more involved. \mathbb{R}^2 , which is the group behind traditional CCNs, is of course not compact. The reason that it is still amenable to our analysis (with small modifications) is that it belongs to one of a handful of families of exceptional non-compact groups that are easy to handle.

ESSENTIAL DEFINITIONS FOR QUOTIENT SPACES

Certain connections between the structure of a group G and its homogeneous space \mathcal{X} are crucial for our exposition. First, by definition, fixing an “origin” $x_0 \in \mathcal{X}$, any $x \in \mathcal{X}$ can be reached as $x = g(x_0)$ for some $g \in G$. This allows us to “index” elements of \mathcal{X} by elements of G . Since we use this mechanism so often, we introduce the shorthand $[g]_{\mathcal{X}} = g(x_0)$, which hides the dependence on the (arbitrary) choice of x_0 .

Second, elementary group theory tells us that the set of group elements that fix x_0 actually form a subgroup H . By further elementary results (see Appendix), the set of group elements that map $x_0 \mapsto x$ is a so-called **left coset** $gH := \{gh \mid h \in H\}$. The set of all such cosets forms the **(left) quotient space** G/H . Therefore, \mathcal{X} can be identified with G/H .

Now for each gH coset we may pick a **coset representative** $g' \in gH$, and let \bar{x} denote the representative of the coset of group elements that map x_0 to x . Note that while the map $g \mapsto [g]_{G/H}$ is well defined, the map $x \mapsto \bar{x}$ going in the opposite direction is more arbitrary, since it depends on the choice of coset representatives.

The **right quotient space** $H \backslash G$ is similarly defined as the space of **right cosets** $Hg := \{hg \mid h \in H\}$. Furthermore, if K is another subgroup of G , we can talk about **double cosets** $HgK = \{h g k \mid h \in H, k \in K\}$ and the corresponding space $H \backslash G / K$.

Given $f: G \rightarrow \mathbb{C}$, we define its **projection** to $\mathcal{X} = G/H$

$$f \downarrow_{\mathcal{X}}: \mathcal{X} \rightarrow \mathbb{C} \quad f \downarrow_{\mathcal{X}}(x) = \frac{1}{|H|} \sum_{g \in \bar{x}H} f(g).$$

Conversely, given $f: \mathcal{X} \rightarrow \mathbb{C}$, we define the **lifting** of f to G

$$f \uparrow^G: G \rightarrow \mathbb{C} \quad f \uparrow^G(g) = f([g]_{\mathcal{X}}).$$

Projection and lifting to/from right quotient spaces and double quotient spaces is defined analogously.

This definition includes $\mathcal{X} = G$ or $\mathcal{Y} = G$ as special cases, since any group is a quotient space of itself with respect to the trivial subgroup $H = \{e\}$.

Definition 4 hides the facts that depending on the choice of \mathcal{X} and \mathcal{Y} : (a) the summation might only have to extend over a quotient space of G rather than the entire group, (b) the result $f * g$ might have symmetries that effectively make it a function on a quotient space rather than G itself (this is exactly what the case will be in generalized convolutional networks). Therefore we now discuss three special cases.

CASE I: $\mathcal{X} = G$ AND $\mathcal{Y} = G/H$

When $f: G \rightarrow \mathbb{C}$ but $g: G/H \rightarrow \mathbb{C}$ for some subgroup H of G , (8) reduces to

$$(f * g)(u) = \sum_{v \in G} f(uv^{-1}) g \uparrow^G(v).$$

Plugging $u' = uh$ into this formula (for any $h \in H$) and changing the variable of summation to $w := vh^{-1}$ gives

$$\begin{aligned} (f * g)(u') &= \sum_{v \in G} f(uhv^{-1}) g \uparrow^G(v) \\ &= \sum_{w \in G} f(uw^{-1}) g \uparrow^G(w). \end{aligned}$$

However, since w and wh are in the same left H -coset, $g \uparrow^G(wh) = g \uparrow^G(w)$, so $(f * g)(u') = (f * g)(u)$, i.e., $f * g$ is constant on left H -cosets. This makes it natural to interpret $f * g$ as a function on G/H rather than the full group. Thus, we have the following definition.

If $f: G \rightarrow \mathbb{C}$, and $g: G/H \rightarrow \mathbb{C}$ then $f * g: G/H \rightarrow \mathbb{C}$ with

$$(f * g)(x) = \sum_{v \in G} f(\bar{x}v^{-1}) g([v]_{G/H}). \quad (9)$$

CASE II: $\mathcal{X} = G/H$ AND $\mathcal{Y} = H \backslash G$

When $f: G/H \rightarrow \mathbb{C}$, but $g: G \rightarrow \mathbb{C}$, (8) reduces to

$$(f * g)(u) = \sum_{v \in G} f \uparrow^G(uv^{-1}) g(v). \quad (10)$$

This time it is not $f * g$, but g that shows a spurious symmetry. Letting $v' = hv$ (for any $h \in H$), by the right H -invariance of $f \uparrow^G$, $f \uparrow^G(uv'^{-1}) = f \uparrow^G(uv^{-1}h^{-1}) = f \uparrow^G(uv)$. Considering that any v can be uniquely written as $v = h\bar{y}$, where \bar{y} is the representative of one of its cosets, while $h \in H$, we get that (10) factorizes in the form

$$\begin{aligned} (f * g)(u) &= \sum_{y \in H \backslash G} f \uparrow^G(u\bar{y}^{-1}) \sum_{h \in H} g(h\bar{y}) \\ &= \sum_{y \in H \backslash G} f \uparrow^G(u\bar{y}^{-1}) \tilde{g}(y), \end{aligned}$$

where $\tilde{g}(y) := \sum_{h \in H} g(h\bar{y})$. In other words, without loss of generality we can take g to be a function on $H \backslash G$ rather than the full group.

If $f: G/H \rightarrow \mathbb{C}$, and $g: H \backslash G \rightarrow \mathbb{C}$, then $f * g: G \rightarrow \mathbb{C}$ with

$$(f * g)(u) = |H| \sum_{y \in H \backslash G} f([u\bar{y}^{-1}]_{G/H}) g(y). \quad (11)$$

CASE III: $\mathcal{X} = G/H$ AND $\mathcal{Y} = H \backslash G/K$

Finally, we consider the case when $f: G/H \rightarrow \mathbb{C}$ and $g: G/K \rightarrow \mathbb{C}$ for two subgroups H, K of G , which might or might not be the same. This combines features of the above two cases in the sense that, similarly to Case I, setting $u' = uk$ for any $k \in K$ and letting $w = vk^{-1}$,

$$\begin{aligned} (f * g)(u') &= \sum_{v \in G} f \uparrow^G(u'v^{-1}) g \uparrow^G(v) = \\ &= \sum_{v \in G} f \uparrow^G(ukv^{-1}) g \uparrow^G(v) = \sum_{w \in G} f \uparrow^G(uw^{-1}) g \uparrow^G(wk) \\ &= \sum_{w \in G} f \uparrow^G(uw^{-1}) g \uparrow^G(w) = (f * g)(u), \end{aligned}$$

showing that $f * g$ is right K -invariant, and therefore can be regarded as a function $G/K \rightarrow \mathbb{C}$. At the same time, similarly to (10), letting $v = h\bar{y}$,

$$\begin{aligned} (f * g)(u) &= \sum_{y \in H \backslash G} f \uparrow^G(u\bar{y}^{-1}) \sum_{h \in H} g \uparrow^G(h\bar{y}) \\ &= \sum_{y \in H \backslash G} f \uparrow^G(u\bar{y}^{-1}) \tilde{g}(y), \end{aligned}$$

where $\tilde{g}(y) := \sum_{h \in H} g(h\bar{y})$, which is left H -invariant. Therefore, without loss of generality, we can take g to be a function $H \backslash G/K \rightarrow \mathbb{C}$.

If $f: G/H \rightarrow \mathbb{C}$, and $g: H \backslash G/K \rightarrow \mathbb{C}$ then we define the **convolution** of f with g as $f * g: G/K \rightarrow \mathbb{C}$ with

$$(f * g)(x) = |H| \sum_{y \in H \backslash G} f([x\bar{y}^{-1}]_{\mathcal{X}}) g([y]_{H \backslash G/K}). \quad (12)$$

Since $f \mapsto f * g$ is a map from one homogeneous space, $\mathcal{X} = G/H$, to another homogeneous space, $\mathcal{Y} = H/K$, it is this last definition that will be of most relevance to us in constructing neural networks.

4.2. Relationship to Fourier analysis

The nature of convolution on homogeneous spaces is further explicated by considering its form in Fourier space (see (Terras, 1999)). Recall that the **Fourier transform** of a function f on a countable group is defined

$$\hat{f}(\rho_i) = \sum_{u \in G} f(u) \rho_i(u), \quad i = 0, 1, 2, \dots, \quad (13)$$

where ρ_0, ρ_1, \dots are matrix valued functions called **irreducible representations** or **irreps** of G (see the Appendix for details). As expected, the generalization of this to the case when f is a function on G/H , $H \backslash G$ or $H \backslash G/K$ is

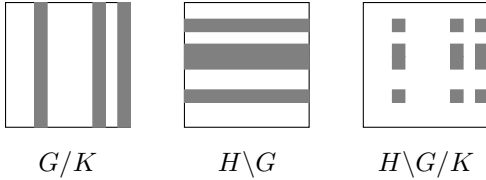
$$\hat{f}(\rho_i) = \sum_{u \in G} \rho_i(u) f \uparrow^G(u), \quad i = 1, 2, \dots$$

Analogous formulae hold for continuous groups, involving integration with respect to the Haar measure.

At first sight it might be surprising that the Fourier transform of a function on a quotient space consists of the same number of matrices of the same sizes as the Fourier transform of a function on G itself, since G/H , $H\backslash G$ or $H\backslash G/K$ are smaller objects than G . This puzzle is resolved by the following proposition, which tells us that in the latter cases, the Fourier matrices have characteristic sparsity patterns.

Proposition 1. *Let ρ be an irrep of G , and assume that on restriction to H it decomposes into irreps of H in the form $\rho|_H = \mu_1 \oplus \mu_2 \oplus \dots \oplus \mu_k$. Let \widehat{f} be the Fourier transform of a function $f: G/H \rightarrow \mathbb{C}$. Then $[\widehat{f}(\rho)]_{*,j} = 0$ unless the block at column j in the decomposition of $\rho|_H$ is the trivial representation. Similarly, if $f: H\backslash G \rightarrow \mathbb{C}$, then $[\widehat{f}(\rho)]_{i,*} = 0$ unless the block of $\rho|_H$ at row i is the trivial representation. Finally, if $f: H\backslash G/K \rightarrow \mathbb{C}$, then $[\widehat{f}(\rho)]_{i,j} = 0$ unless the block of $\rho|_H$ at row i is the trivial representation of H and the block at column j in the decomposition of $\rho|_K$ is the trivial representation of K .*

Schematically, this proposition implies that in the three different cases, the Fourier matrices have three different forms of sparsity:



Fortuitously, just like in the classical, Euclidean case, convolution also takes on a very nice form in the Fourier domain, even when f or g (or both) are defined on homogeneous spaces.

Proposition 2 (Convolution theorem on groups). *Let G be a compact group, H and K subgroups of G , and f, g be complex valued functions on G , G/H , $H\backslash G$ or $H\backslash G/K$. In any combination of these cases,*

$$\widehat{f * g}(\rho_i) = \widehat{f}(\rho_i) \widehat{g}(\rho_i) \quad (14)$$

for any given system of irreps $\mathcal{R}_G = \{\rho_0, \rho_1, \dots\}$.

Plugging in matrices with the appropriate sparsity patterns into (19) now gives us an intuitive way of thinking about Cases I–III above.

CASE I: $\mathcal{X} = G$ AND $\mathcal{Y} = G/H$

Multiplying a column sparse matrix with a dense matrix from the left gives a column sparse matrix with the same

pattern, therefore $f * g$ is a function on G/H :

$$\begin{pmatrix} \text{column sparse} \end{pmatrix} = \begin{pmatrix} \text{dense} \end{pmatrix} \times \begin{pmatrix} \text{column sparse} \end{pmatrix}.$$

$$\widehat{f * g}(\rho) = \widehat{f}(\rho) \widehat{g \uparrow G}(\rho)$$

CASE II: $\mathcal{X} = G/H$ AND $\mathcal{Y} = H\backslash G$

Multiplying a column sparse matrix from the right by another matrix picks out the corresponding rows of the second matrix. Therefore, if f is a function on G/H , then w.l.o.g. we can take g to be a function on $H\backslash G$.

$$\begin{pmatrix} \text{dense} \end{pmatrix} = \begin{pmatrix} \text{column sparse} \end{pmatrix} \times \begin{pmatrix} \text{row sparse} \end{pmatrix}.$$

$$\widehat{f * g}(\rho) = \widehat{f \uparrow G}(\rho) \widehat{g}(\rho)$$

CASE III: $f: G/H \rightarrow \mathbb{C}$ AND $g: H\backslash G/K \rightarrow \mathbb{C}$

Finally, if f is a function on G/H , and we want to make $f * g$ to be a function on G/K , then we should take $g: H\backslash G/K$:

$$\begin{pmatrix} \text{column sparse} \end{pmatrix} = \begin{pmatrix} \text{column sparse} \end{pmatrix} \times \begin{pmatrix} \text{block sparse} \end{pmatrix}.$$

$$\widehat{f * g}(\rho) = \widehat{f \uparrow G}(\rho) \widehat{g \uparrow G}(\rho)$$

5. Main result: the connection between convolution and equivariance

We are finally in a position to define the notion of generalized convolutional networks, and state our main result connecting convolutions and equivariance.

Definition 5. *Let G be a compact group and \mathcal{N} an $L+1$ layer feed-forward network in which the i 'th index set is G/H_i for some subgroup H_i of G . We say that \mathcal{N} is a **G -convolutional neural network** (or **G -CNN** for short) if each of the linear maps ϕ_1, \dots, ϕ_L in \mathcal{N} is a generalized convolution (see Definition 4) of the form*

$$\phi_\ell(f_{\ell-1}) = f_{\ell-1} * \chi_\ell$$

with some filter $\chi_\ell \in L_{V_{\ell-1} \times V_\ell}(H_{\ell-1} \backslash G / H_\ell)$.

Theorem 1. *Let G be a compact group and \mathcal{N} be an $L+1$ layer feed-forward neural network in which the ℓ 'th index set is of the form $\mathcal{X}_\ell = G/H_\ell$, where H_ℓ is some subgroup of G . Then \mathcal{N} is equivariant to the action of G in the sense of Definition 3 if and only if it is a G -CNN.*

Proving this theorem in the forward direction is relatively easy and only requires some elementary facts about cosets and group actions.

Proof of Theorem 1 (forward direction). Assume that we translate $f_{\ell-1}$ by some group element $g \in G$ and get $f'_{\ell-1}$, i.e., $f'_{\ell-1} = \mathbb{T}_g^{\ell-1}(f_{\ell-1})$, where $f'_{\ell-1}(x) = f_{\ell-1}(g^{-1}x)$. Then

$$\begin{aligned}\phi_{\ell}(f'_{\ell-1})(u) &= (f'_{\ell-1} * \chi_{\ell})(u) \\ &= \sum_{v \in G} f'_{\ell-1}([uv^{-1}]_{\mathcal{X}}) \chi_{\ell}(v) \\ &= \sum_{v \in G} f_{\ell-1}(g^{-1}([uv^{-1}]_{\mathcal{X}})) \chi_{\ell}(v).\end{aligned}$$

By $g^{-1}([uv^{-1}]_{\mathcal{X}}) = [g^{-1}uv^{-1}]_{\mathcal{X}}$ this is further equal to

$$\begin{aligned}\sum_{v \in G} f_{\ell-1}([g^{-1}uv^{-1}]_{\mathcal{X}}) \chi_{\ell}(v) \\ = (f_{\ell-1} * \chi_{\ell})(g^{-1}u) = \phi_{\ell}(f_{\ell-1})(g^{-1}u).\end{aligned}$$

Therefore, $\phi_{\ell}(f_{\ell-1})$ is equivariant with $f_{\ell-1}$. Since σ_{ℓ} is a pointwise operator, so is $f_{\ell} = \sigma_{\ell}(\phi_{\ell}(f_{\ell-1}))$. By induction on ℓ , using the transitivity of equivariance, this implies that every layer of \mathcal{N} is equivariant with layer 0. Note that this proof holds not only in the base case, when each f_{ℓ} is a function $\mathcal{X} \rightarrow \mathbb{C}$, but also in the more general case when $f_{\ell}: \mathcal{X}_{\ell} \rightarrow V_{\ell}$ and the filters are $\chi_{\ell}: \mathcal{X}_{\ell} \rightarrow V_{\ell-1} \times V_{\ell}$. ■

Proving the “only if” part of Theorem 1 is more technical, therefore we leave it to the Appendix.

6. Examples of algebraic convolution in neural networks

We are not aware of any prior papers that have exposed the above algebraic theory of equivariance and convolution in its full generality. However, there are a few recent publications that implicitly exploit these ideas in specific contexts.

6.1. Rotation equivariant networks

In image recognition applications it is a natural goal to achieve equivariance to both translation and rotation. The most common approach is to use CNNs, but with filters that are replicated at a certain number of rotational angles (typically multiples of 90 degrees), connected in such a way as to achieve a generalization of equivariance called *steerability*. Steerability also has a group theoretic interpretation, which is most lucidly explained in (Cohen & Welling, 2017).

The recent papers (Marcos et al., 2017) and (Worrall et al., 2017) extend these architectures by considering continuous rotations at each point of the visual field. Thus, putting

aside the steerability aspect for now and only considering the behavior of the network at a single point, both these papers deal with the case where $G = \text{SO}(2)$ (the two dimensional rotation group) and \mathcal{X} is the circle S^1 . The group $\text{SO}(2)$ is commutative, therefore its irreducible representations are one dimensional, and are, in fact, $\rho_j(\theta) = e^{2\pi i j \theta}$, where $i = \sqrt{-1}$. While not calling it a group Fourier transform, Worrall et al. (2017) explicitly expand the local activations in this basis and scale them with weights, which, by virtue of Proposition 2, amounts to convolution on the group, as prescribed by our main theorem.

The form of the nonlinearity in (Worrall et al., 2017) is different from that prescribed in Definition 3, which leads to a coupling between the indices of the Fourier components in any path from the input layer to the output layer. This is compensated by what they call their “equivariance condition”, asserting that only Fourier components for which $M = \sum_{\ell} j_{\ell}$ is the same may mix. This restores equivariance in the last layer, but analyzing it group theoretically is beyond the scope of the present paper.

6.2. Spherical CNNs

Very close in spirit to our present exposition are the recent papers (Cohen et al., 2018; Kondor et al., 2018), which propose convolutional architectures for recognizing images painted on the sphere, satisfying equivariance with respect to rotations. Thus, in this case, $G = \text{SO}(3)$, the group of three dimensional rotations, and \mathcal{X}_{ℓ} is the sphere, S^2 .

The case of rotations acting on the sphere is one of the textbook examples of continuous group actions. In particular, letting x_0 be the North pole, we see that two-dimensional rotations in the x - z plane fix x_0 , therefore, S^2 is identified with the quotient space $\text{SO}(3)/\text{SO}(2)$. The irreducible representations of $\text{SO}(3)$ are given by the so-called Wigner matrices. The ℓ 'th irreducible representation is $2\ell + 1$ dimensional and of the form

$$[\rho_{\ell}(\theta, \phi, \psi)]_{m, m'} = e^{-i m' \phi} d_{m', m}^{\ell}(\theta) e^{-i m \psi},$$

where $m, m' \in \{-\ell, \dots, \ell\}$, (θ, ϕ, ψ) are the Euler angles of the rotation and the $d_{m', m}^{\ell}(\theta)$ function is related to the spherical harmonics. It is immediately clear that on restriction to $\text{SO}(2)$ (corresponding to $\theta, \phi = 0$) only the middle column in each of these matrices reduces to the trivial representation of $\text{SO}(2)$, therefore, by Proposition 1, in the case $f: \text{SO}(3)/\text{SO}(2) \rightarrow \mathbb{C}$, only the middle column of each $\hat{f}(\rho_{\ell})$ matrix will be nonzero. In fact, up to constant scaling factors, the entries in that middle column are just the customary spherical harmonic expansion coefficients.

Cohen et al. (2018) explicitly make this connection between spherical harmonics and $\text{SO}(3)$ Fourier transforms, and store the activations in terms of this representation. Moreover, just like in the present paper, they define convo-

lution in terms of the noncommutative convolution theorem (Proposition 2), use pointwise nonlinearities, and prove that the resulting neural network is $\text{SO}(3)$ -equivariant. However, they do not prove the converse, i.e., that equivariance implies that the network *must* be convolutional. To apply the nonlinearity, the algorithm presented in (Cohen et al., 2018) requires repeated forward and backward $\text{SO}(3)$ fast Fourier transforms. While this leads to a non-conventional architecture, the discussion echoes our observation that when dealing with continuous symmetries such as rotations, one must generalize to more abstract “continuous” neural networks, as afforded by Definition 3.

6.3. Message passing neural networks

There has been considerable interest in extending the convolutional network formalism to learning from graphs (Niepert et al., 2016; Defferrard et al., 2016; Duvenaud et al., 2015), and the current consensus for approaching this problem is to use neural networks based on the message passing idea (Gilmer et al., 2017). Let \mathcal{G} be a graph with n vertices. Message passing neural networks (MPNNs) are usually presented in terms of an iterative process, where in each round ℓ , each vertex v collects the labels of its neighbors w_1, \dots, w_k , and updates its own label \tilde{f}_v^ℓ according to a simple formula such as

$$\tilde{f}_v^\ell = \Phi(\tilde{f}_{w_1}^{\ell-1} + \dots + \tilde{f}_{w_k}^{\ell-1}).$$

An equivalent way of seeing this process, however, is in terms of the “effective receptive fields” \mathcal{S}_v^ℓ of each vertex at round ℓ , i.e., the set of all vertices from which information can propagate to v by round ℓ .

MPNNs can also be viewed as group convolutional networks. A receptive field of size k is just a subset $\{s_1, \dots, s_k\} \subseteq \{1, 2, \dots, n\}$, and the symmetric group \mathbb{S}_n (the group of permutations of $\{1, 2, \dots, n\}$) acts on the set of such subsets transitively by

$$\{s_1, \dots, s_k\} \xrightarrow{\sigma} \{\sigma(s_1), \dots, \sigma(s_k)\} \quad \sigma \in \mathbb{S}_n.$$

Since permuting the $n - k$ vertices *not* in \mathcal{S} amongst themselves, as well as permuting the k vertices that are in \mathcal{S} both leave \mathcal{S} invariant, the stabilizer of this action is $\mathbb{S}_{n-k} \times \mathbb{S}_k$. Thus, the set of all k -subsets of vertices is identified with the quotient space $\mathcal{X} = \mathbb{S}_n / (\mathbb{S}_k \times \mathbb{S}_{n-k})$, and the labeling function for k -element receptive fields is identified with $f^k: \mathcal{X} \rightarrow \mathbb{C}$. Effectively, this turns the MPNN into a generalized feed-forward network in the sense of Definition 3. Note that f^k is a redundant representation of the labeling function because $\mathbb{S}_n / (\mathbb{S}_k \times \mathbb{S}_{n-k})$ also includes subsets that do not correspond to contiguous neighborhoods. However this is not a problem because for such \mathcal{S} we simply set $f^k(\mathcal{S}) = 0$.

The key feature of the message passing formalism is that, by construction, it ensures that the \tilde{f}_v^ℓ labels only depend

on the graph topology and are invariant to renumbering the vertices of \mathcal{G} . In terms of our “ k -subset network” this means that each f^k must be \mathbb{S}_n -equivariant. Thus, in contrast to the previous two examples, now each index set $\mathcal{X}_\ell = \mathbb{S}_n / (\mathbb{S}_{n-\ell} \times \mathbb{S}_\ell)$ is different. The form of the corresponding convolutions $L_{V_{\ell-1}}(\mathcal{X}_{\ell-1}) \rightarrow L_{V_\ell}(\mathcal{X}_\ell)$ are best described in the Fourier domain. Unfortunately, the representation theory of symmetric groups is beyond the scope of the present paper (Sagan, 2001). We content ourselves by stating that the irreps of \mathbb{S}_n are indexed by so-called integer partitions, $(\lambda_1, \dots, \lambda_m)$, where $\lambda_1 \geq \dots \geq \lambda_m$ and $\sum_i \lambda_i = n$. Moreover, the structure of the Fourier transform of a function $f: \mathbb{S}_n / (\mathbb{S}_{n-\ell} \times \mathbb{S}_\ell)$ dictated by Proposition 1 in this case is that each of the Fourier matrices are zero except for a single column in each of the $\hat{f}((n-p, p))$ components, where $0 \leq p \leq \ell$. The main theorem of our paper dictates that the linear map ϕ_ℓ in each layer must be a convolution. In the case of Fourier matrices with such extreme sparsity structure, this means that each of the $\ell + 1$ Fourier matrices can be multiplied by a scalar, χ_p^ℓ . These are the learnable parameters of the network. A real MPNN of course has multiple channels and various corresponding parameters, which could also be introduced in the k -subset network. The above observation about the form of χ_ℓ is nonetheless interesting, because it at once implies that permutation equivariance is a severe constraint the significantly limits the form of the convolutional filters, yet the framework is still richer than traditional MPNNs where the labels of the neighbors are simply summed.

7. Conclusions

Convolution has emerged as one of the key organizing principles of deep neural network architectures. Nonetheless, depending on their background, the word “convolution” means different things to different researchers. The goal of this paper was to show that in the common setting when there is a group acting on the data that the architecture must be equivariant to, convolution has a specific mathematical meaning that has far reaching consequences: we proved that a feed forward network is equivariant to the group action if and only if it respects this notion of convolution.

Our theory gives a clear prescription to practitioners on how to design neural networks for data with non-trivial symmetries, such as data on the sphere, etc.. In particular, we argue for Fourier space representations, similar to those that have appeared in (Worrall et al., 2017; Cohen et al., 2018; Kondor et al., 2018)), and, even more recently, since the submission of the original version of the present paper in (Thomas et al., 2018; Kondor, 2018; Weiler et al., 2018).

Acknowledgements

This work was supported in part by DARPA Young Faculty Award D16AP00112.

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Appendix

A. Background from group and representation theory

For a more detailed background on representation theory, we point the reader to Serre, 1977.

Groups. A **group** is a set G endowed with an operation $G \times G \rightarrow G$ (usually denoted multiplicatively) obeying the following axioms:

- G1. for any $g_1, g_2 \in G$, $g_1 g_2 \in G$ (closure);

- G2. for any $g_1, g_2, g_3 \in G$, $g_1(g_2g_3) = (g_1g_2)g_3$ (associativity);
- G3. there is a unique $e \in G$, called the **identity** of G , such that $eg = ge = g$ for any $u \in G$;
- G4. for any $g \in G$, there is a corresponding element $g^{-1} \in G$ called the **inverse** of g , such that $gg^{-1} = g^{-1}g = e$.

We do *not* require that the group operation be commutative, i.e., in general, $g_1g_2 \neq g_2g_1$. Groups can be finite or infinite, countable or uncountable, compact or non-compact. While most of the results in this paper would generalize to any compact group, to keep the exposition as simple as possible, throughout we assume that G is finite or countably infinite. As usual, $|G|$ will denote the size (cardinality) of G , sometimes also called the **order** of the group. A subset H of G is called a **subgroup** of G , denoted $H \leq G$, if H itself forms a group under the same operation as G , i.e., if for any $g_1, g_2 \in H$, $g_1g_2 \in H$.

Homogeneous Spaces.

Definition 6. Let G be a group acting on a set \mathcal{X} . We say that \mathcal{X} is a **homogeneous space** of G if for any $x, y \in \mathcal{X}$, there is a $g \in G$ such that $y = g(x)$.

The significance of homogeneous spaces for our purposes is that once we fix the “origin” x_0 , the above correspondence between points in \mathcal{X} and the group elements that map x_0 to them allows to lift various operations on the homogeneous space to the group. Because expressions like $g(x_0)$ appear so often in the following, we introduce the shorthand $[g]_{\mathcal{X}} := g(x_0)$. Note that this hides the dependency on the (arbitrary) choice of x_0 .

For some examples, we see that \mathbb{Z}^2 is a homogeneous space of itself with respect to the trivial action $(i, j) \mapsto (g_1+i, g_2+j)$, and the sphere is a homogeneous space of the rotation group with respect to the action:

$$x \mapsto R(x) \quad R(x) = Rx \quad x \in S^2, \quad (15)$$

On the other hand, the entries of the adjacency matrix are *not* a homogeneous space of \mathbb{S}_n with respect to

$$(i, j) \mapsto (\sigma(i), \sigma(j)) \quad \sigma \in \mathbb{S}_n. \quad (16)$$

, because if we take some (i, j) with $i \neq j$, then 16 can map it to any other (i', j') with $i' \neq j'$, but not to any of the diagonal elements, where $i' = j'$. If we split the matrix into its “diagonal”, and “off-diagonal” parts, individually these two parts are homogeneous spaces.

Representations. A (finite dimensional) **representation** of a group G over a field \mathbb{F} is a matrix-valued function $\rho: G \rightarrow \mathbb{F}^{d_\rho \times d_\rho}$ such that $\rho(g_1)\rho(g_2) = \rho(g_1g_2)$ for any

$g_1, g_2 \in G$. In this paper, unless stated otherwise, we always assume that $\mathbb{F} = \mathbb{C}$. A representation ρ is said to be **unitary** if $\rho(g^{-1}) = \rho(g)^\dagger$ for any $g \in G$. One representation shared by every group is the **trivial representation** ρ_{tr} that simply evaluates to the one dimensional matrix $\rho_{\text{tr}}(g) = (1)$ on every group element.

Equivalence, reducibility and irreps. Two representations ρ and ρ' of the same dimensionality d are said to be **equivalent** if for some invertible matrix $Q \in \mathbb{C}^{d \times d}$, $\rho(g) = Q^{-1}\rho'(g)Q$ for any $g \in G$. A representation ρ is said to be **reducible** if it decomposes into a direct sum of smaller representations in the form

$$\begin{aligned} \rho(g) &= Q^{-1} (\rho_1(g) \oplus \rho_2(g)) Q \\ &= Q^{-1} \left(\begin{array}{c|c} \rho_1(g) & 0 \\ \hline 0 & \rho_2(g) \end{array} \right) Q \quad \forall g \in G \end{aligned}$$

for some invertible matrix $Q \in \mathbb{C}^{d_\rho \times d_\rho}$. We use \mathcal{R}_G to denote a complete set of inequivalent irreducible representations of G . However, since this is quite a mouthful, in this paper we also use the alternative term **system of irreps** to refer to \mathcal{R}_G . Note that the choice of irreps in \mathcal{R}_G is far from unique, since each $\rho \in \mathcal{R}_G$ can be replaced by an equivalent irrep $Q^\top \rho(g) Q$, where Q is any orthogonal matrix of the appropriate size.

Complete reducibility and irreps. Representation theory takes on its simplest form when G is compact (and $\mathbb{F} = \mathbb{C}$). One of the reasons for this is that it is possible to prove (“theorem of complete reducibility”) that any representation ρ of a compact group can be reduced into a direct sum of irreducible ones, i.e.,

$$\rho(g) = Q^{-1} (\rho_{(1)}(g) \oplus \rho_{(2)}(g) \oplus \dots \oplus \rho_{(k)}(g)) Q, g \in G \quad (17)$$

for some sequence $\rho_{(1)}, \rho_{(2)}, \dots, \rho_{(k)}$ of irreducible representations of G and some $Q \in \mathbb{C}^{d \times d}$. In this sense, for compact groups, \mathcal{R}_G plays a role very similar to the primes in arithmetic. Fixing \mathcal{R}_G , the number of times that a particular $\rho' \in \mathcal{R}_G$ appears in (17) is a well-defined quantity called the **multiplicity** of ρ' in ρ , denoted $m_\rho(\rho')$. Compactness also has a number of other advantages:

1. When G is compact, \mathcal{R}_G is a countable set, therefore we can refer to the individual irreps as ρ_1, ρ_2, \dots . (When G is finite, \mathcal{R}_G is not only countable but finite.)
2. The system of irreps of a compact group is essentially unique in the sense that if \mathcal{R}'_G is any other system of irreps, then there is a bijection $\phi: \mathcal{R}_G \rightarrow \mathcal{R}'_G$ mapping each irrep $\rho \in \mathcal{R}_G$ to an equivalent irrep $\phi(\rho) \in \mathcal{R}'_G$.
3. When G is compact, \mathcal{R}_G can be chosen in such a way that each $\rho \in \mathcal{R}$ is unitary.

Restricted representations. Given any representation ρ of G and subgroup $H \leq G$, the *restriction* of ρ to H is defined as the function $\rho|_H: H \rightarrow \mathbb{C}^{d_\rho \times d_\rho}$, where $\rho|_H(h) = \rho(h)$ for all $h \in H$. It is trivial to check that $\rho|_H$ is a representation of H , but, in general, it is not irreducible (even when ρ itself is irreducible).

Fourier Transforms. In the Euclidean domain convolution and cross-correlation have close relationships with the Fourier transform

$$\widehat{f}(k) = \int e^{-2\pi i k x} f(x) dx, \quad (18)$$

where i is the imaginary unit, $\sqrt{-1}$. In particular, the Fourier transform of $f * g$ is just the pointwise product of the Fourier transforms of f and g ,

$$\widehat{f * g}(k) = \widehat{f}(k) \widehat{g}(k), \quad (19)$$

while cross-correlation is

$$\widehat{f \star g}(k) = \widehat{f}(k)^* \widehat{g}(k). \quad (20)$$

The concept of *group representations* (see Section A) allows generalizing the Fourier transform to any compact group. The **Fourier transform** of $f: G \rightarrow \mathbb{C}$ is defined as:

$$\widehat{f}(\rho_i) = \int_G \rho_i(u) f(u) d\mu(u), \quad i = 1, 2, \dots, \quad (21)$$

which, in the countable (or finite) case simplifies to

$$\widehat{f}(\rho_i) = \sum_{u \in G} f(u) \rho_i(u), \quad i = 1, 2, \dots \quad (22)$$

Despite \mathbb{R} not being a compact group, (18) can be seen as a special case of (21), since $e^{-2\pi i k x}$ trivially obeys $e^{-2\pi i k(x_1+x_2)} = e^{-2\pi i k x_1} e^{-2\pi i k x_2}$, and the functions $\rho_k(x) = e^{-2\pi i k x}$ are, in fact, the irreducible representations of \mathbb{R} . The fundamental novelty in (21) and (22) compared to (18), however, is that since, in general (in particular, when G is not commutative), irreducible representations are matrix valued functions, each “Fourier component” $\widehat{f}(\rho)$ is now a matrix. In other respects, Fourier transforms on groups behave very similarly to classical Fourier transforms. For example, we have an inverse Fourier transform

$$f(u) = \frac{1}{|G|} \sum_{\rho \in \mathcal{R}} d_\rho \operatorname{tr}[f(\rho) \rho(u)^{-1}],$$

and also an analog of the convolution theorem, which is stated in the main body of the paper.

B. Convolution of vector valued functions

Since neural nets have multiple channels, we need to further extend equations 6-12 to vector/matrix valued functions. Once again, there are multiple cases to consider.

Definition 7. Let G be a finite or countable group, and \mathcal{X} and \mathcal{Y} be (left or right) quotient spaces of G .

1. If $f: \mathcal{X} \rightarrow \mathbb{C}^m$, and $g: \mathcal{Y} \rightarrow \mathbb{C}^m$, we define $f * g: G \rightarrow \mathbb{C}$ with

$$(f * g)(u) = \sum_{v \in G} f \uparrow^G(uv^{-1}) \cdot g \uparrow^G(v), \quad (23)$$

where \cdot denotes the dot product.

2. If $f: \mathcal{X} \rightarrow \mathbb{C}^{n \times m}$, and $g: \mathcal{Y} \rightarrow \mathbb{C}^m$, we define $f * g: G \rightarrow \mathbb{C}^n$ with

$$(f * g)(u) = \sum_{v \in G} f \uparrow^G(uv^{-1}) \times g \uparrow^G(v), \quad (24)$$

where \times denotes the matrix/vector product.

3. If $f: \mathcal{X} \rightarrow \mathbb{C}^m$, and $g: \mathcal{Y} \rightarrow \mathbb{C}^{n \times m}$, we define $f * g: G \rightarrow \mathbb{C}^m$ with

$$(f * g)(u) = \sum_{v \in G} f \uparrow^G(uv^{-1}) \tilde{\times} g \uparrow^G(v), \quad (25)$$

where $v \tilde{\times} A$ denotes the “reverse matrix/vector product” Av .

Since in cases 2 and 3 the nature of the product is clear from the definition of f and g , we will omit the \times and $\tilde{\times}$ symbols. The specializations of these formulae to the cases of Equations 6-12 are as to be expected.

C. Proof of Proposition 1

Proposition 1 has three parts. To proceed with the proof, we introduce two simple lemmas.

Recall that if H is a subgroup of G , a function $f: G \rightarrow \mathbb{C}$ is called **right H -invariant** if $f(uh) = f(u)$ for all $h \in H$ and all $u \in G$, and it is called **left H -invariant** if $f(hu) = f(u)$ for all $h \in H$ and all $u \in G$.

Lemma 1. Let H and K be two subgroups of a group G . Then

1. If $f: G/H \rightarrow \mathbb{C}$, then $f \uparrow^G: G \rightarrow \mathbb{C}$ is right H -invariant.
2. If $f: H \backslash G \rightarrow \mathbb{C}$, then $f \uparrow^G: G \rightarrow \mathbb{C}$ is left H -invariant.
3. If $f: K \backslash G/H \rightarrow \mathbb{C}$, then $f \uparrow^G: G \rightarrow \mathbb{C}$ is right H -invariant and left K -invariant.

Lemma 2. Let ρ be an irreducible representation of a countable group G . Then $\sum_{u \in G} \rho(u) = 0$ unless ρ is the trivial representation, $\rho_{\text{tr}}(u) = (1)$.

Proof. Let us define the functions $r_{i,j}^\rho(u) = [\rho(u)]_{i,j}$. Recall that for $f, g: G \rightarrow \mathbb{C}$, the inner product $\langle f, g \rangle$ is

defined $\langle f, g \rangle = \sum_{u \in G} f(u) * g(u)$. The Fourier transform of a function f can then be written element-wise as $[\widehat{f}(\rho)]_{i,j} = \langle r_{i,j}^\rho, f \rangle$. However, since the Fourier transform is a unitary transformation, for any $\rho, \rho' \in \mathcal{R}_G$, unless $\rho = \rho'$, $i = i'$ and $j = j'$, we must have $\langle r_{i,j}^\rho, r_{i',j'}^{\rho'} \rangle = 0$. In particular, $[\sum_{u \in G} \rho(u)]_{i,j} = \langle r_{1,1}^{\rho_{\text{tr}}}, r_{i,j}^\rho \rangle = 0$, unless $\rho = \rho_{\text{tr}}$ (and $i = j = 1$). ■

Now recall that given an irrep ρ of G , the *restriction* of ρ to H is $\rho|_H: H \rightarrow \mathbb{C}^{d_\rho \times d_\rho}$, where $\rho|_H(h) = \rho(h)$ for all $h \in H$. It is trivial to check that $\rho|_H$ is a representation of H , but, in general, it is not irreducible. Thus, by the Theorem of Complete Decomposability (see section A), it must decompose in the form $\rho|_H(h) = Q(\mu_1(h) \oplus \mu_2(h) \oplus \dots \oplus \mu_k(h))Q^\dagger$ for some sequence μ_1, \dots, μ_k of irreps of H and some unitary matrix Q . In the special case when the irreps of G and H are adapted to $H \leq G$, however, Q is just the unity.

This is essentially the case that we consider in Proposition 1. Now, armed with the above lemmas, we are in a position to prove Proposition 1.

C.0.1. PROOF OF PART 1

Proof. The fact that any $u \in G$ can be written uniquely as $u = gh$ where g is the representative of one of the gH cosets and $h \in H$ immediately tells us that $\widehat{f}(\rho)$ factors as

$$\begin{aligned} \widehat{f}(\rho) &= \sum_{u \in G} f \uparrow^G(u) \rho(u) = \sum_{x \in G/H} \sum_{h \in H} f \uparrow^G(\overline{x}h) \rho(\overline{x}h) \\ &= \sum_{x \in G/H} \sum_{h \in H} f(x) \rho(\overline{x}h) = \sum_{x \in G/H} \sum_{h \in H} f(x) \rho(\overline{x}) \rho(h) \\ &= \sum_{x \in G/H} f(x) \rho(\overline{x}) \left[\sum_{h \in H} \rho(h) \right]. \end{aligned}$$

However, $\rho(h) = \mu_1(h) \oplus \mu_2(h) \oplus \dots \oplus \mu_k(h)$ for some sequence of irreps μ_1, \dots, μ_k of H , so

$$\sum_{h \in H} \rho(h) = \left[\sum_{h \in H} \mu_1(h) \right] \oplus \left[\sum_{h \in H} \mu_2(h) \right] \oplus \dots \oplus \left[\sum_{h \in H} \mu_k(h) \right],$$

and by Lemma 2 each of the terms in this sum where μ_i is *not* the trivial representation (on H) is a zero matrix, zeroing out all the corresponding columns in $\widehat{f}(\rho)$. ■

C.0.2. PROOF OF PART 2

Proof. Analogous to the proof of part 1, using $u = hg$ and a factorization similar to that of $\widehat{f}(\rho)$ in C.0.1 except that $\sum_{h \in H} \rho(h)$ will now multiply $\sum_{x \in H \setminus G} f(x) \rho(\overline{x})$ from the left. ■

C.0.3. PROOF OF PART 3

Proof. Immediate from combining case 3 of Lemma 1 with Parts 1 and 2 of Proposition 1. ■

D. Proof of Proposition 2

Proof. Let us assume that G is countable. Then

$$\begin{aligned} \widehat{f * g}(\rho_i) &= \sum_{u \in G} \left[\sum_{v \in G} f(uv^{-1}) g(v) \right] \rho_i(u) \\ &= \sum_{u \in G} \sum_{v \in G} f(uv^{-1}) g(v) \rho_i(uv^{-1}) \rho_i(v) \\ &= \sum_{v \in G} \sum_{u \in G} f(uv^{-1}) g(v) \rho_i(uv^{-1}) \rho_i(v) \\ &= \sum_{v \in G} \left[\sum_{u \in G} f(uv^{-1}) \rho_i(uv^{-1}) \right] g(v) \rho_i(v) \\ &= \sum_{v \in G} \left[\sum_{w \in G} f(w) \rho_i(w) \right] g(v) \rho_i(v) \\ &= \left[\sum_{w \in G} f(w) \rho_i(w) \right] \left[\sum_{v \in G} g(v) \rho_i(v) \right] \\ &= \widehat{f}(\rho_i) \widehat{g}(\rho_i). \end{aligned}$$

The continuous case is proved similarly but with integrals with respect Haar measure instead of sums. ■

E. Proof of Theorem 1

E.1. Reverse Direction

Proving the “only if” part of Theorem 1 requires concepts from representation theory and the notion of generalized Fourier transforms (Section A)). We also need two versions of Schur’s Lemma.

Lemma 3. (Schur’s lemma I) Let $\{\rho(g): U \rightarrow U\}_{g \in G}$ and $\{\rho'(g): V \rightarrow V\}_{g \in G}$ be two irreducible representations of a compact group G . Let $\phi: U \rightarrow V$ be a linear (not necessarily invertible) mapping that is equivariant with these representations in the sense that $\phi(\rho(g)(u)) = \rho'(g)(\phi(u))$ for any $u \in U$. Then, unless ϕ is the zero map, ρ and ρ' are equivalent representations.

Lemma 4. (Schur’s lemma II) Let $\{\rho(g): U \rightarrow U\}_{g \in G}$ be an irreducible representation of a compact group G on a space U , and $\phi: U \rightarrow U$ a linear map that commutes with each $\rho(g)$ (i.e., $\rho(g) \circ \phi = \phi \circ \rho(g)$ for any $g \in G$). Then ϕ is a multiple of the identity.

We build up the proof through a sequence of lemmas.

Lemma 5. Let U and V be two vector spaces on which a compact group G acts by the linear actions $\{T_g: U \rightarrow$

$U\}_{g \in G}$ and $\{T'_g: V \rightarrow V\}_{g \in G}$, respectively. Let $\phi: U \rightarrow V$ be a linear map that is equivariant with the $\{T_g\}$ and $\{T'_g\}$ actions, and W be an irreducible subspace of U (with respect to $\{T_g\}$). Then $Z = \phi(W)$ is an irreducible subspace of V , and the restriction of $\{T_g\}$ to W , as a representation, is equivalent with the restriction of $\{T'_g\}$ to Z .

Proof. Assume for contradiction that Z is reducible, i.e., that it has a proper subspace $\mathcal{Z} \subset Z$ that is fixed by $\{T'_g\}$ (in other words, $T'_g(v) \in \mathcal{Z}$ for all $v \in \mathcal{Z}$ and $g \in G$). Let v be any nonzero vector in \mathcal{Z} , $u \in U$ be such that $\phi(u) = v$, and $\mathcal{W} = \text{span}\{T_g(u) \mid g \in G\}$. Since W is irreducible, \mathcal{W} cannot be a proper subspace of W , so $\mathcal{W} = W$. Thus,

$$\begin{aligned} Z &= \phi(\text{span}\{T_g(u) \mid g \in G\}) \\ &= \text{span}\{T'_g(\phi(u)) \mid g \in G\} = \text{span}\{T'_g(v) \mid g \in G\} \subseteq \mathcal{Z}, \end{aligned} \quad (26)$$

contradicting our assumption. Thus, the restriction $\{T_g|_W\}$ of $\{T_g\}$ to W and the restriction $\{T'_g|_Z\}$ of $\{T'_g\}$ to Z are both irreducible representations, and $\phi: W \rightarrow Z$ is a linear map that is equivariant with them. By Schur's lemma it follows that $\{T_g|_W\}$ and $\{T'_g|_Z\}$ are equivalent representations. ■

Lemma 6. Let U and V be two vector spaces on which a compact group G acts by the linear actions $\{T_g: U \rightarrow U\}_{g \in G}$ and $\{T'_g: V \rightarrow V\}_{g \in G}$, and let $U = U_1 \oplus U_2 \oplus \dots$ and $V = V_1 \oplus V_2 \oplus \dots$ be the corresponding isotypic decompositions. Let $\phi: U \rightarrow V$ be a linear map that is equivariant with the $\{T_g\}$ and $\{T'_g\}$ actions. Then $\phi(U_i) \subseteq V_i$ for any i .

Proof. Let $U_i = U_i^1 \oplus U_i^2 \oplus \dots$ be the decomposition of U_i into irreducible G -modules, and $V_i^j = \phi(U_i^j)$. By Lemma 5, each V_i^j is an irreducible G -module that is equivalent with U_i^j , hence $V_i^j \subseteq V_i$. Consequently, $\phi(U_i) = \phi(U_i^1 \oplus U_i^2 \oplus \dots) \subseteq V_i$. ■

Lemma 7. Let $\mathcal{X} = G/H$ and $\mathcal{X}' = G/K$ be two homogeneous spaces of a compact group G , let $\{\mathbb{T}_g: L(\mathcal{X}) \rightarrow L(\mathcal{X})\}_{g \in G}$ and $\{\mathbb{T}'_g: L(\mathcal{X}') \rightarrow L(\mathcal{X}')\}_{g \in G}$ be the corresponding translation actions, and let $\phi: L(\mathcal{X}) \rightarrow L(\mathcal{X}')$ be a linear map that is equivariant with these actions. Given $f \in L(\mathcal{X})$ let \widehat{f} denote its Fourier transform with respect to a specific choice of origin $x_0 \in \mathcal{X}$ and system or irreps $\mathcal{R}_G = \{\rho_1, \rho_2, \dots\}$. Similarly, \widehat{f}' is the Fourier transform of $f' \in L(\mathcal{X}')$, with respect to some $x'_0 \in \mathcal{X}'$ and the same system of irreps.

Now if $f' = \phi(f)$, then each Fourier component of f' is a linear function of the corresponding Fourier component of f , i.e., there is a sequence of linear maps $\{\Phi_i\}$ such that $\widehat{f}'(\rho_i) = \Phi_i(\widehat{f}(\rho_i))$.

Proof. Let $U_1 \oplus U_2 \oplus \dots$ and $V_1 \oplus V_2 \oplus \dots$ be the isotypic decompositions of $L(\mathcal{X})$ and $L(\mathcal{X}')$ with respect to the $\{\mathbb{T}_g\}$ and $\{\mathbb{T}'_g\}$ actions. By our discussion in Section ??, each Fourier component $\widehat{f}(\rho_i)$ captures the part of f falling in the corresponding isotypic subspace U_i . Similarly, $\widehat{f}'(\rho_j)$ captures the part of f' falling in V_j . Lemma 6 tells us that because ϕ is equivariant with the translation actions, it maps each U_i to the corresponding isotypic V_i . Therefore, $\widehat{f}'(\rho_i) = \Phi_i(\widehat{f}(\rho_i))$ for some function Φ_i . By the linearity of ϕ , each Φ_i must be linear. ■

Lemma 7 is a big step towards describing what form equivariant mappings take in Fourier space, but it doesn't yet fully pin down the individual Φ_i maps. We now focus on a single pair of isotypics (U_i, V_i) and the corresponding map Φ_i taking $\widehat{f}(\rho_i) \mapsto \widehat{f}'(\rho_i)$. We will say that Φ_i is an *allowable* map if there is some equivariant ϕ such that $\widehat{\phi(f)}(\rho_i) = \Phi_i(\widehat{f}(\rho_i))$. Clearly, if Φ_1, Φ_2, \dots are individually allowable, then they are also jointly allowable.

Lemma 8. All linear maps of the form $\Phi_i: M \mapsto MB$ where $B \in \mathbb{C}^{\delta \times \delta}$ are allowable.

Proof. Recall that the $\{\mathbb{T}_g\}$ action takes $f \mapsto f^g$, where $f^g(x) = f(g^{-1}x)$. In Fourier space,

$$\begin{aligned} \widehat{f^g}(\rho_i) &= \sum_{u \in G} \rho_i(u) f^g \uparrow^G(u) \\ &= \sum_{u \in G} \rho_i(u) f \uparrow^G(g^{-1}u) \\ &= \sum_{w \in G} \rho_i(gw) f \uparrow^G(w) \\ &= \rho_i(g) \sum_{w \in G} \rho_i(w) f \uparrow^G(w) \\ &= \rho_i(g) \widehat{f}(\rho_i). \end{aligned} \quad (27)$$

(This is actually a general result called the (left) translation theorem.) Thus,

$$\Phi_i(\widehat{\mathbb{T}_g(f)}(\rho_i)) = \Phi_i(\rho_i(g) \widehat{f}(\rho_i)) = \rho_i(g) \widehat{f}(\rho_i) B.$$

Similarly, the $\{\mathbb{T}'_g\}$ action maps $\widehat{f}'(\rho_i) \mapsto g(\rho_i) \widehat{f}'(\rho_i)$, so

$$\mathbb{T}'_g(\Phi_i(\widehat{f}(\rho_i))) = \mathbb{T}'_g(\widehat{f}(\rho_i) B) = \rho_i(g) \widehat{f}(\rho_i) B.$$

Therefore, Φ_i is equivariant with the $\{\mathbb{T}\}$ and $\{\mathbb{T}'\}$ actions. ■

Lemma 9. Let $\Phi_i: M \mapsto BM$ for some $B \in \mathbb{C}^{\delta \times \delta}$. Then Φ_i is not allowable unless B is a multiple of the identity. Moreover, this theorem also hold in the columnwise sense that if $\Phi_i: M \rightarrow M'$ such that $[M']_{*,j} = B_j [M]_{*,j}$ for some sequence of matrices B_1, \dots, B_d , then Φ_i is not allowable unless each B_j is a multiple of the identity.

Proof. Following the same steps as in the proof of Lemma 8, we now have

$$\begin{aligned}\Phi_i(\widehat{\mathbb{T}_g(f)}(\rho_i)) &= B\rho_i(g)\widehat{f}(\rho_i), \\ \mathbb{T}'_g(\Phi_i(\widehat{f}(\rho_i))) &= \rho_i(g)B\widehat{f}(\rho_i).\end{aligned}$$

However, by the second form of Schur's Lemma, we cannot have $B\rho_i(g) = \rho_i(g)B$ for all $g \in G$, unless B is a multiple of the identity. ■

Lemma 10. Φ_i is allowable if and only if it is of the form $M \mapsto MB$ for some $B \in \mathbb{C}^{\delta \times \delta}$.

Proof. For the “if” part of this lemma, see Lemma 8. For the “only if” part, note that the set of allowable Φ_i form a subspace of all linear maps $\mathbb{C}^{\delta \times \delta} \rightarrow \mathbb{C}^{\delta \times \delta}$, and any allowable Φ_i can be expressed in the form

$$[\Phi_i(M)]_{a,b} = \sum_{c,d} \alpha_{a,b,c,d} M_{c,d}.$$

By Lemma 9, if $a \neq c$ but $b = d$, then $\alpha_{a,b,c,d} = 0$. On the other hand, by Lemma 8 if $a = c$, then $\alpha_{a,b,c,d}$ can take on any value, regardless of the values of b and d , as long as $\alpha_{a,b,a,d}$ is constant across varying a .

Now consider the remaining case $a \neq c$ and $b \neq d$, and assume that $\alpha_{a,b,c,d} \neq 0$ while Φ_i is still allowable. Then, by Lemma 8, it is possible to construct a second allowable map Φ'_i (namely one in which $\alpha'_{a,d,a,b} = 1$ and $\alpha'_{a,d,x,y} = 0$ for all $(x,y) \neq (c,d)$) such that in the composite map $\Phi''_i = \Phi'_i \circ \Phi_i$, $\alpha''_{a,d,c,d} \neq 0$. Thus, Φ''_i is not allowable. However, the composition of one allowable map with another allowable map is allowable, contradicting our assumption that Φ_i is allowable.

Thus, we have established that if Φ_i is allowable, then $\alpha_{a,b,c,d} = 0$, unless $a = c$. To show that any allowable Φ_i of the form $M \mapsto MB$, it remains to prove that additionally $\alpha_{a,b,a,d}$ is constant across a . Assume for contradiction that Φ_i is allowable, but for some (a,e,b,d) indices $\alpha_{a,b,a,d} \neq \alpha_{e,b,e,d}$. Now let Φ_0 be the allowable map that zeros out every column except column d (i.e., $\alpha_{x,d,x,d} = 1$ for all x , but all other coefficients are zero), and let Φ' be the allowable map that moves column b to column d (i.e., $\alpha'_{x,d,x,b} = 1$ for any x , but all other coefficients are zero). Since the composition of allowable maps is allowable, we expect $\Phi'' = \Phi' \circ \Phi \circ \Phi^0$ to be allowable. However Φ'' is a map that falls under the purview of Lemma 9, yet $\alpha''_{a,d,a,d} \neq \alpha''_{e,d,e,d}$ (i.e., M_j is not a multiple of the identity) creating a contradiction. ■

Since \mathcal{N} is a G-CNN, each of the mappings $(\sigma_\ell \circ \phi_\ell): L(\mathcal{X}_{\ell-1}) \rightarrow L(\mathcal{X}_\ell)$ is equivariant with the corresponding translation actions $\{\mathbb{T}_g^{\ell-1}\}_{g \in G}$ and $\{\mathbb{T}_g^\ell\}_{g \in G}$. Since σ_ℓ is a pointwise operator, this is equivalent to asserting that ϕ_ℓ is equivariant with $\{\mathbb{T}_g^{\ell-1}\}_{g \in G}$ and $\{\mathbb{T}_g^\ell\}_{g \in G}$.

Letting $\mathcal{X} = \mathcal{X}_{\ell-1}$ and $\mathcal{X}' = \mathcal{X}_\ell$, Lemma 8 then tells us the the Fourier transforms of $f_{\ell-1}$ and $\phi_\ell(f_{\ell-1})$ are related by

$$\phi_\ell(\widehat{f_{\ell-1}})(\rho_i) = \Phi(\widehat{f_{\ell-1}}(\rho_i))$$

for some fixed set of linear maps Φ_1, Φ_2, \dots . Furthermore, by Lemma 10, each Φ_i must be of the form $M \mapsto MB_i$ for some appropriate matrix $B_i \in \mathbb{C}^{d_\rho \times d_\rho}$. If we then define χ_ℓ as the inverse Fourier transform of (B_1, B_2, \dots) , then by the convolution theorem (Proposition 2), $\phi_\ell(f_{\ell-1}) = f_{\ell-1} * \chi$, confirming that \mathcal{N} is a G-CNN. The extension of this result to the vector valued case, $f_\ell: \mathcal{X}_\ell \rightarrow V_\ell$, is straightforward. ■

Proof of Theorem 1 (reverse direction). For simplicity we first prove the theorem assuming $\mathcal{Y}_\ell = \mathbb{C}$ for each ℓ .