EQUIVARIANT NEURAL NETWORKS AND EQUIVARIFICATION

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ABSTRACT. We provide a process to modify a neural network to an equivariant one, which we call equivarification. As an illustration, we build an equivariant neural network for image classification by equivarifying a convolutional neural network.

1. INTRODUCTION

One key issue in deep neural network training is the difficulty of tuning parameters, especially when the network size grows large [4]. Many techniques have been used to solve this issue by analyzing the structural characteristics of data, for example, sparsity [6], invariance in movement [3]. In particular, convolutional neural network is a type of network that uses filters to reduce the number of parameters compared with fully connected networks by observing the invariance of various movement, such as the shift of an object in the photo [5]. However, to handle the case of rotation, they usually use the data augmentation approach to generate redundant input data that has a bunch of training images with different rotation angles of the object to identify.

In this paper, we take advantage of the symmetry property of the data and design a scalable equivariant neural network that is able to capture and preserve the symmetries, e.g., the rotation symmetries. One key property of our designed scalable equivariant neural network is that although the network size grows linearly in the number of rotations we want to detect, the number of parameters we need to train is still the same as the original network. In addition, we can also output the rotation using the same network.

To be precise, for example, consider the space of all images. One can build a cat classifier that assigns a number between 0 and 1 to each image indicating the “probability” that it is an image of a cat. If one image is a rotation (say 90 degree counterclockwise) of another one, then the classifier better assigns the same “probability” to these two images. A classifier that satisfies this property is said to be invariant under 90-degree rotation,
which is a special case of being *equivariant*. Furthermore, we can require
our classifier not only produces the “probability” of being a cat image, but
also provides an angle, say in \( \{0, 90, 180, 270\} \) (more precisely, the “prob-
bility” of each angle). Suppose the classifier maps one image to probability
1 and degree 90, then we expect that it assigns the 180 degrees rotated one
to probability 1 and degree \( 90 + 180 = 270 \).

We provide a way to modify an existing neural network to an equivari-
ant one, the process of which is called *equivarification*. We equivarify a
convolutional neural network as an illustration. In particular, we use the
MNIST data set and we prepare the data by randomly rotating each image
by an angle in \( \{0, 90, 180, 270\} \). The neural network predicts the number
and also the angle. In particular, if we forget the angle and keep only the
number, we get an invariant neural network. The equivariance of our neural
network is built into the structure, and it is independent of how we train it.
Moreover, for the training data, it does not make any difference in results
whether we prepare it by randomly rotating and recording the angles, or not
rotating and labeling everything as degree 0.

1.1. **Relations to other works.** Among the existing nontrivial neural net-
work structures, the one that is closest in spirit to an invariant one is the
convolutional neural network [5], when it comes to translation (not rota-
tion) symmetries. But due to the absence of exact translational symmetries
on data and the usage of strides, one does not get translational invariance.
The notion of equivariant neural network is explicitly mentioned and stud-
ied in [1, 2].

To the best of our knowledge and understanding, this paper gives the
first non-trivial (non-invariant) equivariant neural network and the also first
non-trivial invariant neural network.

1.2. **Guide to the rest of the paper.** For the benefits of future development
and quotation, we present our idea a little bit more general and clearer than it
seems to be needed at the current stage. A hasty reader can go directly to the
examples. Note that our method is suitable for various types of networks,
and here we demonstrate it through the example of a CNN.

2. **Setup**

Let \( X \) be a set, and \( G \) be a group.

**Definition 2.0.1.** We say that \( G \) acts on \( X \) if there exists a map
\[
a : G \times X \to X
\]
such that for any \( x \in X \)
\[
- a(e, x) = x, \text{ where } e \in G \text{ is the identity element,}
\]
for any \( g_1, g_2 \in G \), we have
\[
a(g_1g_2, x) = a(g_1, a(g_2, x)).
\]

For convenience, instead of \( a(g, x) \) we simply write \( gx \), and the above formula becomes \((g_1g_2)x = g_1(g_2x)\).

Let \( X, Y \) be two sets, and \( G \) be a group that acts on both \( X \) and \( Y \).

**Definition 2.0.2.** A map \( F : X \to Y \) is said to be \( G \)-equivariant, if \( F(gx) = gF(x) \) for all \( x \in X \) and \( g \in G \). Moreover, if \( G \) acts trivially on \( Y \) then we say \( F \) is \( G \)-invariant.

**Example 2.0.3.** Let \( X \) be the space of all images of \( 28 \times 28 \) pixels, which contains the MNIST data set. Let \( G \) be the cyclic group of order 4. Pick a generator \( g \) of \( G \), and we define the action of \( g \) on \( X \) by setting \( gx \) to be the image obtained from rotating \( x \) counterclockwise by 90 degrees. Let \( Y \) be the set \( \{0, 1, 2, ..., 9\} \times \{0, 90, 180, 270\} \), and for any \( y = (\text{num}, \theta) \in Y \) we define
\[
gy := (\text{num}, (\theta + 90) \mod 360).
\]

An equivariant neural network that classifies the number and rotation angle can be viewed as a map \( F \) from \( X \) to \( Y \). Equivariance means if \( F(x) = (\text{num}, \theta) \) then \( F(gx) = (\text{num}, (\theta + 90) \mod 360) \), for all \( x \in X \).

3. EQUIFARICATION

In this section we fix \( X \) and \( Z \) to be two sets, and \( G \) to be a group that acts on \( X \). Define \( Z^G := \{ s : G \to Z \} \), the space of all maps from \( G \) to \( Z \). Clearly, \( Z^G \) admits a \( G \)-action
\[
G \times Z^G \to Z^G
\]
\[
(g, s) \mapsto gs,
\]
where \( gs \) as a map from \( G \) to \( Z \) is defined as
\[
(gs)(g') := s(g^{-1}g'),
\]
for any \( g' \in G \).

We have the projection map \( p : Z^G \to Z \) that is define by \( p(s) = s(e) \) for any \( s \in Z^G \) where \( e \in G \) is the identity element. Then \( p \) satisfies

**Lemma 3.0.1.** For any map \( F : X \to Z \), there exits a unique \( G \)-equivariant map \( \hat{F} : X \to Z^G \) such that \( p(\hat{F}(x)) = F(x) \) for all \( x \in X \).

**Proof.** For any \( x \in X \), we define \( \hat{F}(x) \) as a map from \( G \) to \( Z \) by
\[
(\hat{F}(x))(g) = F(g^{-1}x),
\]
for any $g \in G$. To see that $\hat{F}$ is $G$-equivariant, we need to check for any $x \in X$ and $g \in G$, $\hat{F}(gx) = g(\hat{F}(x))$ as elements in $Z \times G$. For any $h \in G$, $(\hat{F}(gx))(h) = F(h^{-1}gx)$ by the definition of $\hat{F}$, while $(g(\hat{F}(x)))(h) = (\hat{F}(x))(g^{-1}h) = F(h^{-1}gx)$. We do not need the uniqueness part, so we leave it to the readers. □

This lemma can be summarized as the commutative diagram in Figure 1.

Given any map $F : X \to Z$,

**Definition 3.0.2.** We call a tuple $(\hat{Z}, \hat{F}, p)$ an equivarification of $F$ if

- $\hat{Z}$ is a set with a $G$-action;
- $\hat{F} : X \to \hat{Z}$ is a $G$-equivariant map;
- $p : \hat{Z} \to Z$ is a map such that $p \circ \hat{F} = F$.

From Lemma 3.0.1 we know that equivarifications always exist. It is not unique for example, if $Z$ admits a $G$-action and $F$ is already $G$-invariant, then we can simply take $\hat{Z} = Z$ and $\hat{F} = F$. See Appendix for more discussion.

**Example 3.0.3.** Let $G$ be the cyclic group of order 4. More concretely, we order elements of $G$ by $(e, g, g^2, g^3)$. The set $Z \times G$ can be identified to $Z \times Z \times Z \times Z$ via the map

$$s \mapsto (s(e), s(g), s(g^2), s(g^3)).$$

(3.0.2)

Then $G$ acts on $Z_{4}^{Z}$ by $g(z_0, z_1, z_2, z_3) = (z_3, z_0, z_1, z_2)$, and the projection map $p : Z \times Z \times Z \times Z \to Z$ is given by $(z_0, z_1, z_2, z_3) \mapsto z_0$. Let $F : X \to Z$ be an arbitrary map, then after identification $\hat{F}$ becomes a map from $Z$ to $Z \times Z \times Z \times Z$ and

$$\hat{F}(x) = (F(x), F(g^{-1}x), F(g^{-2}x), F(g^{-3}x)).$$

One can check that $\hat{F}$ is $G$-equivariant. The map $p$ is given by

$$p(z_0, z_1, z_2, z_3) = z_0.$$

It is easy to see that $p \circ \hat{F} = F$. 

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**Figure 1.**
4. APPLICATION TO NEURAL NETWORKS

Let \( \{ L_i : X_i \to X_{i+1} \}_{i=0}^n \) be an \( n \)-layer neural network. In particular, \( X_0 \) is the input data set, and \( X_{n+1} \) is the output data set. Let \( G \) be a finite group that acts on \( X_0 \). Let \( L \) be the composition of all layers 
\[
L = L_n \circ L_{n-1} \circ \cdots \circ L_0 : X_0 \to X_n.
\]

Then we can equivarify \( L \) and get a map \( \hat{L} : X_0 \to \hat{X}_n \), an equivariant neural network. Alternatively, one can construct an equivariant neural network layer by layer. More precisely, the equivariant neural network is given by 
\[
\{ \hat{L}_i \circ p_i : \hat{X}_i \to \hat{X}_{i+1} \}_{i=0}^n,
\]
where \( \hat{L}_i \circ p_i \) is the equivarification of \( L_i \circ p_i \) for \( i \in \{0, 1, \ldots, n\} \), \( \hat{X}_0 = X_0 \) and \( p_0 = \text{id} \) is the identity map (See Figure 2).

Unfortunately, this does not give us anything new, since 
\[
\hat{L}_n \circ p_n \circ L_{n-1} \circ p_{n-1} \circ \cdots \circ L_0 \circ p_0 = \hat{L}.
\]

Sometimes, other than equivarifying the map \( L_i \circ p_i : \hat{X}_i \to X_{i+1} \), it makes sense to construct some other map \( L'_i \) from \( \hat{X}_i \) to some set \( X'_{i+1} \), and then we can equivarify \( L'_i \). This makes the equivariant neural network more interesting (see the example below).

**Example 4.0.1.** Let the 0-th layer \( L_0 : X_0 \to X_1 \) of a neural network that defined on the MNIST data set be a convolutional layer, and \( X_1 = \mathbb{R}^{\ell_1} \), where \( \ell_1 = 28 \times 28 \times c_1 \), and \( c_1 \) is the number of channels (strides = \( (1, 1) \), padding = ‘same’). Let \( G = \{ e, g, g^2, g^3 \} \) be the cyclic group of order 4 such that \( g \) acts on \( X_0 \) as the 90-degree counterclockwise rotation. Then we construct \( \hat{L}_0 : X_0 \to \mathbb{R}^{4\ell_1} \) by 
\[
x_0 \mapsto (L_0(x_0), L_0(g^{-1}x_0), L_0(g^{-2}x_0), L_0(g^{-3}x_0)).
\]

For the next layer, instead of equivarifying \( L_1 \circ p_1 : \mathbb{R}^{4\ell_1} \to \mathbb{R}^{\ell_2} \), we can construct another convolution layer directly from \( \mathbb{R}^{4\ell_1} \) by concatenating the four copies of \( \mathbb{R}^{\ell_1} \) along the channel axis to obtain \( \mathbb{R}^{28 \times 28 \times 4c_1} \), and build a standard convolution layer on it. (This new construction of course changes the number of variables compared to that of the original network.)
Now we discuss the labeling of the input data. Since the neural network is \( G \)-equivariant, it makes sense to encode the labels \( G \)-equivariantly. We continue with the MNIST example.

**Example 4.0.2.** For \( m \in \{0, 1, 2, \ldots, 9\} \) denote
\[
e_m = (0, \cdots, 0, 1, 0, \cdots, 0) \in \mathbb{R}^{10}.
\]
↑

\( m \)-th spot

For an unrotated image \( x_0 \in X_0 \) that represents the number \( m \), we assign the label \( e_m \oplus 0 \oplus 0 \oplus 0 \in \mathbb{R}^{40} \). Then based on the equivariance, we assign
\[
g x_0 \mapsto 0 \oplus e_m \oplus 0 \oplus 0,
g^2 x_0 \mapsto 0 \oplus 0 \oplus e_m \oplus 0,
g^3 x_0 \mapsto 0 \oplus 0 \oplus 0 \oplus e_m.
\]

In the MNIST data set, only the unrotated images are available. For each testing image, we randomly rotate it by an angle of degree in \( \{0, 90, 180, 270\} \), and we prepare the label as above. For the training images, we can do the same, but just for convenience, we actually do not rotate them, since it won’t affect the training result.

5. **APPENDIX**

5.1. **Network graph.** The graph of our neural network can be found in Figure [3]. Note that equivarification process does not increase the the number of variables. In our case, in order to illustrate flexibility we choose not to simply equivarify the original neural network, so the layer conv2 and conv3 have four times the number of variables compared to the corresponding original layers.

5.2. **Truly equivariance.** To spot check the equivariance after implementation, we print out probability vectors in \( \mathbb{R}^{40} \) of an image of number seven and its rotations. We see that the probability vectors are identical after a shift by 10 slots. See Figure [4].

5.3. **Accuracy.** The accuracy of our neural network on the test data is 96.8\%, which is quite good considering the fact that some numbers are quite hard to determine the angles, such as 0, 1, and 8. Here we count the prediction as correct if both the number and the angle are predicted correctly.

\[\footnote{When we implemented, instead of Formula 3.0.2, we used \( s \mapsto (s(e), s(g), s(g^2), s(g^3)) \), which explains the shift in the opposite direction.}

\[\footnote{The code in tensorflow can be found at https://github.com/symplecticgeometry/equivariant-neural-network-and-equivarification.} \]
Figure 3. In this figure, conv1 is a standard convolution layer with input $X_0$ and output $X_1$. After equivarification of conv1, we get four copies of $X_1$. Then we stack the four copies along the channel direction, and take this whole thing as an input of a standard convolution layer conv2. We equivarify conv2, stack the four copies of $X_2$, and feed it to another convolution layer conv3. Now instead of equivarifying conv3, we add layer pool and layer dense (logistic layer), and then we equivarify their composition dense $\circ$ pool $\circ$ conv3 $\circ g^{-1}$ and get $\hat{X}_5 = \mathbb{R}^{40}$. To get the predicted classes, we can take an argmax afterwards.

5.4. More about equivarification. In Section 3 we define $Z \times G$ as an example of equivarification. In this section, we construct a “minimal” model of equivarification. Let $H$ be the subgroup of $G$ defined by

$$H = \{ g \in G \mid F(gx) = F(x) \text{ for all } x \in X \},$$

and $G/H$ be the left coset of $H$ in $G$. Then define

$$\hat{Z} = G^{\times G/H} = \{ s : G/H \to Z \},$$

the space of maps from $G/H$ to $Z$; a projection map $p : \hat{Z} \to Z$ by $p(s) = s(H)$; and equivariant lift $\hat{F} : X \to \hat{Z}$ by $\hat{F}(gH)(x) = F(g^{-1}x)$. We leave it for the readers to check that this is a well-defined equivarification, and it is minimal in the sense that every other equivarification factors through it. Note that this construction of $\hat{Z}$ depends on the map $F$. In the application to neural network, $F$ usually depends on variables $\alpha$ that are to be trained,
FIGURE 4. On the left, we have the rotated images; on the right, we have the predicted number, angle, and the probability vector in $\mathbb{R}^{40}$, each component of which corresponds to the probability of a (number, angle) combination.

then we can modify the definition of $H$ by

$$H = \{ g \in G \mid F_\alpha(gx) = F_\alpha(x) \text{ for all } \alpha, \text{ and } x \in X \}.$$
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