EQUIVARIANCE-AWARE ARCHITECTURAL OPTIMIZATION OF NEURAL NETWORKS

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ABSTRACT

Incorporating equivariance to symmetry groups as a constraint during neural network training can improve performance and generalization for tasks exhibiting those symmetries, but such symmetries are often not perfectly nor explicitly present. This motivates algorithmically optimizing the architectural constraints imposed by equivariance. We propose the equivariance relaxation morphism, which preserves functionality while reparameterizing a group equivariant layer to operate with equivariance constraints on a subgroup, as well as the $[G]$-mixed equivariant layer, which mixes layers constrained to different groups to enable within-layer equivariance optimization. We further present evolutionary and differentiable neural architecture search (NAS) algorithms that utilize these mechanisms respectively for equivariance-aware architectural optimization. Experiments across a variety of datasets show the benefit of dynamically constrained equivariance to find effective architectures with approximate equivariance. [1]

1 INTRODUCTION

Constraining neural networks to be equivariant to symmetry groups present in the data can improve their task performance, efficiency, and generalization capabilities (Bronstein et al., 2021), as shown by translation-equivariant convolutional neural networks (Fukushima & Miyake, 1982; LeCun et al., 1989) for image-based tasks (LeCun et al., 1998). Seminal works have developed general theories and architectures for equivariance in neural networks, providing a blueprint for equivariant operations on complex structured data (Cohen & Welling, 2016; Ravanbakhsh et al., 2017; Kondor & Trivedi, 2018; Weiler et al., 2021). However, these works design model constraints based on an explicit equivariance property. Furthermore, their architectural assumption of full equivariance in every layer may be overly constraining; e.g., in handwritten digit recognition, full equivariance to 180° rotation may lead to misclassifying samples of "6" and "9". Weiler & Cesa (2019) found that local equivariance from a final subgroup convolutional layer improves performance over full equivariance. If appropriate equivariance constraints are instead learned, the benefits of equivariance could extend to applications where the data may have unknown or imperfect symmetries.

Learning approximate equivariance has been recently approached through novel layer operations (Wang et al., 2022; Finzi et al., 2021; Zhou et al., 2020; Yeh et al., 2022; Basu et al., 2021). Separately, the field of neural architecture search (NAS) aims to optimize full neural network architectures (Zoph & Le, 2017; Real et al., 2017; Elsken et al., 2017; Liu et al., 2018; Lu et al., 2019). Existing NAS methods have not yet been developed for explicitly optimizing equivariance, although partial or soft equivariant approaches like Romero & Lohit (2022) and van der Ouderaa et al. (2022) do allow for custom equivariant architectures. An important aspect of NAS is network morphisms: function-preserving architectural changes (Wei et al., 2016) which can be used during training to change the loss landscape and gradient descent trajectory while immediately maintaining the current functionality and loss value (Maile et al., 2022). Developing tools for searching over a space of architectural representations of equivariance would allow for existing NAS algorithms to be applied towards architectural optimization of equivariance.

Contributions First, we present two mechanisms towards equivariance-aware architectural optimization. The *equivariance relaxation morphism* for group convolutional layers partially expands

[1] Our code will be made available in the camera-ready version: `https://github.com/`

the representation and parameters of the layer to enable less constrained learning with a prior on symmetry. The $[G]$-*mixed equivariant layer* parameterizes a layer as a weighted sum of layers equivariant to different groups, permitting the learning of architectural weighting parameters.

Second, we implement these concepts within two algorithms for architectural optimization of partially-equivariant networks. Evolutionary Equivariance-Aware NAS (EquiNAS$_E$) utilizes the equivariance relaxation morphism in a greedy evolutionary algorithm, dynamically relaxing constraints throughout the training process. Differentiable Equivariance-Aware NAS (EquiNAS$_D$) implements $[G]$-mixed equivariant layers throughout a network to learn the appropriate approximate equivariance of each layer, in addition to their optimized weights, during training.

Finally, we analyze the proposed mechanisms via their respective NAS approaches in multiple image classification tasks, investigating how the dynamically learned approximate equivariance affects training and performance over baseline models and other approaches.

2 Related works

Approximate equivariance Although no other works on approximate equivariance explicitly study architectural optimization, some approaches are architectural in nature. We compare our contributions with the most conceptually similar works to our knowledge.

The main contributions of Basu et al. (2021) and Agrawal & Ostrowski (2022) are similar to our proposed equivariant relaxation morphism. Basu et al. (2021) also utilizes subgroup decomposition but instead algorithmically builds up equivariances from smaller groups, while our work focuses on relaxing existing constraints. Agrawal & Ostrowski (2022) presents theoretical contributions towards network morphisms for group-invariant shallow neural networks: in comparison, our work focuses on deep group convolutional architectures and implements the morphism in a NAS algorithm.

The main contributions of Wang et al. (2022) and Finzi et al. (2021) are similar to our proposed $[G]$-mixed equivariant layer. Wang et al. (2022) also uses a weighted sum of kernels, but uses the same group for each kernel and defines the weights over the domain of group elements. Finzi et al. (2021) uses an equivariant layer in parallel to a linear layer with weighted regularization, thus only using two layers in parallel and weighting them through regularization rather than parameterization.

In more diverse approaches, Zhou et al. (2020) and Yeh et al. (2022) represent symmetry-inducing weight sharing through learnable matrices. Romero & Lohit (2022) and van der Ouderaa et al. (2022) learn partial or soft equivariances for each layer.

Neural architecture search Neural architecture search (NAS) aims to optimize both the architecture and its parameters for a given task. Liu et al. (2018) approaches this difficult bi-level optimization by creating a large super-network containing all possible elements and continuously relaxing the discrete architectural parameters to enable search by gradient descent. Other NAS approaches include evolutionary algorithms (Real et al., 2017; Lu et al., 2019; Elsken et al., 2017) and reinforcement learning (Zoph & Le, 2017), which search over discretely represented architectures.

3 Background

We assume familiarity with group theory (Herstein, 2006). Let G be a discrete group. The lth G-equivariant group convolutional layer (Cohen & Welling, 2016) of a group convolutional neural network (G-CNN) convolves the feature map $f\colon G \to \mathbb{R}^{C_{l-1}}$ output from the previous layer with a filter with kernel size k represented as learnable parameters $\psi\colon G \to \mathbb{R}^{C_l \times C_{l-1}}$. For each output channel $d \in [C_l]$, where $[C] := \{1, \ldots, C\}$, and group element $g \in G$, the layer's output is defined via the convolution operator[2]:

$$[f \star_G \psi]_d(g) = \sum_{h \in G} \sum_{c=1}^{C_{l-1}} f_c(h) \psi_{d,c}(g^{-1}h). \tag{1}$$

[2]We identify the correlation and convolution operators as they only differ where the inverse group element is placed and refer to both as "convolution" throughout this work.

The first layer is a special case: the input to the network needs to be lifted via this operation such that the output feature map of this layer has a domain of G. In the case of image data, an image x with C channels may be interpreted as a function $x\colon \mathbb{Z}^2 \to \mathbb{R}^C$ mapping each pixel in coordinate space to a real number for each channel, where the cth channel of x is referred to as x_c. The input is $x\colon \mathbb{Z}^2 \to \mathbb{R}^{C_0}$, so the layer is instead a *lifting* convolution:

$$[x \star_G \psi]_d(g) = \sum_{y \in \mathbb{Z}^2} \sum_{c=1}^{C_0} x_c(y) \psi_{d,c}(g^{-1}y). \tag{2}$$

We present our contributions in the group convolutional layer case, although similar claims apply for the lifting convolutional layer case.

4 Towards Architectural Optimization over Subgroups

We propose two mechanisms to enable search over subgroups: the equivariance relaxation morphism and a $[G]$-mixed equivariant layer. The proposed morphism, described in Section 4.1, changes the equivariance constraint from one group to another subgroup while preserving the learned weights of the initial group convolutional operator. The $[G]$-mixed equivariant layer, presented in Section 4.2, allows for a single layer to represent equivariance to multiple subgroups through a weighted sum.

4.1 Equivariance Relaxation Morphism

The *equivariance relaxation morphism* reparameterizes a G-equivariant group (or lifting) convolutional layer to operate over a subgroup of G, partially removing weight-sharing constraints from the parameter space while maintaining the functionality of the layer.

Let $G' \leq G$ be a subgroup of G. Let R be a system of representatives of the left quotient (including the neutral element), so that $G' \setminus G = \{G'r \mid r \in R\}$, where $G'r \coloneqq \{g'r \mid g' \in G'\}$. Given a G-equivariant group convolutional layer with feature map f and kernel ψ, we define the relaxed feature map $\tilde{f}\colon G' \to \mathbb{R}^{(C_{l-1} \times |R|)}$ and relaxed kernel $\tilde{\psi}\colon G' \to \mathbb{R}^{(C_l \times |R|) \times (C_{l-1} \times |R|)}$ as follows. For $c \in [C_{l-1}]$, $s, t \in R$, $d \in [C_l]$:

$$\tilde{f}_{(c,s)}(g') \coloneqq f_c(g's), \tag{3}$$

$$\tilde{\psi}_{(d,t),(c,s)}(g') \coloneqq \psi_{d,c}(t^{-1}g's). \tag{4}$$

We define the *equivariance relaxation morphism* from G to G' as the reparameterization of ψ as $\tilde{\psi}$ (Eq. 4) and reshaping of f as $\tilde{f}$ (Eq. 3). We will show that the new output layer, $[\tilde{f} \star_{G'} \tilde{\psi}]_{(d,t)}(g')$, is equivalent to $[f \star_G \psi]_d(g't)$ down to reshaping. Since the mapping $G' \times R \to G$, $(g', t) \mapsto g't$, is bijective, every g can uniquely be written as $g = g't$ with $g' \in G'$ and $t \in R$. For $g \in G$, $G'g \in G' \setminus G$ has a unique representative $t \in R$ with $G'g = G't$, and $g' \coloneqq gt^{-1} \in G'$. By the same argument, $h \in G$ may be written as $h = h's$ with unique $h \in G'$ and $s \in R$. With these preliminaries, we get:

$$\begin{aligned}
[f \star_G \psi]_d(g't) &= [f \star_G \psi]_d(g) && (5)\\
&= \sum_{h \in G} \sum_{c=1}^{C_{l-1}} f_c(h) \psi_{d,c}(g^{-1}h), && (6)\\
&= \sum_{h' \in G'} \sum_{s \in R} \sum_{c=1}^{C_{l-1}} f_c(h's) \psi_{d,c}(t^{-1}g'^{-1}h's), && (7)\\
&= \sum_{h' \in G'} \sum_{c=1}^{C_{l-1}} \sum_{s \in R} \tilde{f}_{(c,s)}(h') \tilde{\psi}_{(d,t),(c,s)}(g'^{-1}h'), && (8)\\
&= \left[\tilde{f} \star_{G'} \tilde{\psi}\right]_{(d,t)}(g'), && (9)
\end{aligned}$$

which shows the claim. Thus, the convolution of $\tilde{f}$ with $\tilde{\psi}$ is equivariant to G but parametrized as a G'-equivariant group convolutional layer, where the representatives are expanded into independent

channels. This morphism can be viewed as initializing a G'-equivariant layer with a pre-trained prior of equivariance to G, maintaining any previous training.

Standard convolutional layers are a special case of group-equivariant layers, where the group is translational symmetry over pixel space. Regular group convolutions are often implemented by relaxation to the translational symmetry group by expanding the kernel via the appropriate group actions, allowing a standard convolution implementation from a deep learning library to be used. The equivariance relaxation morphism generalizes this concept to any subgroup. This, as well as how the equivariance relaxation morphism is implemented, is discussed further in Appendix A.

4.2 $[G]$-MIXED EQUIVARIANT LAYER

Towards learning equivariance, we additionally propose partial equivariance through a mixture of layers, each constrained to equivariance to different groups and applied in parallel to the same input then all combined via a weighted sum. The equivariance relaxation morphism provides a mapping of group elements between pairs of groups where one is a subgroup of the other. For a set of groups $[G]$ where each group is a subgroup or supergroup of all other groups within the set, we define a $[G]$-*mixed equivariant layer* as:

$$\left[f \hat{\star}_{[G]} [\psi]\right]_{(d,t)} (g) = \sum_{G \in [G]} z_G \left[f \star_{G'} \widetilde{\psi^G}\right]_{(d,t)} (g) \tag{10}$$

$$= \left[f \star_{G'} \sum_{G \in [G]} z_G \widetilde{\psi^G}\right]_{(d,t)} (g), \tag{11}$$

where each element z_G of $[z] \coloneqq \{z_G | G \in [G]\}$ is an architectural weighting parameter such that $\sum_{G \in [G]} z_G = 1$, G' is a subgroup of all groups in $[G]$, each element ψ^G of $[\psi]$ is a kernel with a domain of G, and $\widetilde{\psi^G}$ is the transformation of ψ^G from a domain of G to G' as defined in Equation 4. Thus, the layer is parametrized by $[\psi]$ and $[z]$, computing a weighted sum of operations that are equivariant to different groups of $[G]$. The layer may be equivalently computed by convolution of the input with the weighted sum of transformed kernels, shown in Equation 11. We provide further implementation details in Appendix A.

5 EQUIVARIANCE-AWARE NEURAL ARCHITECTURE ALGORITHMS

We present two neural architecture search methods that utilize the presented mechanisms for discovering appropriate equivariance during neural network training: Evolutionary Equivariance-Aware NAS (EquiNAS$_E$) and Differentiable Equivariance-Aware NAS (EquiNAS$_D$). Both methods optimizffe an architecture while learning network weights, returning a final trained network adapted to the equivariances present in the training data. However, they differ in NAS paradigm and approximate equivariance representation: EqufiNAS$_E$, described in Section 5.1, searches for networks composed of layers each fully equivariant to possibly different groups, while EquiNAS$_D$, described in Section 5.2, searches for smooth mixtures of equivariant layers.

5.1 EVOLUTIONARY EQUIVARIANCE-AWARE NAS

Towards finding the optimal full equivariance per layer, the equivariance relaxation morphism presented in Section 4.1 is applied as the genetic operator in an evolutionary hill-climbing algorithm. The Evolutionary Equivariance-Aware NAS (EquiNAS$_E$) algorithm, given in Algorithm 1, is similar to other evolutionary NAS methods such as Elsken et al. (2017) with pareto selection as in Falanti et al. (2022). A population of networks, which starts with an individual with all layers equivariant to the largest possible group, undergoes mutation via equivariance relaxation and selection based on accuracy and parameter count to optimize neural architecture while learning network parameters.

In each generation, candidate networks are evaluated based on maximizing validation accuracy and minimizing parameter count: the entire Pareto front is kept, then additional high-accuracy individuals are added if necessary until the desired parent population size is reached. Offspring are generated from each parent separately through mutation using the relaxation morphism. This preserves the

Algorithm 1 Evolutionary equivariance-aware neural architecture search.

procedure EQUINAS$_E$(Initial symmetry group G)
  Initialize population with a G-equivariant group convolutional network.
  for each generation **do**
    for each network in population **do**
      Add children of network with relaxed equivariance constraints into population.
    for each network in population **do**
      Partially train network on dataset.
    Select Pareto-efficient and high accuracy networks as new population.
  return population

Algorithm 2 Differentiable equivariance-aware neural architecture search.

procedure EQUINAS$_D$(Set of groups $[G]$)
  Initialize network with $[G]$-mixed equivariant layers, parameterized by Ψ and Z.
  while not converged **do**
    Update Z by $\nabla_Z \mathcal{L}(\Psi, Z)$.
    Update Ψ by $\nabla_\Psi \mathcal{L}(\Psi, Z)$.
  return trained network

weights of the parameterized equivariance during mutation, allowing for the continuous training of networks over evolution through inheritance from parent individuals. Specifically, mutation reduces a single layer's parameterized equivariance to a subgroup within the constraint that each layer has parametrized equivariance to a subgroup of all preceding layers. This constraint yields local equivariance properties for the network, as shown in Weiler & Cesa (2019) and Elsayed et al. (2020) to be empirically favorable in image classification tasks. The resulting individuals are each trained independently for a given training time, and then this process repeats.

The second objective of minimizing parameter count is intended to advance efficient networks, such as those with large symmetry groups. Accuracy-based selection alone would necessarily prefer larger networks as mutation via the equivariance relaxation morphism results in two networks with identical performance but different size, the relaxed network having more parameters, until training; potentially short-term increases in validation accuracy after training would then result in the selection of individuals with more parameters. Thus, the proposed strategy of selecting both pareto-front and high-accuracy individuals is intended to maintain a diverse yet efficient population without succumbing to overly greedy selections too early.

5.2 DIFFERENTIABLE EQUIVARIANCE-AWARE NAS

In a contrasting paradigm, the $[G]$-mixed equivariant layer presented in Section 4.2 allows for smoothly searching across a spectrum of equivariance for each layer via a differentiable NAS algorithm. Our Differentiable Equivariance-Aware NAS (EquiNAS$_D$) algorithm, defined in Algorithm 2, is inspired by DARTS (Liu et al., 2018) with significant changes detailed in the following paragraphs. EquiNAS$_D$ simplifies the bilevel optimization of the architecture weighting parameters Z and kernel weights Ψ into alternating independent updates, computing the gradient update for Z with the current, rather than optimal, Ψ for the current architecture encoded by Z, to boost search efficiency with minimal performance loss compared to higher order approximations (Liu et al., 2018).

In most differentiable NAS search spaces, the desired output architecture is discretized to select a subset of architectural options within constraints, then the weights are re-initialized and trained within the static architecture. In our formulation, this is not necessary as any mixed operation can be equivalently expressed as a single layer equivariant to any group G' that is a common subgroup to all groups of the mixed operation (Eq. 11): in our experimental case, this is a standard translation-equivariant convolutional layer, so the final model can be equivalently expressed as a standard convolutional model with encoded partial equivariance. Thus, the final optimized architecture and trained weights are output from the single search process.

In order to enforce that the scaling of each kernel does not confound the architecture weighting parameters, we use the weight normalizing reparameterization (Salimans & Kingma, 2016) and do not update the scalar norm parameter of each kernel after initialization.

We do not use disjoint datasets for updating Ψ and Z, but rather draw one batch for Ψ and another for Z independently and randomly from the same training split. This allows for a standard dataset split and to use the validation set for hyperparameter tuning.

These two NAS approaches present adaptations of two standard types of NAS, evolutionary and differentiable, to the search for optimal partial equivariance. The equivariance relaxation morphism and the $[G]$-mixed equivariant layer that enable the evolutionary and differentiable search methods respectively are the main focus; the other characteristics of the NAS methods are adapted from existing methods, but further study could advance specialization of equivariance-aware NAS. We next study empirically the two EquiNAS methods on three datasets, one with known rotational symmetry and two with unknown but visually significant rotational and reflectional symmetry.

6 EXPERIMENTS

We focus on the regular representation of groups and show experiments with reflectional and up to 4-fold rotational symmetry groups applied to image classification tasks. Examples of symmetry groups acting on pixel space, which corresponds to $\mathbb{Z}^2$, include $T(2)$, which consists of discrete translations in both dimensions; the cyclical groups C_n, which consist of n-fold rotations; and the dihedral groups D_n, which consist of reflections with n-fold rotations, where $n \in \{1, 2, 4\}$ for exact symmetry without interpolation. The $p4$ group consists of discrete translations and multiples of 90° rotations and may be represented as $T(2) \rtimes C_4$. The $p4m$ group consists of discrete translations, reflections, and multiples of 90° rotations and may be represented as $T(2) \rtimes D_4$. As standard convolutional layers are already equivariant to $T(2)$, we refer to layers also equivariant to n-fold rotations with or without reflections as D_n or C_n-equivariant, respectively. So, a C_1 equivariant convolutional layer is a standard translation-equivariant convolutional layer. We use $\{C_1, D_1, C_2, D_2, C_4, D_4\}$ as the set of potential groups for mutation in EquiNAS$_E$ and as $[G]$ in EquiNAS$_D$.

We present experiments on image classification for a variety of datasets. The Rotated MNIST dataset (Larochelle et al., 2007, rotMNIST) is a version of the MNIST handwritten digit dataset but with the images rotated by any angle. This task serves as a simple investigational study with known symmetry, while the following two tasks are more realistic and complex. The Galaxy10 DECals dataset (Leung & Bovy, 2019, Galaxy10) contains galaxy images in 10 broad categories. The ISIC 2019 dataset (Codella et al., 2018; Tschandl et al., 2018; Combalia et al., 2019, ISIC) contains dermascopic images of 8 types of skin cancer plus a null class. For Galaxy10 and ISIC, we downsample the images to 64×64 due to computational constraints, which adds notable difficulty to the tasks. These tasks exhibit varying levels of rotational and reflectional symmetry, motivating architectural optimization to determine the most effective application of equivariance constraints.

Across all experiments, the architectures are designed to have consistent channel dimensions once expanded to a standard translation-equivariant convolutional layer for each layer across models. Thus, constrained equivariance to a larger symmetry group results in fewer learnable parameters. A layer constrained to C_4 equivariance has $|C_4 \setminus D_4| = 2$ times as many independent channels and as many parameters as a layer constrained to D_4 equivariance. This is a notably different paradigm than other works that equate parameter counts across architectures with different equivariance properties.

As baseline comparisons, we train and test G-CNNs with static architectures. In addition to the static baselines, we re-implement the residual pathway priors (RPP) approach by Finzi et al. (2021) as a C_1 equivariant layer with regularization in parallel with a D_4 equivariant convolutional layer.

Further experiment details such as architecture details and other hyperparameters can be found in Appendix B. For each paradigm of experiments, we present their results in the following subsections, with general discussion following in Section 7.

6.1 EVOLUTIONARY EQUIVARIANCE-AWARE NAS

The classification test errors are listed in Table 1. The evolutionary progress on rotMNIST is shown in Figure 1. The selected population maintains a fully equivariant network in every generation. The

Method	rotMNIST	Galaxy10	ISIC
EquiNAS$_E$	**1.78 ± 0.04**	51.5 ± 16.0	**32.7 ± 0.6**
RPP (Finzi et al., 2021)	2.18 ± 0.04	85.8 ± 2.9	33.9 ± 2.0
D_4 baseline	**1.78 ± 0.11**	68.1 ± 14.6	**32.6 ± 0.8**
C_4 baseline	**1.64 ± 0.22**	87.3 ± 4.2	33.9 ± 1.3
C_1 baseline	5.02 ± 1.15	86.9 ± 3.6	35.0 ± 1.7
C_4 (prior: D_4)	1.93 ± 0.05	**47.0 ± 9.3**	33.4 ± 2.2
C_1 (prior: D_4)	3.40 ± 0.07	**47.1 ± 16.3**	33.7 ± 1.5
C_1 (prior: C_4)	2.96 ± 0.05	53.8 ± 20.8	**32.6 ± 1.4**

Table 1: Test error percentages (lower is better) across tasks and approaches. Statistics are aggregated over the final selected population of 5 individuals for EquiNAS$_E$ and across 5 random seeds for all other methods. The **best** and **second best** average errors for each task are highlighted. See Figure 3 in Appendix C for individual trial results.

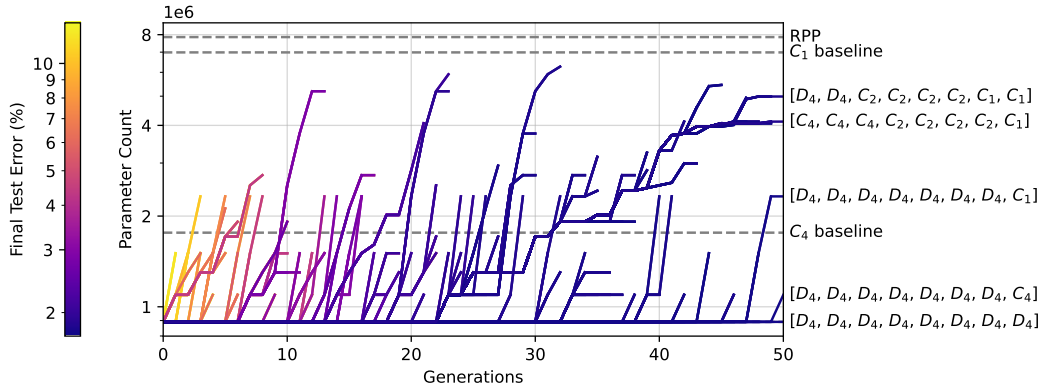

Figure 1: Historical parameter counts of each selected individual for EquiNAS$_E$ on rotMNIST. The architectures of the final selected population are labeled. Each parameter count history is colored according to the final test accuracy, which is measured of each individual upon removal. For other tasks, see Figure 4 in Appendix C.

final selected population originates from two main lineages, one diverging from the fully equivariant network midway through and the other staying fully equivariant until the last few generations.

Experiments on the Galaxy10 task have high, nearly random errors. This may be due to the nature of the dataset and the necessary resizing causing high signal loss, but this also represents many real-world applications with low signal-to-noise ratios. EquiNAS$_E$ found the best model on this task, achieving a test error of 22.4% with all C_1-equivariant layers. This architecture was relaxed from a fully D_4 equivariant architecture in the latter half of evolution, shown in Figure 4a in Appendix C, but outperforms both the C_1 and D_4 baselines, demonstrating that training through relaxation can arrive at better parameters than only training in an equivalent but statically equivariant architecture.

In addition to the normally initialized static baselines, we also train and test baselines that are initialized with priors to larger symmetry groups. These are implemented by initializing all layers to be constrained to the prior symmetry group, then using the equivariance relaxation morphism on each layer. EquiNAS$_E$ searches for relaxation schedules that yield trained priors on equivariance, while these additional baselines yield untrained priors. The results in Table 1 show that, the C_1-equivariant networks generally improve with either equivariance prior, while the C_4 equivariant networks perform better with D_4 equivariance initialization only when the D_4 constrained baselines also work well. The untrained prior methods do not perform as well as EquiNAS$_E$ on rotMNIST, showing the benefit of investing some training time to the constrained equivariance. However, for the Galaxy10 task, the baselines with priors have the best average performances.

Method	rotMNIST	Galaxy10	ISIC
EquiNAS$_D$	**2.29 ± 0.27**	**46.6 ± 20.3**	32.8 ± 0.6
RPP (Finzi et al., 2021)	2.89 ± 0.27	88.7 ± 5.4	**31.5 ± 0.9**
D_4 Baseline	2.97 ± 1.50	86.3 ± 6.5	**32.0 ± 1.0**
C_4 Baseline	**2.43 ± 0.54**	**77.3 ± 14.3**	32.8 ± 1.0
C_1 Baseline	3.97 ± 0.75	84.5 ± 6.8	32.9 ± 3.1

Table 2: Test error percentages (lower is better) in percent of incorrect classifications across tasks and approaches. The **best** and **second best** average errors for each task are highlighted. See Figure 5 in Appendix C for individual trial results.

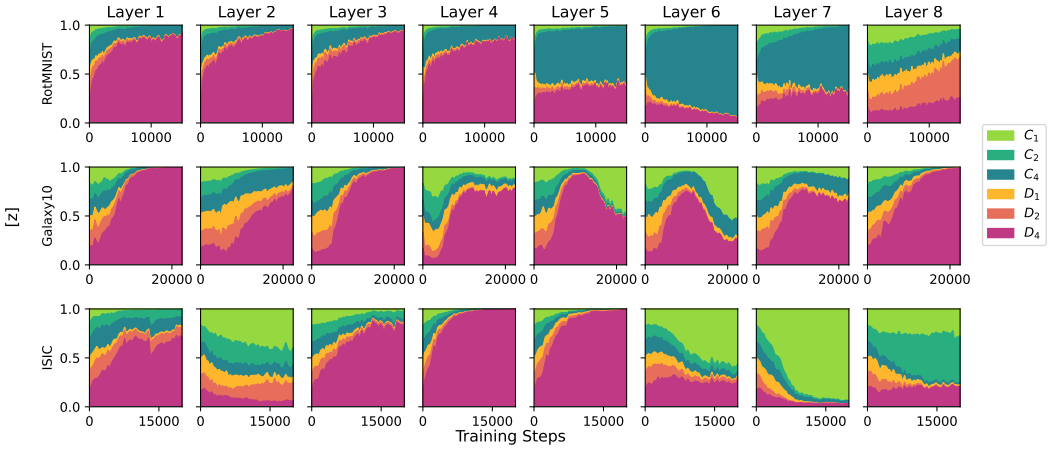

Figure 2: Architecture weighting parameters by layer for one selected trial from each task. For other trials, see Figures 6-8 in Appendix C.

6.2 Differentiable Equivariance-aware NAS

The classification test errors are listed in Table 2. EquiNAS$_D$ achieves better test accuracy than the other comparable methods on rotMNIST and Galaxy10. Due to differences in training protocol, only comparisons of relative rankings with Table 1 are possible: baseline methods accuracies followed similar patterns to ranking between experimental paradigms, suggesting the benefit of general C_4 equivariance for rotMNIST and Galaxy10 and general D_4 equivariance, including RPP, for ISIC.

The architecture weighting parameter dynamics for one exemplary trial per task are shown in Figure 2. The general trend of less constrained layers toward the end of the network supports the conjecture of local equivariance being beneficial. However, this effect is less consistent for Galaxy10 and especially ISIC with less inherent symmetry: trials on ISIC, the only task where EquiNAS$_D$ did not exceed baselines, had the most varied architectures. As seen in Appendix C, the final mixing of architectures for ISIC, and somewhat for Galaxy10, included a high level of C_1, indicating that feature analysis outside of symmetry groups is important for these benchmarks.

Similar to EquiNAS$_E$, EquiNAS$_D$ found the best model for Galaxy10, shown as the selected trial in Figure 2. The layers of this model learn mostly strong equivariance to D_4, but the small contributions from less constrained layers may allow it to specialize enough to adapt to the level of symmetry present in the dataset while still generalizing to classify the unseen test data effectively.

Previous differentiable NAS works often used regularization of network size or even architecture weighting parameters themselves to encourage efficient architectures with a single highly weighted choice for each layer. However, our algorithm shows strong preference for more equivariant and thus more expressive layers, notably to D_4 or C_4 equivariance, without such regularization. This may be due to the bilevel optimization dynamics: more constrained layers may be able to make more effective updates to more closely approximate the correct gradient computation that assumes optimal weights and thus become favorable compared to the lagging larger layers.

7 DISCUSSION

To our knowledge, this is the first work which proposes search methods for networks with dynamically constrained equivariance. Many NAS approaches separately search for an architecture and then reinitialize and retrain the weights, while our two proposed approaches find an optimal architecture with trained weights in a single process, notably with dynamically constrained weights. Gradient-based tuning (Maclaurin et al., 2015) has shown the benefit not only of optimizing hyperparameters but also of dynamically adjusting them during training (Lichtarge et al., 2022). There is an inherent trade-off between accuracy and generalization capabilities with more constrained equivariance: dynamically constrained weights can reap both over the course of training.

Our two equivariance-aware NAS approaches have distinct approaches: EquiNAS$_E$ searches for architectures composed of discretely equivariant layers, while EquiNAS$_D$ searches for continuous mixtures of equivariance within each layer. The EquiNAS$_D$ algorithm avoids many known problems in differentiable NAS such as the discretization gap that occurs when searching over a continuous relaxation of a discrete architectural search space (Xie et al., 2021), such as that of EquiNAS$_E$. Towards searching for discretely equivariant layers using the $[G]$-mixed equivariant layer, proximal NAS algorithms use techniques such as projection (Yao et al., 2020) and straight-through estimation (Li et al., 2022) to avoid the discretization gap and thus may be effective for this application.

The EquiNAS$_E$ algorithm is innately greedy. At each selection step, the population is evaluated on the known current performance rather than the unknown final performance, so this metric is biased to architectures that train quickly. Networks constrained to higher symmetry group equivariance tend to learn faster, but this could be confounded by the equivariance relaxation causing large gradients for the newly unconstrained parameters and thus potentially fast increases in performance. Further work could utilize other metrics for final performance, such as proxies (White et al., 2022).

All of the theoretical and algorithmic contributions of this work are applicable beyond the image classification experiments presented to architectures with parametrized equivariance to any discrete group. We leave the extension to other group representations and domains as future work.

Our proposed equivariance-aware NAS problems can be practically applied to find effective networks for datasets with hypothesizable symmetry. EquiNAS$_E$ may particularly work well on tasks that benefit from local equivariance, which can be determined by analyzing the architecture weighting parameters from first applying the more efficient EquiNAS$_D$. For tasks where EquiNAS$_D$ models have less consistent equivariance patterns, EquiNAS$_E$ could be adapted to propose candidates that relax any layer in the network, removing our constraint of non-increasing equivariance. We thus recommend EquiNAS$_D$ for practical applications if the final model is not restricted to discrete equivariance, in which case it can be used to inform design decisions for applying EquiNAS$_E$.

Beyond NAS, the equivariance relaxation morphism could be used in other applications such as fine-tuning and distillation. Layers of a pre-trained equivariant network could be expanded via equivariance relaxation before fine-tuning on the same or a new task. Similarly, a network could be distilled to a wider architecture for additional performance benefits.

The proposed equivariance-aware NAS algorithms are intentionally simple to focus on studying the architectural mechanisms presented in Section 4, although we have already discussed potential improvements to these algorithms. We include all valid results, even those that do not favor our own techniques, for transparency. This work aims to build a foundation for the intersection of equivariant architectures and NAS, rather than over-engineer the algorithms and experiments for incremental performance gains on selected benchmarks.

Conclusion We present two mechanisms towards equivariance-aware architectural optimization, the equivariance relaxation morphism and the $[G]$-mixed equivariant layer, as well as two NAS algorithms that implement these mechanisms respectively in an evolutionary approach, EquiNAS$_E$, and a differentiable approach, EquiNAS$_D$. We investigate how the dynamic equivariance achieved by these algorithms affects the training and performance of networks across multiple image classification tasks of varying complexity and assumed symmetry, demonstrating that these techniques can search for performant architectures and weights even on noisy tasks. The proposed mechanisms and algorithms are extendable beyond vision tasks to any architecture with parametrized equivariance to any discrete group.

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A Implementation Details

Group convolutional layers The implementation of regular group convolutional layers can be viewed as a special case of our proposed equivariance relaxation morphism. With the preliminaries given in Section 4.1 and the case of $G' = T(2)$, $\tilde{f}$ and $\tilde{\psi}$ are computed such that $\tilde{f}_{(c,s)}(g') \coloneqq f_c(g's)$ and $\tilde{\psi}_{(d,t),(c,s)}(g') \coloneqq \psi_{d,c}(t^{-1}g's)$ for each $g' \in T(2)$, $c \in [C_{l-1}]$, $s, t \in R$, and $d \in [C_l]$.

Let $S_G := |R|$. The learnable parameters of the G_l-equivariant lth layer with C_l output channels, corresponding to ψ, are stored as a tensor of size $C_l \times C_{l-1} \times S_{G_l} \times K_l \times K_l$. The kernel transformation expands this kernel tensor by performing the action of each $r \in R$ on another copy of the tensor to expand its shape along a new dimension, resulting in a tensor of size $C_l \times S_{G_l} \times C_{l-1} \times S_{G_l} \times K_l \times K_l$, which is reshaped to $C_l S_{G_l} \times C_{l-1} S_{G_l} \times K_l \times K_l$. The input tensor to the lth layer, corresponding to f, is in the shape of $B \times C_{l-1} \times S_{G_l} \times H_{l-1} \times W_{l-1}$, which is reshaped to $B \times C_{l-1} S_{G_l} \times H_{l-1} \times W_{l-1}$ and convolved with the expanded kernel. The output of shape $B \times C_l S_{G_l} \times H_l \times W_l$ is reshaped to $B \times C_l \times S_{G_l} \times H_l \times W_l$.

Equivariance relaxation morphism To implement the equivariance relaxation morphism, the new kernel tensor is initialized by applying Equation 4 such that result of applying the preceding kernel transformation is equivalent. Our implementation of group actions relies on group channel indexing to represent the order of group elements: to ensure this is consistent before and after the morphism, the appropriate reordering of the output and input channels of the expanded filter are applied upon expansion. The new kernel tensor has a shape of $C_l|R| \times C_{l-1}|R| \times S_{G_l}/|R| \times K_l \times K_l$. The $[G]$-mixed equivariant layer is built on top of this implementation, also using proper input and output channel reordering between layers to ensure correct mixing of group channels.

B Experimental Details

Architecture backbone For both EquiNAS$_E$ and EquiNAS$_D$ experiments, we use the same backbone architecture, such that the static baselines have the same architecture across experiments. The architectures have a lifting layer followed by 7 group convolutional layers, for a total of 8 convolutional layers. After 4 layers, the channel count doubles, from 16 to 32 for a D_4 equivariant network and scaling up for smaller symmetry group equivariance constraints. An average pooling layer is placed after every other layer for all architectures and additionally after the fifth and seventh convolutional layers for Galaxy10 and ISIC. After the final group convolutional layer is a group-dimension average pooling followed by two linear layers to the output dimension. Every convolutional and linear layer except the output layer is immediately followed by a batchnorm then a ReLU.

Hyperparameters The hyperparameters for each algorithm are selected such that baselines only differ by training time and optimizers. The learning rates were selected by grid search over baselines on rotMNIST. For all experiments in Section 6.1, we use a simple SGD optimizer with learning rate 0.1 to avoid confounding effects such as momentum during the morphism. For EquiNAS$_E$, the parent selection size is 5, the training time per generation is 0.5 epochs, and the number of generations is 50 for rotMNIST and Galaxy10 and 25 for ISIC. Baselines were trained for the equivalent number of epochs. For all experiments in Section 6.2, we use separate Adam optimizers for Ψ and Z, each with a learning rate of 0.01 and otherwise default settings. The total training time was 100 epochs

for rotMNIST and 50 epochs for Galaxy10 and ISIC. For RPP, we use a C_1-equivariant layer with an $L2$ regularization parameter of $1\mathrm{e}{-6}$ in parallel with a D_4-equivariant layer without regularization.

For rotMNIST, we use the standard training and test split with a batch size of 64, reserving 10% of the training data as the validation set. For Galaxy10, we set aside 10% of the dataset as the test set, reserving 10% of the remaining training data as the validation set. For ISIC, we set aside 10% of the available training dataset as the test set, reserving 10% of the remaining training data as the validation. For the latter two datasets, we resize the images to 64×64 due to computational constraints and use a batchsize of 32. The validation sets were previously used for hyperparameter tuning: for experimental results, they are only used for the experiments in Section 6.1 as necessary for the EquiNAS$_E$ algorithm. No data augmentation is performed, although the datasets are normalized.

C Additional Figures

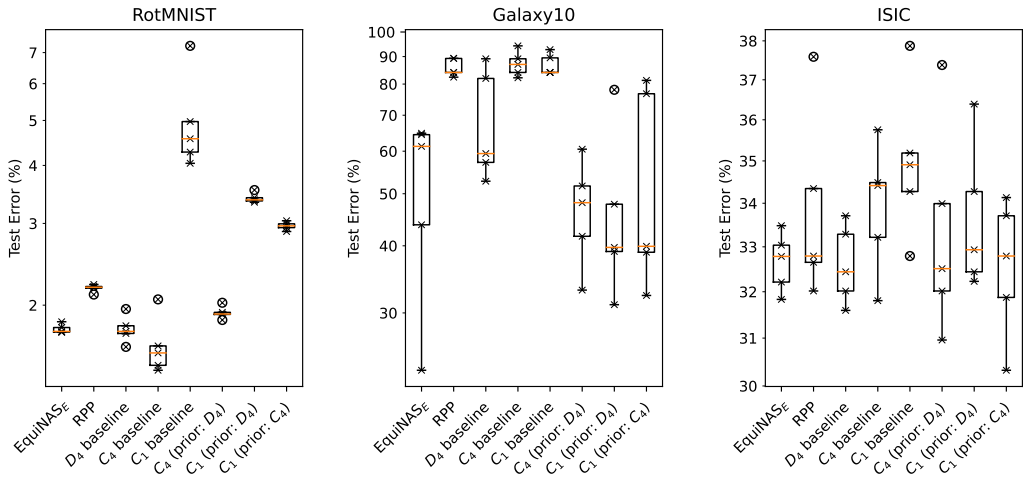
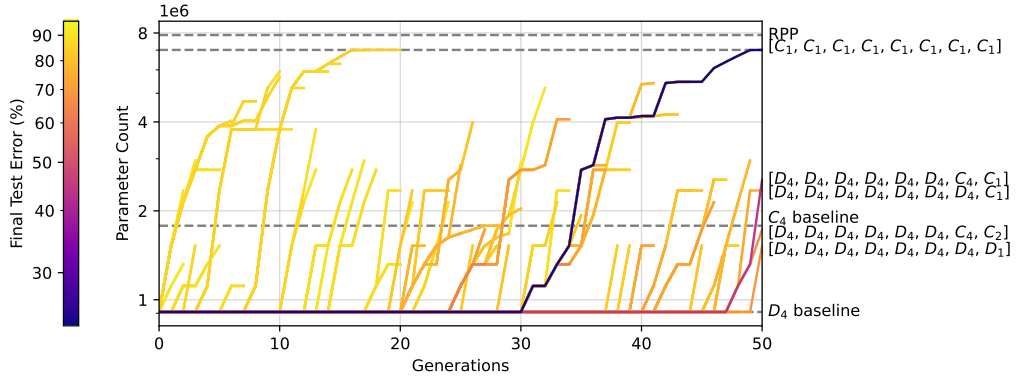
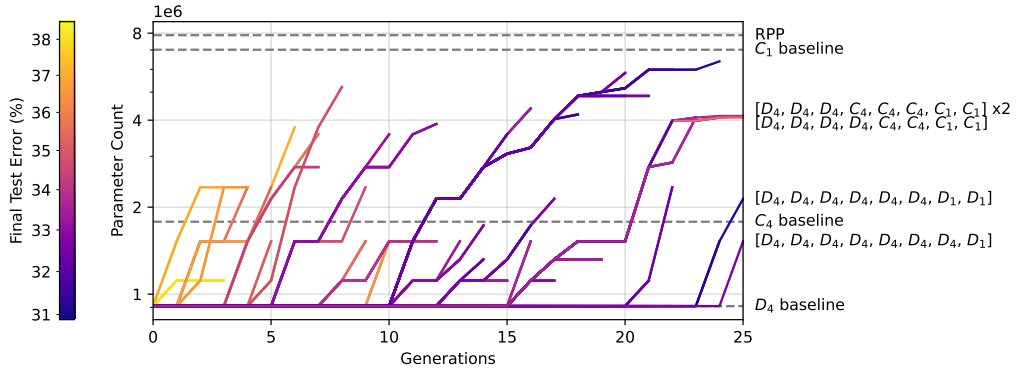


Figure 3: Test errors for experiments of Section 6.1.



(a) Galaxy10



(b) ISIC

Figure 4: Historical parameter counts of each selected individual for EquiNAS$_E$ (see Figure 1 for rotMNIST).

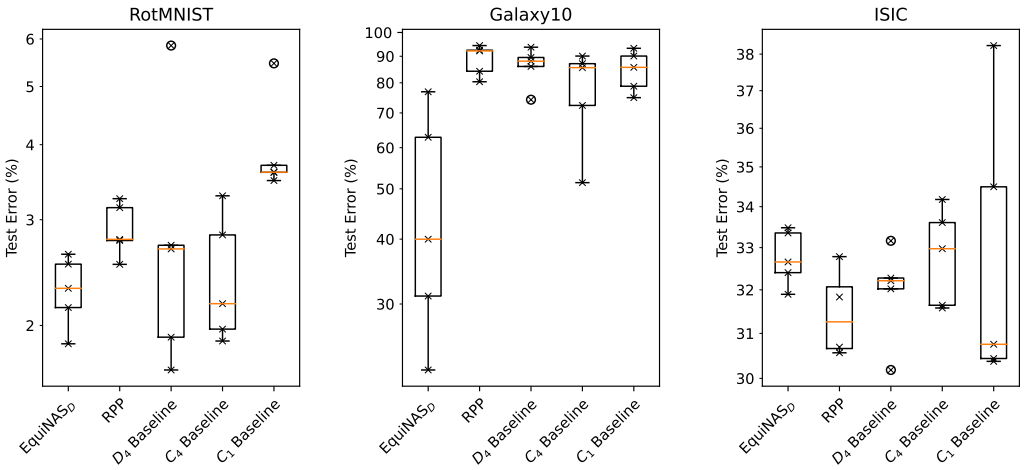


Figure 5: Test errors for experiments of Section 6.2.

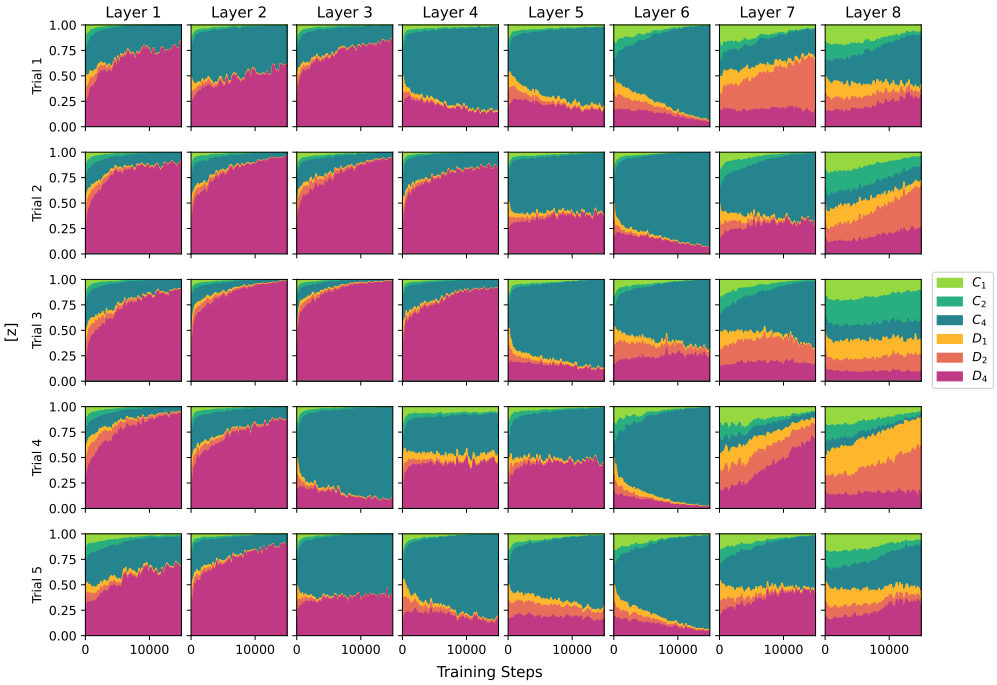


Figure 6: Architecture weighting parameters by layer for all trials on rotMNIST.

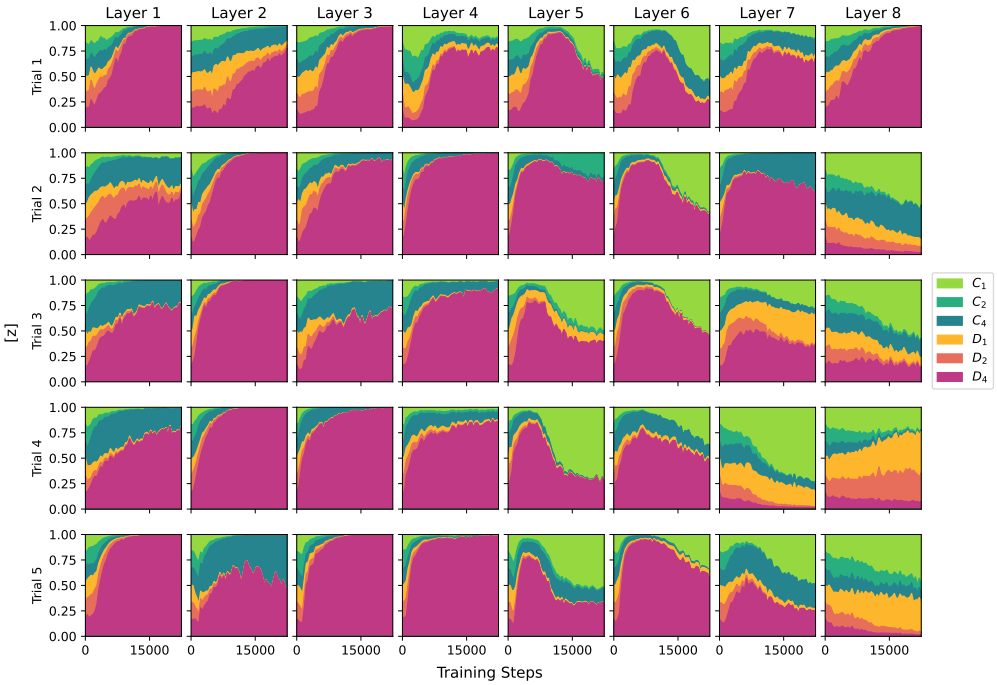


Figure 7: Architecture weighting parameters by layer for all trials on Galaxy10.

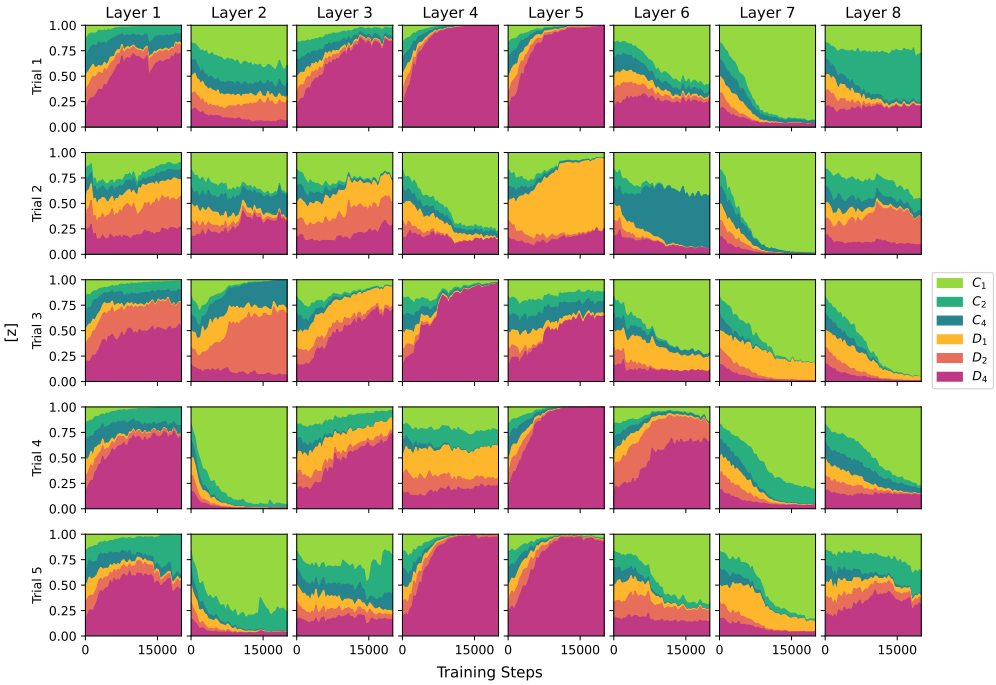


Figure 8: Architecture weighting parameters by layer for all trials on ISIC.