Meta-Learning Symmetries by Reparameterization

Allan Zhou, Tom Knowles, Chelsea Finn
Stanford University
{ayz,tknowles,cbfinn}@stanford.edu

Abstract

Many successful deep learning architectures are equivariant to certain transformations in order to conserve parameters and improve generalization: most famously, convolution layers are equivariant to shifts of the input. This approach only works when practitioners know a priori symmetries of the task and can manually construct an architecture with the corresponding equivariances. Our goal is a general approach for learning equivariances from data, without needing prior knowledge of a task’s symmetries or custom task-specific architectures. We present a method for learning and encoding equivariances into networks by learning corresponding parameter sharing patterns from data. Our method can provably encode equivariance-inducing parameter sharing for any finite group of symmetry transformations, and we find experimentally that it can automatically learn a variety of equivariances from symmetries in data. We provide our experiment code and pre-trained models at https://github.com/AllanYangZhou/metalearning-symmetries.

1 Introduction

In deep learning, the convolutional neural network (CNN) [29] is a prime example of exploiting equivariance to a symmetry transformation to conserve parameters and improve generalization. In image classification [40, 27] and audio processing [18, 22] tasks, we may expect the layers of a deep network to learn feature detectors that are translation equivariant: if we translate the input, the output feature map is also translated. Convolution layers satisfy translation equivariance by definition, and produce remarkable results on these tasks. The success of convolution’s “built in” inductive bias suggests that we can similarly exploit other equivariances to solve machine learning problems.

However, there are substantial challenges with building in inductive biases. Identifying the correct biases to build in is challenging, and even if we do know the correct biases, it is often difficult to build them into a neural network. Practitioners commonly avoid this issue by “training in” desired equivariances (usually the special case of invariances) using data augmentation. However, data augmentation can be challenging in many problem settings and we would prefer to build the equivariance into the network itself. Additionally, building in incorrect biases may actually be detrimental to final performance [33].

In this work we aim for an approach that can automatically learn and encode equivariances into a neural network. This would free practitioners from having to design custom equivariant architectures for each task, and allow them to transfer any learned equivariances to new tasks. Neural network layers can achieve various equivariances through parameter sharing patterns, such as the spatial parameter sharing of standard convolutions. The particular sharing pattern depends on the equivariance, and in this paper we reparameterize network layers to learnably represent sharing patterns. We leverage meta-learning to learn the sharing patterns that help a model to generalize on new tasks.

The primary contribution of this paper is a general approach to automatically learn and build in equivariances to symmetries observed in data, without requiring custom designed equivariant architectures and using only generic neural network components. We show theoretically that this

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method can produce networks equivariant to any finite symmetry group. Our experiments show
that our method can not only recover various convolutional architectures from data, but also learns
invariances to a variety of transformations usually obtained via data augmentation.

2 Related Work

A number of works have studied designing layers with equivariances to certain transformations such
as permutation, rotation, reflection, and scaling \([17,6,54,53,7,51,52]\). These approaches focus on
manually constructing layers analogous to standard convolution, but equivariant to other symmetry
groups besides translation. More theoretical work has characterized the nature of equivariant layers
for various symmetry groups \([26,43,39]\). Rather than building symmetries into the architecture, data
augmentation \([4,56]\) trains a network to satisfy them. There is also a hybrid approach that pre-trains
a basis of rotated filters in order to define roto-translation equivariant convolution \([11]\). Unlike these
works, we aim to automatically build in symmetries by acquiring them from data.

Prior work on automatically learning symmetries is more sparse, and includes works that focus on
Gaussian processes \([49]\) and symmetries of physical systems \([20,8]\). Automatically discovering data
augmentation strategies \([9,34]\) can also be considered a way of learning symmetries, but does not
embed these symmetries into the model itself.

Our work is related to neural network architecture search \([55,5,32,14]\), which also aims to automate
part of the model design process. Although architecture search methods are varied, they are generally
not designed to exploit symmetry or learn equivariances. Evolutionary methods for learning both
network weights and topology \([46,47]\) are also not motivated by symmetry considerations.

Our method learns to exploit symmetries that are shared by a collection of tasks, a form of meta-
learning \([48,42,3,23]\). We extend gradient based meta-learning \([15,31,2]\) to separately learn
parameter sharing patterns (which enforce equivariance) and actual parameter values. Separately
representing network weights in terms of a sharing pattern and parameter values is a form of
reparameterization. Prior work has used weight reparameterization in order to “warp” the loss surface
\([30,16]\) and to learn good latent spaces \([41]\) for optimization, rather than to encode equivariance.

HyperNetworks \([21]\) generate network layer weights using a separate smaller network, which can
be viewed as a nonlinear reparameterization, albeit not one that encourages learning equivariances.
Modular meta-learning \([1]\) is a related technique that aims to achieve combinatorial generalization
on new tasks by stacking meta-learned “modules,” each of which is a neural network. This can
be seen as parameter sharing by re-using and combining these modules, rather than by layerwise
reparameterization as in our work.

3 Preliminaries

In Sec. 3.1, we review gradient based meta-learning, which underlies our algorithm. Sections 3.2
and 3.3 build up a formal definition of equivariance and group convolution \([6]\), a generalization
of standard convolution which defines equivariant operations for other groups such as rotation and
reflection. These concepts are important for a theoretical understanding of our work as a method for
learning group convolutions in Sec. 4.2.

3.1 Gradient Based Meta-Learning

Our method is a gradient-based meta-learning algorithm that extends MAML \([15]\), which we briefly
review here. Suppose we have some task distribution \(p(T)\), where each task is split into training and
validation datasets \(T_i = \{D_i^{tr}, D_i^{val}\}\). For a model with parameters \(\theta\), loss \(\mathcal{L}\), and learning rate \(\alpha\), the
“inner loop” updates \(\theta\) using the task’s training data, shown here with one gradient descent step:

\[
\theta' = \theta - \alpha \nabla_{\theta} \mathcal{L}(\theta, D^{tr})
\]

In the “outer loop,” MAML meta-learns a good initialization \(\theta\) using the loss of the new parameters
\(\theta'\) on the task’s validation data:

\[
\theta \leftarrow \theta - \eta \nabla_{\theta} \mathcal{L}(\theta', D^{val})
\]
with respect to these transformations: A function (like a neural network layer) is equivariant to some transformation if transforming the input changes the output in the same way. To be more precise, we must define what equivariance means in terms of functions on some underlying space. We denote the vector space of all real-valued functions on \( X \) by \( \mathcal{F}_X \). For group \( G \), we can define how \( G \) acts on \( \mathcal{F}_X \) by a representation \( \pi : G \rightarrow GL(\mathcal{F}_X) \) which maps each \( g \in G \) to an invertible linear transformation on \( \mathcal{F}_X \). If \( G \) already acts on \( X \), the “natural” representation of the action is \( \pi(g)f(x) = f(g^{-1}x) \). To provide a concrete example, consider images as functions \( f : \mathbb{R}^2 \rightarrow \mathbb{R} \) mapping pixel locations to intensities, and let \( G = \mathbb{R}^2 \) act on \( X = \mathbb{R}^2 \) by translation as defined above. Then \( \pi(g)f(x) = f((g^{-1}x)) = f(x-g) \) for any \( g, x \in \mathbb{R}^2 \). Hence this representation of \( \mathbb{R}^2 \) on images translates images by translating their underlying space (the 2-D plane).

### 3.3 Equivariance and Convolution

A function (like a neural network layer) is equivariant to some transformation if transforming the function’s input is the same as transforming its output. To be more precise, we must define what those transformations of the input and output are. Consider a neural network layer as a function on functions \( \phi : \mathcal{F}_X \rightarrow \mathcal{F}_Y \) for two underlying spaces \( X,Y \). Assume we have some group \( G \) and two representations \( \pi_1 : G \rightarrow GL(\mathcal{F}_X), \pi_2 : G \rightarrow GL(\mathcal{F}_Y) \), where \( \pi_1(g) \) defines how \( g \in G \) transforms the input, while \( \pi_2(g) \) defines how \( g \) transforms the output. We define \( G \)-equivariance with respect to these transformations:

\[
\phi(\pi_1(g)f) = \pi_2(g)\phi(f), \quad \forall g \in G, f \in \mathcal{F}_X
\]

If we choose \( \pi_2 \equiv \text{id} \) we get \( \phi(\pi_1(g)f) = \phi(f) \), showing that invariance is a type of equivariance.

Deep networks contain many layers, but fortunately function composition preserves equivariance. So if we achieve equivariance in each individual layer, the whole network will be equivariant. Pointwise

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**Figure 1:** Convolution as translating filters. Left: Standard 1-D convolution slides a filter \( w \) along the length of input \( x \). This operation is translation equivariant: translating \( x \) will translate \( g \). Right: Standard convolution is equivalent to a fully connected layer with a parameter sharing pattern: each row contains translated copies of the filter. Other equivariant layers will have their own sharing patterns.
nonlinearities such as ReLU and sigmoid are already equivariant to any permutation of the input and output indices, which includes translation, reflection, and rotation. Hence we are primarily focused on enforcing equivariance in the linear layers.

Prior work [26] has shown that a linear layer $\phi$ is equivariant to the action of some group if and only if it is a group convolution, which generalizes standard convolutions to arbitrary groups. For a specific $G$, we call the corresponding group convolution “$G$-convolution” to distinguish it from standard convolution. Intuitively, $G$-convolution transforms a filter according to each $g \in G$, then computes a dot product between the transformed filter and the input. In standard convolution, the filter transformations correspond to translation (Fig. 1). More formally, assume $X$ is a finite set. $G$-equivariant layers convolve an input $f : X \to \mathbb{R}$ with a filter $\psi : X \to \mathbb{R}$:

$$
[\phi(f)](g) = (f * \psi)(g) = \sum_{x \in X} f(x)[\pi(g)\psi](x) = \sum_{x \in X} f(x)\psi(g^{-1}x)
$$

(4)

In this work, we present a method that represents and learns parameter sharing patterns for existing layers, such as fully connected layers. These sharing patterns can force the layer to implement various group convolutions, and hence equivariant layers.

4 Encoding and Learning Equivariance

In order to learn equivariances automatically, our method introduces a flexible representation that can encode possible equivariances, and an algorithm for learning which equivariances to encode. Here we describe this method, which we call Meta-learning Symmetries by Reparameterization (MSR).

4.1 Learnable Parameter Sharing

As Fig. 1 shows, a fully connected layer can implement standard convolution if its weight matrix is constrained with a particular sharing pattern, where each row contains a translated copy of the same underlying filter parameters. This idea generalizes to equivariant layers for other transformations like rotation and reflection, but the sharing pattern depends on the transformation. Since we do not know the sharing pattern a priori, we “reparameterize” fully connected weight matrices to represent them in a general and flexible fashion. A fully connected layer $\phi : \mathbb{R}^n \to \mathbb{R}^m$ has weight matrix $W$:

$$
y = \phi(x) = Wx, \quad W \in \mathbb{R}^{m \times n}
$$

(5)

We can optionally incorporate biases by appending a dimension with value “1” to the input $x$. We factorize $W$ as the product of a “symmetry matrix” $U$ and a vector $v$ of $k$ “filter parameters”:

$$
\text{vec}(W) = Uv, \quad v \in \mathbb{R}^k, U \in \mathbb{R}^{mn \times k}
$$

(6)

For fully connected layers, we reshape the vector $\text{vec}(W) \in \mathbb{R}^{mn}$ into a weight matrix $W \in \mathbb{R}^{m \times n}$. Intuitively, $U$ encodes the pattern by which the weights $W$ will “share” the filter parameters $v$. Crucially, we can now separate the problem of learning the sharing pattern (learning $U$) from the problem of learning the filter parameters $v$. In Sec. 4.3 we discuss how to learn $U$ from data.

The symmetry matrix for each layer has $mnk$ entries, which can become too expensive in larger layers. Kronecker factorization is a common approach for approximating a very large matrix with smaller ones [35,37]. In Appendix A, we describe how we apply Kronecker approximation to Eq. 6 and analyze memory and computation efficiency.

In practice, there are certain equivariances that would be expensive to meta-learn, but that we know to be useful: for example, standard 2D convolutions for image data. However, there may be still other symmetries of the data (i.e., rotation, scaling, reflection, etc.) that we still wish to learn automatically. This suggests a “hybrid” approach, where we bake-in certain equivariances we know to be useful, and learn the others. Indeed, we can directly reparameterize a standard convolution layer by reshaping $\text{vec}(W)$ into a convolution filter bank rather than a weight matrix. By doing so we bake in translational equivariance, but we can still learn things like rotation equivariance from data.

4.2 Parameter sharing and group convolution

Here we show that by properly choosing the symmetry matrix $U$ of Eq. 6 we can force the layer to implement arbitrary group convolutions (Eq. 4) by filter $v$. Recall that group convolutions generalize...
We reparameterize the weights of each layer in terms of a symmetry matrix $U$ which can enforce equivariant sharing patterns of the filter parameters $v$. Here we show a $U$ that enforces permutation equivariance. More technically, the layer implements group convolution on the permutation group $S_2$: $U$’s block submatrices $\pi(e), \pi(g)$ define the action of each permutation on filter $v$. Note that $U$ need not be binary in general.

For each task, the inner loop updates the filter parameters $v$ to the task using the inner loop loss. Note that the symmetry matrix $U$ does not change in the inner loop, and is only updated by the outer loop.

**Algorithm 1: MSR: Meta-Training**

**Input**: $(T_j)_{j=1}^N \sim p(\mathcal{T})$: Meta-training tasks

**Input**: $(U, v)$: Randomly initialized symmetry matrices and filters.

**Input**: $\alpha, \eta$: Inner and outer loop step sizes.

**While not done**

- Sample minibatch $(T_i)_{i=1}^n \sim \{T_j\}_{j=1}^N$.
- For all $T_i \in \{T_i\}_{i=1}^n$
  - $(D_{i}^{tr}, D_{i}^{val}) \leftarrow T_i$; // task data
  - $\delta_i \leftarrow \nabla_v L(D_i^{tr}, U, v)$; // inner step
  - $v' \leftarrow v - \alpha \delta_i$;
  - $G_i \leftarrow \frac{d}{dv} L(D_i^{val}, U, v')$; /* outer gradient */
  - $G_i \leftarrow \frac{d}{dv} L(D_i^{val}, U, v')$; /* outer step */
- $U \leftarrow U - \eta \sum_i G_i$;

standard convolution to define operations that are equivariant to other groups, such as rotation and permutation. Hence by choosing $U$ properly we can enforce arbitrary equivariances, which will be preserved regardless of the value of $v$.

For simplicity, we’ll work with an input of the form $f : X \to \mathbb{R}$, although the result easily generalizes to multi-channel inputs $f : X \to \mathbb{R}^c$. We assume that $f$ has finite support $\{x_1, \ldots, x_s\}$ on $X$ and can therefore be represented as a vector $\mathbf{f} \in \mathbb{R}^s$, where $\mathbf{f}(x_i)$. In practice, this is always the case: for example, a discretized image is only nonzero at a finite number of pixel locations. Then we can formalize our claim:

**Proposition 1** Suppose $G$ is a finite group $\{g_1, \ldots, g_n\}$. There exists a $U \in \mathbb{R}^{ns \times s}$ such that for any $v \in \mathbb{R}^s$, the layer with weights $\text{vec}(W) = U^G v$ implements $G$-convolution on input $\mathbf{f} \in \mathbb{R}^s$. Moreover, with this fixed choice of $U^G$, any $G$-convolution can be represented by a weight matrix $\text{vec}(W) = U^G v$ for some $v \in \mathbb{R}^s$.

We present a proof in Appendix B.

Intuitively, $U$ can store the symmetry transformations $\pi(g)$ for each $g \in G$, thus capturing how the filters should transform during $G$-convolution. For example, Fig. 2 shows how to choose $U$ to implement convolution on the permutation group $S_2$.

Subject to having a correct $U^G$, $v$ is precisely the convolution filter in a $G$-convolution. This will motivate the notion of separately learning the convolution filter $v$ and the symmetry structure $U$ in the inner and outer loops of a meta-learning process, respectively.

**4.3 Meta-learning equivariances**

Meta-learning generally applies when we want to learn and exploit some shared structure in a distribution of tasks $p(\mathcal{T})$. In this case, we assume the task distribution has some common underlying
We now introduce a series of synthetic meta-learning problems, where each problem contains translation symmetry. MSR with a fully connected model (MSR-FC) is comparable to MAML with a convolution model (MAML-Conv) on translation equivariant \((k = 1)\) data. On higher rank data (less symmetry), MSR outperforms all other approaches.

| Method         | \(k = 1\) | \(k = 2\) | \(k = 5\) |
|----------------|-----------|-----------|-----------|
| MAML-FC        | 3.2 ± .29 | 2.1 ± .15 | .89 ± .05 |
| MAML-LC        | 2.4 ± .23 | 1.6 ± .11 | .81 ± .05 |
| MAML-Conv      | .16 ± .02 | .52 ± .05 | .44 ± .02 |
| MSR-FC (Ours)  | .18 ± .03 | .21 ± .02 | .22 ± .01 |

Table 1: Meta-test mean squared error (MSE) of MSR and MAML using different models on synthetic data with (partial) translation symmetry. MSR with a fully connected model (MSR-FC) is comparable to MAML with a convolution model (MAML-Conv) on translation equivariant \((k = 1)\) data. On higher rank data (less symmetry), MSR outperforms all other approaches.

We illustrate the inner and outer loop updates in Fig.\(3\). Note that in addition to meta-learning the LC filter weights with a rank \(k\) we use the inner loop (Eq.\(8\)) to update only the filter parameters \(U\) after meta-training is complete, we freeze the symmetry matrices \(U\) and only updates \(v\) using the task training data:

\[
v' \leftarrow v - \alpha \nabla_v \mathcal{L}(D_i^{\text{val}}, U, v)
\]

where \(\mathcal{L}\) is simply the supervised learning loss, and \(\alpha\) is the inner loop step size. During meta-training, the outer loop then computes the loss on the task’s validation data using \(v'\), and update \(U\):

\[
U \leftarrow U - \eta \frac{d}{dU} \mathcal{L}(D_i^{\text{val}}, U, v')
\]

We illustrate the inner and outer loop updates in Fig.\(3\). Note that in addition to meta-learning the symmetry matrices, we can also still meta-learn the filter initialization \(v\) as in prior work. In practice we also take outer updates averaged over mini-batches of tasks, as we describe in Alg.\(1\).

After meta-training is complete, we freeze the symmetry matrices \(U\). On a new test task \(T_k \sim p(T)\), we use the inner loop (Eq.\(8\)) to update only the filter parameters \(v\). The frozen \(U\) enforces the meta-learned equivariance-inducing parameter sharing in each layer. This sharing improves generalization by reducing the number of task-specific inner loop parameters. For example, the sharing pattern of standard convolution guarantees that the weight matrix is constant along any diagonal, reducing the number of per-task parameters (see Fig.\(1\)).

## 5 Can we recover convolutional structure?

We now introduce a series of synthetic meta-learning problems, where each problem contains regression tasks that are guaranteed to have some symmetries, such as translation, rotation, or reflection. We combine meta-learning methods with general architectures not designed with these symmetries in mind to see whether each method can automatically meta-learn these equivariances.

### 5.1 Learning (partial) translation symmetry

Our first batch of synthetic problems contains tasks with translational symmetry: we generate regression data by feeding random input vectors to a 1-D locally connected (LC) layer with filter size 3 to generate output vectors. Each task corresponds to the values of the LC filter, and the meta-learner must minimize mean squared error (MSE) after observing a single input-output pair. For each problem we constrain the LC filter weights with a rank \(k \in \{1, 2, 5\}\) factorization\(13\), implementing a form of partial translation symmetry. In the extreme case where rank \(k = 1\), the LC layer is equivalent to convolution (ignoring the biases) and thus generates exactly translation equivariant task data. We apply both MSR and MAML to this problem using a single layer fully connected model (MSR-FC and MAML-FC, respectively), so these models have no translational equivariance built in and must meta-learn it to solve the tasks efficiently. For comparison, we also train convolutional and locally...
connected models with MAML (MAML-Conv and MAML-LC, respectively). Since MAML-Conv’s architecture builds in translation equivariance, we expect it to at least perform well on the rank $k = 1$ problem. We train each method to convergence on the meta-training tasks of each problem, then evaluate the meta-test MSE. Appendix D.1 further explains the experimental setup.

Table 1 shows how each method performs on each of the synthetic problems, listed by column denoting the rank $k$ of the LC filter generating task data. On completely translation equivariant data ($k = 1$), MSR-FC performs comparably to MAML-Conv despite not having built in symmetry assumptions. MSR-FC actually meta-learns symmetry matrices that enforce convolutional sharing structure on the weights (Fig. 4), essentially “learning convolution” from translation-equivariant data. In Appendix C we inspect the meta-learned symmetry matrix $U$, which we find implements convolution using filter $v$ just as Sec. 4.2 predicted. Meanwhile, MAML-FC and MAML-LC perform significantly worse as they are unable to meta-learn this structure.

On partially symmetric data (rank $k = 2$ or $k = 5$), MSR-FC outperforms all other methods due to its ability to flexibly meta-learn even partial symmetries. MAML-Conv performs worse in these settings since the convolution assumption is overly restrictive, while MAML-FC and MAML-LC are not able to meta-learn much structure at all.

## 5.2 Learning equivariance to rotations and flips

We also created synthetic problems with 2-D synthetic image inputs and outputs, in order to study rotation and flip equivariance. We generate task data by passing randomly generated inputs through a single layer $E(2)$-equivariant steerable CNN [51] configured to be equivariant to combinations of translations, discrete rotations by increments of $45^\circ$, and reflections. Hence our synthetic task data contains rotation and reflection in addition to translation symmetry. Each task corresponds to different values of the data-generating network’s weights. We apply MSR and MAML to a single standard convolution layer. By reparameterizing a convolution layer, we have already guaranteed translational equivariance, but each method must still meta-learn rotation and reflection (flip) equivariance from the data. Table 2 shows that MSR easily learns rotation and rotation+reflection equivariance on top of the convolutional model’s built in translational equivariance.

## 6 Can we learn invariances from augmented data?

Practitioners commonly use data augmentation to train their models to have certain invariances. Since invariance is a special case of equivariance, we can also view data augmentation as a way of learning equivariant models. The downside is that we need augmented data for each task. While augmentation is often possible during meta-training, there are many situations where its impractical at meta-test time. For example, in robotics we may meta-train a robot in simulation and then deploy (meta-test) in the real world, a kind of sim2real transfer strategy [45]. During meta-training we can augment data using the simulated environment, but we cannot do the same at meta-test time in the real world.

Can we instead use MSR to learn equivariances from data augmentation at training time, and encode those learned equivariances into the network itself? This way, the network would preserve learned equivariances on new meta-test tasks without needing any additional data augmentation.

### Algorithm 2: Augmentation Meta-Training

```
input : $\{T_i\}_{i=1}^N$; Meta-training tasks
input : META-TRAIN; Any meta-learner
input : AUGMENT; Data augmenter
forall $T_i \in \{T_i\}_{i=1}^N$ do
    $\{D_i^{tr}, D_i^{val}\} \leftarrow T_i$; // task data split
    $D_i^{val} \leftarrow$ AUGMENT($D^{val}$);
    $\hat{T}_i \leftarrow \{D_i^{tr}, D_i^{val}\}$
META-TRAIN ($\{\hat{T}_i\}_{i=1}^N$)
```

Table 2: MSR learns rotation and flip equivariant parameter sharing on top of a standard convolution model, and thus achieves much better generalization error on meta-test tasks compared to MAML on rotation and flip equivariant data.
We introduce a method for automatically meta-learning equivariances in neural network models, by encoding learned equivariance-inducing parameter sharing patterns in each layer. On new tasks, these sharing patterns reduce the number of task-specific parameters and improve generalization. Our experiments show that this method can improve few-shot generalization on task distributions with shared underlying symmetries. We also introduce a strategy for meta-training invariances into networks using data augmentation, and show that it works well with our method. By encoding equivariances into the network as a parameter sharing pattern, our method has the benefit of preserving learned equivariances on new tasks so it can learn more efficiently.

Table 3: Meta-test accuracies on Aug-Omniglot and Aug-MiniImagenet few-shot classification, which requires generalizing to augmented validation data from un-augmented training data. MSR performs comparably to or better than other methods under this augmented regime. Results shown with 95% CIs.

Alg. 2 describes our approach for meta-learning invariances from data augmentation, which wraps around any meta-learning algorithm using generic data augmentation procedures. Recall that each task is split into training and validation data \( T_i = \{ D_{i}^{tr}, D_{i}^{val} \} \). We use the data augmentation procedure to only modify the validation data, producing a new validation dataset \( \hat{D}_{i}^{val} \) for each task. We re-assemble each modified task using the original training data and modified validation data \( \hat{T}_i \leftarrow \{ D_{i}^{tr}, \hat{D}_{i}^{val} \} \). For each task, the meta-learner observes unaugmented training data, but must generalize to perform well on augmented validation data. This forces the model to be invariant to the augmentation transforms without actually seeing any augmented training data.

We apply this augmentation strategy to Omniglot [28] and MiniImagenet [50] few shot classification to create the Aug-Omniglot and Aug-MiniImagenet benchmarks. Our data augmentation function contains a combination of random rotations, flips, and resizes (rescaling), which we apply only to each task’s validation data as described above. Aside from the augmentation procedure, the benchmarks are identical to prior work [15]: for each task, the model must classify images into one of either 5 or 20 classes \((n\text{-way})\) and receives either 1 or 5 examples of each class in the task training data \((k\text{-shot})\).

We tried combining Alg. 2 with our MSR method and three other meta-learning algorithms: MAML [15], ANIL [38], and Prototypical Networks (ProtoNets) [44]. While the latter three methods all have the potential to learn equivariant features through Alg. 2, we hypothesize that since MSR enforces learned equivariance through its symmetry matrices it should outperform those feature-metalearning methods. Appendix D.2 describes the experimental setup and methods implementations in more detail.

Table 3 shows each method’s meta-test accuracies on both benchmarks. Across different settings MSR performs either comparably to the best method, or the best. MAML and ANIL perform similarly to each other, and usually worse than MSR, suggesting that learning equivariant or invariant features is not as helpful as learning equivariant layer structures. ProtoNets perform well on the easier Aug-Omniglot benchmark, but evidently struggle with learning a transformation invariant metric space on the harder Aug-MiniImagenet problems. Note that MSR’s reparameterization increases the number of meta-learned parameters at each layer, so MSR models contain more total parameters than corresponding MAML models. The “MAML (Big)” results show MAML performance with more total parameters containing more total parameters than the corresponding MSR models. The results show that MSR also outperforms these larger MAML models despite having fewer total parameters.

7 Discussion and Future Work

We introduce a method for automatically meta-learning equivariances in neural network models, by encoding learned equivariance-inducing parameter sharing patterns in each layer. On new tasks, these sharing patterns reduce the number of task-specific parameters and improve generalization. Our experiments show that this method can improve few-shot generalization on task distributions with shared underlying symmetries. We also introduce a strategy for meta-training invariances into networks using data augmentation, and show that it works well with our method. By encoding equivariances into the network as a parameter sharing pattern, our method has the benefit of preserving learned equivariances on new tasks so it can learn more efficiently.

Machine learning thus far has benefited from exploiting human knowledge of problem symmetries, and we believe this work presents a step towards learning and exploiting symmetries automatically. This work leads to numerous directions for future investigation. In addition to generalization
benefits, standard convolution is practical since it exploits the parameter sharing structure to improve computational efficiency, relative to a fully connected layer of the same input/output dimensions. While MSR we can improve computational efficiency by reparameterizing known structured layers (such as standard convolution), it does not exploit learned structure to further optimize its computation. Can we automatically learn or find efficient implementations of these more structured operations? Additionally, our method is best for learning symmetries which are shared across a distribution of tasks. Further research on quickly discovering symmetries which are particular to a single task would make deep learning methods significantly more useful on many difficult real world problems.

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A Approximation and Tractability

A.1 Fully connected

From Eq. 6, we see that for a layer with \( m \) output units, \( n \) input units, and \( k \) filter parameters the
symmetry matrix \( U \) has \( mnk \) entries. This is too expensive for larger layers, so in practice, we need
a factorized reparameterization to reduce memory and compute requirements when \( k \) is larger.

For fully connected layers, we use a Kronecker factorization to scalably reparameterize each layer.
First, we assume that the filter parameters \( v \in \mathbb{R}^{kl} \) can be arranged in a matrix \( V \in \mathbb{R}^{k \times l} \). Then we
reparameterize each layer’s weight matrix \( W \) similar to Eq. 6 but assume the symmetry matrix is the
Kronecker product of two smaller matrices:

\[
\text{vec}(W) = (U_2 \otimes U_1) \text{vec}(V), \quad U_1 \in \mathbb{R}^{m \times k}, U_2 \in \mathbb{R}^{n \times l}
\]

(10)

Since we only store the two Kronecker factors \( U_1 \) and \( U_2 \), we reduce the memory requirements of \( U \)
from \( mnl \) to \( mk + nl \). In our experiments we generally choose \( V \in \mathbb{R}^{m \times n} \) so \( U_1 \in \mathbb{R}^{m \times m} \) and
\( U_2 \in \mathbb{R}^{n \times n} \). Then the actual memory cost of each reparameterized layer (including both \( U \) and \( V \)) is
\( m^2 + n^2 + mn \), compared to \( mn \) for a standard fully connected layer. So in the case where \( m \approx n \),
MSR increases memory cost by roughly a constant factor of \( 3 \).

After approximation MSR also increases computation time (forward and backward passes) by roughly
a constant factor of 3 compared to MAML. A standard fully connected layer requires a single matrix-
matrix multiply \( Y = WX \) in the forward pass (here \( Y \) and \( X \) are matrices since inputs and outputs
are in batches). Applying the Kronecker-vec trick to Eq. 10 gives:

\[
W = U_1 V U_2^T \iff \text{vec}(W) = (U_2 \otimes U_1) \text{vec}(V)
\]

(11)

So rather than actually form the (possibly large) symmetry matrix \( U_2 \otimes U_1 \), we can directly construct
\( W \) simply using 2 additional matrix-matrix multiplies \( W = U_1 V U_2^T \). Again assuming \( V \in \mathbb{R}^{m \times n} \)
and \( m \approx n \), each matrix in the preceding expression is approximately the same size as \( W \).

A.2 2D Convolution

When reparameterizing 2-D convolutions, we need to produce a filter (a rank-4 tensor \( W \in \mathbb{R}^{C_i \times C_i \times H \times W} \)). We assume the filter parameters are stored in a rank 3 tensor \( V \in \mathbb{R}^{p \times q \times s} \),
and factorize the symmetry matrix \( U \) into three separate matrices \( U_1 \in \mathbb{R}^{C_i \times p}, U_2 \in \mathbb{R}^{C_i \times q} \) and
\( U_3 \in \mathbb{R}^{H \times W} \). A similar Kronecker product approximation gives:

\[
\tilde{W} = V \times_1 U_1 \times_2 U_2 \times_3 U_3, \quad \tilde{W} \in \mathbb{R}^{C_i \times C_i \times H \times W}
\]

(12)

\[
W = \text{reshape}(\tilde{W}), \quad W \in \mathbb{R}^{C_i \times C_i \times H \times W}
\]

(13)

where \( \times_n \) represents \( n \)-mode tensor multiplication [25]. Just as in the fully connected case, this
convolution reparameterization is equivalent to a Kronecker factorization of the symmetry matrix \( U \).

An analysis of the memory and computation requirements of reparameterized convolution layers
proceeds similarly to the above analysis for the fully connected case. As we describe below, in our
augmented experiments using convolutional models each MSR outer step takes roughly 30%-40% longer
than a MAML outer step.

B Proof of Proposition [1]

We’ll model an input signal as a function \( f : X \to \mathbb{R} \) on some underlying space \( X \). We then consider
a finite group \( G = \{g_1, \ldots, g_n\} \) of symmetries acting transitively on \( X \), over which we desire
\( G \)-equivariance. Many (but not all) of the groups discussed in [51] are finite groups of this form.

It is proven by [26] that a function is equivariant to \( G \) if and only if it is a \( G \)-convolution. Following the
original paper on group-equivariant CNNs [6], we in fact consider a slight simplification of this
notion: a finite “\( G \) cross-correlation” of \( f \) with a filter \( \psi : X \to \mathbb{R} \). This can be defined as:

\[
[f \ast \psi]_G(g) = \sum_{x \in X} f(x) \psi(g^{-1} x^T)
\]

(14)

This definition avoids notions such as lifting of \( X \) to \( G \) and the possibility of more general group representations, for the sake of simplicity. We recommend Kondor and Trivedi [26] for a more complete theory of \( G \)-convolutions.
We consider $W \in \mathbb{R}^{n \times s}$ allows arbitrary $G$ cross-correlations—and only $G$ cross-correlations—to be represented by fully connected layers with weight matrices of the form

$$W = \text{reshape}(U^G v),$$

where $v \in \mathbb{R}^s$ is any arbitrary vector of appropriate dimension. The reshape specifically gives $W \in \mathbb{R}^{n \times s}$, which transforms the vector $\overline{f} \in \mathbb{R}^s$.

With this in mind, we first use that the action of the group can be represented as a matrix representation on this vector space, using the matrix representation $\pi$:

$$[\pi(g)\overline{f}]_i = f(g^{-1}x_i)$$

where notably $\pi(g) \in \mathbb{R}^{s \times s}$.

We consider $U^G \in \mathbb{R}^{s \times s}$, and $v \in \mathbb{R}^s$. Since $v \in \mathbb{R}^s$, we can also treat $v$ as the “dual” vector of a function $\hat{v} : X \rightarrow \mathbb{R}$ with support $\{x_1, \ldots, x_s\}$, described by $\hat{v}(x_i) = v_i$. We can interpret $\hat{v}$ as a convolutional filter, just like $\hat{\psi}$ in Eq. (14) $W$ then acts on $\hat{v}$ just as it acts on $\overline{f}$, namely:

$$[\pi(g)v]_i = \hat{v}(g^{-1}x_i).$$

Now, we define $U^G$ by stacking the matrix representations of $g_i \in G$:

$$U^G = \begin{bmatrix} \pi(g_1) \\ \vdots \\ \pi(g_n) \end{bmatrix}$$

which implies the following value of $W$:

$$W = \text{reshape}(U^G v) = \text{reshape} \begin{bmatrix} \pi(g_1)v \\ \vdots \\ \pi(g_n)v \end{bmatrix} = \begin{bmatrix} \pi(g_1)v & \cdots & \pi(g_n)v \\ \vdots & \ddots & \vdots \\ \pi(g_1)v & \cdots & \pi(g_n)v \end{bmatrix}$$

This then grants that the output of the fully connected layer with weights $W$ is:

$$(W\overline{f})_i = \sum_{j=1}^{s} (\pi(g_i)v)_j \overline{f}_j.$$ Using that $f$ has finite support $\{x_1, \ldots, x_s\}$, and that $(\pi(g_i)v)_j = \hat{v}(g_i^{-1}x_j)$, we have that:

$$(W\overline{f})_i = \sum_{j=1}^{s} \hat{v}(g_i^{-1}x_j)f(x_j) = \sum_{x \in X} \hat{v}(g_i^{-1}x)f(x).$$

Lastly, we can interpret $W_G\overline{f}$ as a function $\phi^G(f)$ mapping each $g_i \in G$ to its $i^{th}$ component:

$$[\phi^G(f)](g_i) = (W\overline{f})_i = \sum_{x \in X} \hat{v}(g_i^{-1}x)f(x)$$

---

This is using the natural linear algebraic dual of the free vector space on $\{x_1, \ldots, x_s\}$. 

---

Figure 5: The theoretical convolutional weight symmetry matrix for the group $(g) \cong C_4$, where $g$ is a $\frac{2\pi}{N}$-radian rotation of a $3 \times 3$ image ($N \in \{0, 1, 2, 3\}$). Notice that the image is flattened into a length 9 vector. The matrix $\pi(g)$ describes the action of a $\frac{2\pi}{N}$-radian rotation on this image.
Figure 6: The submatrices of the meta-learned symmetry matrix of MSR-FC on the translation equivariant problem (Sec. 5.1). Intensity corresponds to each entry’s absolute value. We see that the symmetry matrix has been meta-learned to implement standard convolution: each $\pi(i)$ translates the size filter $v \in \mathbb{R}^3$ by $i$ spaces. Note that in actuality the submatrices are stacked on top of each other in $U$ as in Eq. [18] but we display them side-by-side for visualization.

which is precisely the cross-correlation as described in Eq. [14] with filter $\psi = \hat{v}$. This implies that $\phi^G$ must be equivariant with respect to $G$. Moreover, all such $G$-equivariant functions are $G$ cross-correlations parameterized by $v$, so with $U^G$ fixed as in Eq. [18] we have that $W = U^G v$ can represent all $G$-equivariant functions.

This means that if $v$ is chosen to have the same dimension as the input, and the weight symmetry matrix is sufficiently large, any equivariance to a finite group can be meta-learned. Moreover, in this case the symmetry matrix has a very natural and interpretable structure, containing a representation of the group in block submatrices. Lastly, notice that $v$ corresponds (dually) to the convolutional filter, justifying the notion that we learn the convolutional filter in the inner loop, and the group action in the outer group.

In the above proof, we’ve used the original definition of group convolution [6] for the sake of simplicity. It is useful to note that a slight generalization of the proof applies for more general equivariance between representations, as defined in equation (3)—i.e. the case when $\pi(g)$ is an arbitrary linear transformation, and not necessarily of the form $\pi(g)f(x) = f(g^{-1}x)$. This is subject to a unitarity condition on the group representation [52].

Without any modification to the method, arbitrary linear approximations to group convolution can be learnt when the group $G$ is not a subgroup of the symmetric group—i.e. when $G$ does not consist purely of permutations of indices. For example, non axis-aligned rotations can be easily approximated through bilinear and bicubic interpolation, whereby the value of a pixel $x$ after rotation is a linear interpolation of the 4 or 16 pixels nearest to the “true” value of this pixel before rotation $g^{-1}x$. This allows us to practically learn groups like $C_8$, which is generated by 45 degree rotations.

C Visualizing the meta-learned symmetry matrix

Fig. 6 visualizes the actual symmetry matrix $U$ that MSR-FC meta-learns from translation equivariant data. Each column is one of the submatrices $\pi(i)$ corresponding to the action of the discrete translation group element $i \in \mathbb{Z}$ on the filter $v$. In other words, MSR automatically meta-learned $U$ to contain these submatrices $\pi(i)$ such that each $\pi(i)$ translates the filter by $i$ spaces, effectively meta-learning standard convolution! In the actual symmetry matrix the submatrices are stacked on top of each other as in Eq. [18] but we display each submatrix side-by-side for easy visualization. The figure is also cropped for space: there are a total of 68 submatrices but we show only the first 20, and each submatrix is cropped from $70 \times 3$ to $22 \times 3$. 

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D Experimental details

Throughout this work we implemented all gradient based meta-learning algorithms in PyTorch using the Higher [19] library.

D.1 Synthetic Problems

In the synthetic problems we generated regression data using either a single locally connected layer (Sec. 5.1) or a single E(2)-steerable layer (Sec. 5.2). Each task corresponds to different weights of the data generating network, whose entries we sample independently from a standard normal distribution. For rank $k$ locally connected filters we sampled $k$ width-3 filters and then set the filter value at each spatial location to be a random linear combination of those $k$ filters. We generated 10,000 tasks for each synthetic problem and randomly split them into 8,000 meta-train and 2,000 meta-test tasks.

For each particular task, we generated 20 data points by randomly sampling the input vector or “image” entries from a standard normal distribution, passing the input vector into the data generating network, and saving the input and output as a pair. We then randomly split the task data into task training data (1 data point) and task validation data (19 datapoints). Hence the model has to solve each task after viewing a single task training datapoint.

During meta-training we trained each method for 5,000 steps, which was sufficient for the training loss to converge for every method in every problem. We used the Adam [24] optimizer in the outer loop with learning rate .001. In the inner loop we used SGD with meta-learned per-layer learning rates, initialized to 0.1. We used a single inner loop step for all experiments, and a task batch size of 32 during meta-training. At meta-test time we evaluated average performance and error bars using 300 random held-out tasks.

We ran all experiments on a single machine with a single NVidia RTX 2080Ti GPU. Our MSR-FC experiments took about 9.5 (outer loop) steps per second, while our MSR-Conv experiments took about 2.8 (outer loop) steps per second.

D.2 Augmentation Experiments

To create Aug-Omniglot and Aug-MiniImagenet, we extended the Omniglot and MiniImagenet benchmarks from TorchMeta [10]. Each task in these benchmarks is split into support (train) and query (validation) datasets. For the augmented benchmarks we applied data augmentation to only the query dataset of each task, which consisted of randomly resized crops, reflections, and rotations by up to 30°. Using the torchvision library, the augmentation function is:

```python
# Data augmentation applied to ONLY the query set.
size = 28 # Omniglot image size. 84 for MiniImagenet.
augment_fn = Compose(
    RandomResizedCrop(28, scale=(0.8, 1.0)),
    RandomVerticalFlip(p=0.5),
    RandomHorizontalFlip(p=0.5),
    RandomRotation(30, resample=Image.BILINEAR),
)
```

For all experiments except MiniImagenet 5-shot, MAML and MSR used exactly the same convolutional architecture (same number of layers, number of channels, filter sizes, etc.) as prior work on Omniglot and MiniImagenet [50]. For MSR we reparameterize each layer’s weight matrix or convolutional filter. For MiniImagenet 5-shot, we found that increasing architecture size helped both methods: for the first 3 convolution layers, we increased the number of output channels to 128 and increased the kernel size to 5. We then inserted a $1 \times 1$ convolution layer with 64 output channels right before the linear output layer. For fair comparison we also increased the ProtoNet architecture size on MiniImagenet 5-shot, using 128 output channels at each layer. We found that increasing the kernel size to 5 at each layer in the ProtoNet worsened performance, so we left it at 3.

For “MAML (Big)” experiments we increased the architecture size of the MAML model to exceed the number of meta-parameters (symmetry matrices + filter parameters) in the corresponding MSR model. For MiniImagenet 5-Shot we increased the number of output channels at each of the 3
convolution layers to 128, then inserted an additional linear layer with 3840 output units before the final linear layer. For MiniImagenet 1-Shot we increased the number of output channels at each of the 3 convolution layers to 64, then inserted an additional linear layer with 1920 output units before the final linear layer. For the Omniglot experiments we increased the number of output channels at each of the 3 convolution layers to 150.

For all experiments and gradient based methods we trained for 60,000 (outer) steps using the Adam optimizer with learning rate .0005 for MiniImagenet 5-shot and .001 for all other experiments. In the inner loop we used SGD with meta-learned per-layer learning rates initialized to 0.4 for Omniglot and .05 for MiniImagenet. We meta-trained using a single inner loop step in all experiments, and used 3 inner loop steps at meta-test time. Although MAML originally meta-trained with 5 inner loop steps on MiniImagenet, we found that this destabilized meta-training on our augmented version. We hypothesize that this is due to the discrepancy between support and query data in our augmented problems. During meta-training we used a task batch size of 32 for Omniglot and 10 for MiniImagenet. At meta-test time we evaluated average performance and error bars using 1000 held-out meta-test tasks.

We ran all experiments on a machine with a single NVidia Titan RTX GPU. For our Aug-Omniglot, we ran two experiments at simultaneously on the same machine, which likely slowed each invididual experiment down. Our MSR method took about 0.6 steps per second, whereas the MAML baseline took about 0.86 steps per second. For Aug-Miniimagenet we ran one experiment per machine. MSR took 4.2 steps per second, while MAML took 5.6 steps per second on these experiments.