In What Ways Are Deep Neural Networks Invariant and How Should We Measure This?

Abstract

It is often said that a deep learning model is "invariant" to some specific type of transformation. However, what is meant by this statement strongly depends on the context in which it is made. In this paper we explore the nature of invariance and equivariance of deep learning models with the goal of better understanding the ways in which they actually capture these concepts on a formal level. We introduce a family of invariance and equivariance metrics that allows us to quantify these properties in a way that disentangles them from other metrics such as loss or accuracy. We use our metrics to better understand the two most popular methods used to build invariance into networks: data augmentation and equivariant layers. We draw a range of conclusions about invariance and equivariance in deep learning models, ranging from whether initializing a model with pretrained weights has an effect on a trained model's invariance, to the extent to which invariance learned via training can generalize to out-of-distribution data.

1 Introduction

The notions of invariance and equivariance have been guiding concepts across a diverse range of scientific domains, from physics to psychology. In machine learning (ML) the concept of invariance is frequently invoked to describe models whose output does not change when its input is transformed in ways that are irrelevant to the task the model was designed for. For a dog or cat image classifier, for example, it is desirable for the model to be reflection invariant so that the same prediction is made whether or not the input image is reflected across its vertical axis. This type of invariance is useful in this model because although an image generally changes when reflected, whether it contains a dog or cat does not. Equivariance is used to describe models whose output changes in a manner that is aligned with the way that input is transformed. For example, as an image is rotated, the position of bounding boxes predicted by an object detector should also rotate (thus, the object detector should be rotation equivariant).

While mathematicians have developed rigorous theory that can describe invariance and equivariance, the amount of this that is actually used in the context of ML varies dramatically among different works. Within computer vision, research on relatively simple image transformations (i.e., rotations or translations) is often presented within a solid group-theoretic framework [5; 53; 8]. Other work dealing with more complex types of transformations such as changes in image background have (by necessity) needed to be more informal [52]. Furthermore, while model invariance and equivariance are frequently a central component in a broad range of ML research, limited effort has been put into trying to measure them directly with the purpose of understanding the general invariance and equivariance properties of deep learning models. Rather, most works measure them indirectly through other ML metrics that align with the ultimate purpose of the model (e.g., loss or accuracy). While such a strategy makes sense when optimizing model performance is the primary objective, we miss an opportunity to better understand how and why deep neural networks work (or fail). The purpose

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of this paper is to propose a group-theoretic family of metrics, associated to an arbitrary group of symmetries G, which we call *G-empirical equivariance deviation* (G-EED), that quantify the G-equivariance (and G-invariance) of a model.

Informally, the G-EED of a model measures the extent to which it fails to be equivariant on a specific data distribution and with respect to a specific notion of distance in output space. This aligns with needs in ML where the user of a model may care only that their model is equivariant on data that the model will actually encounter in practice and not on any possible input. Further, since invariance is a special case of equivariance, G-EED also measures the extent to which a model fails to be invariant to the action of G. To show the breadth of the G-EED concept, we give a number of different ways it can be applied to measure different aspects of equivariance in a model. For example, we show how G-EED can be applied to a model's latent space representations to measure the extent to which a model extracts G-invariant features.

Finally, we use G-EED to answer a range of questions about invariance and equivariance in neural networks, with a focus on the two most popular ways of inducing invariance in these models: data augmentation and equivariant architectures. Some of the conclusions we draw from our experiments include the following. (1) Training with augmentation does not tend to induce invariance through learned equivariant layers; rather, invariance arises through some other mechanism. (2) Invariance learned through augmentation does generalize mildly to out-of-distribution data (e.g., common image corruptions), but apparent invariance seen for far out-of-distribution data (e.g., images from a completely different domain) could be the result of model insensitivity. (3) Invariance should not be assumed to correlate with model performance: models with random weights can be more invariant (in the usual mathematical sense) than models with learned or hard-coded invariance. The authors propose that the ML community needs to identify new notions that describe invariance that specifically captures ideas of invariance that are relevant to ML.(4) Models initialized with pretrained weights tend to have different invariance or equivariance properties than models initialized with random weights though whether these models are judged to be more invariant depends on specific notion of distance one chooses to use.

In summary, the contributions of this paper include:

- The introduction of G-empirical equivariance deviation, the first family of metrics that can rigorously and directly measure invariance and equivariance in deep learning models.

- A demonstration of the flexibility of G-EED, showing that it can be applied easily to a range of different components of a deep learning model to measure different forms of invariance and equivariance.

- Use of G-EED to answer a range of questions, shedding light on the extent to which neural networks are or are not invariant and equivariant.

2 Related Work

The literature on invariance and equivariance in machine learning can roughly be partitioned into two groups: those works that focus on how to build invariance and equivariance into a model or its components [27; 8; 53; 46; 9; 47; 19; 11; 37; 42; 1] and those works that focus on the theory behind invariance or equivariance [2; 5; 4; 34; 41].

Three common approaches are used to build invariance into deep learning models: data augmentation, feature averaging, and equivariant architectures. In this paper we focus on the first and third of these. Outside of a few ubiquitous layer types (such as standard translation equivariant convolutional layers), data augmentation is by far the most commonly used method, being a standard component of many training routines, particularly in computer vision. Although the details differ between different approaches, the basic idea is to randomly transform training examples as they are fed to the model, thereby encouraging the model to give the same prediction for different transformations of the same input [38]. Since it has become a common procedure when training deep learning models, data augmentation research has expanded in many directions [11; 37; 42; 1].

The idea that G-invariance can be hard coded into a model by combining multiple G-equivariant layers with data reduction layers (e.g., pooling) has a long history in deep learning. The most famous example of this idea is the conventional convolutional neural network (CNN) [32]. Since then a multitude of other group equivariant layers have been designed including two-dimensional rotation

equivalent layers [48; 51; 36; 39; 40], three-dimensional rotational equivariant layers [47; 10; 15], layers equivariant to the Euclidean group and its subgroups [46] (which we test against in this paper), and layers that are equivariant with respect to the symmetric group [33].

Our work is not the first to analyze various aspects of invariance in neural network models. Lyle et al. [34] analyzed invariance with respect to the benefits and limitations of data augmentation and feature averaging, presenting both theoretical and empirical arguments for using feature averaging over data augmentation. More recently, Chen et al. [5] presented a useful group-theoretic framework with which to understand data augmentation. Relevant to the present work, Chen et al. [4] introduced a notion of *approximate invariance*. Unlike that work, however, which focused on theoretical results related to data augmentation, this paper aims to introduce metrics that can be applied to modern deep learning architectures and answers questions about invariance from an empirical perspective. There are a number of existing works that proposed metrics aimed at measuring the extent to which a model is not equivariant (e.g. [7; 22; 17; 44; 50]). Our work differs from these in two ways: (1) we build general metrics based on basic group theory that are designed to work across groups and datatypes and (2) unlike other works that use their metric to evaluate the equivariance of a specific model, we use our metrics to explore how models learn (or do not learn) to be equivariant generally.

Finally, a range of recent works have shown that even beyond the standard evaluation statistics (e.g., accuracy), invariance is an important concept to consider when studying deep learning models. For example, Kaur et al. [25] showed that lack of invariance can be used to identify out-of-distribution inputs. A further series of works investigated whether excessive invariance can reduce adversarial robustness [23; 24; 41]. All of this work reinforces one of the primary messages of this paper, that it is important to be able to measure invariance and equivariance directly in a model.

3   Quantifying Invariance and Equivariance

We begin this section by recalling the mathematical definitions of equivariance and invariance. We present these definitions in terms of the mathematical concept of a group, which formally captures the notion of symmetry [14].

Assume that G is a group. We say that G *acts* on sets X and Y if there are maps $\phi_X : G \times X \to X$ and $\phi_Y : G \times Y \to Y$ that respect the composition operation of G. That is, for $g_1, g_2 \in G$ and $x \in X$,

$$\phi_X(g_2, \phi_X(g_1, x)) = \phi_X(g_2 g_1, x),$$

with an analogous condition for ϕ_Y. Whenever the meaning is clear, we simplify notation by writing $\phi_X(g, x) = gx$ (with an analogous convention for ϕ_Y). A map $f : X \to Y$ is said to be *G-equivariant* if for all $x \in X$ and $g \in G$,

$$f(gx) = gf(x). \tag{1}$$

In the case where the map ϕ_Y is trivial so that $gy = y$ for all $g \in G$ and $y \in Y$, we say that f is *G-invariant*. Thus, invariance is a special case of equivariance.

Assume that $f : X \to Y$ is a neural network where X is the ambient space of input data and Y is the target space. In many cases there is a natural way to factorize f into a composition $f = f_2 \circ f_1$ where $f_1 : X \to Z$ is known as the feature extractor, Z is the latent space of f, and $f_2 : Z \to Y$ is the classifier. For example, if f is a ResNet50 CNN [20] then f_1 may consist of all residual blocks while f_2 would consist of the final affine classification and softmax layers. We say that machine learning model f *extracts G-equivariant features* if f_1 is a G-equivariant function. This is an especially meaningful distinction in the context of transfer learning where invariance or equivariance can be transferred to a new task via the invariance or equivariance of f_1. Note that the definition of G-equivariant feature extraction requires a well-defined action of G on Z, which may not be obvious in many cases. Because the trivial action is defined for any G and Z, we can always ask whether f *extracts G-invariant features*.

The following proposition provides some insight into how the invariance (or lack of invariance) of f_1 relates to the invariance (or lack of invariance) of f.

Proposition 3.1. Let $f : X \to Y$ be a function that decomposes into $f = f_2 \circ f_1$ where $f_1 : X \to Z$ and $f_2 : Z \to Y$. Suppose that G acts on X, Z, and Y.

    1. f can be G-invariant even if f_1 and f_2 are not.

141   2. If f_1 is G-invariant, then f is G-invariant.

142 A proof of Proposition 3.1 can be found in Section A.6. Note that Proposition 3.1.2 implies that if
143 earlier layers of a network achieve invariance with respect to some group, then this invariance will
144 persist into later layers. This may be seen as part of the justification of the common practice within
145 the equivariant architectures community of building invariance through successive combinations of
146 G-equivariant layers and pooling layers. Of course, the statement holds only when exact invariance is
147 achieved. We see below that this is not generally the case.

3.1 Measuring equivariance

149 In this section we assume that both X and Y are vector spaces and the action of G on both X and Y
150 is linear. In all of our experiments we assume that the action of G on X and Y is known. In the case
151 that f is also a linear map, the equivariance of f can be checked directly by checking equivariance on
152 a basis for X. By extension, the equivariance of many common types of neural network layers can be
153 checked when these can be framed as linear maps (e.g., convolutional layers). However, there is no
154 systematic procedure for checking the equivariance of a nonlinear function f. If f is the composition
155 of a sequence of functions $f_1, f_2, \ldots, f_n$ and we can check that each is equivariant, then we know
156 that f is equivariant, but we cannot prove that a function is not equivariant just by proving that each
157 layer is not equivariant (this follows from Proposition 3.1.1). We are thus motivated to introduce a
158 family of metrics that can be used to empirically measure the extent to which a function deviates
159 from being equivariant on a data distribution $\mathcal{D}$ on X.

160 Since we assume in this section that the action of G on Y is linear, we can define the kernel of this
161 action, $\ker(\phi_Y)$, which is a subgroup of G. $\ker(\phi_Y)$ consists of all those $g \in G$ such that g acts as
162 the identity on Y. For $x \in X$, we define $\hat{f}(x)$ to be the expected value of $f(gx)$ over $\ker(\phi_Y)$,

$$\hat{f}(x) := \mathbb{E}_{g \in \ker(\phi_Y)}(f(gx)) = \int_{g \in \ker(\phi_Y)} f(gx) d\mu \tag{2}$$

163 where μ is the usual normalized Haar measure on subgroup $\ker(G)$. Note that when f is G-equivariant,
164 then for each $g \in \ker(\phi_Y)$, $f(gx) = gf(x) = f(x)$ and hence $\hat{f} = f$.

165 Let $(\mathcal{D}, \nu)$ be a probability distribution on X and let $m : Y \times Y \to \mathbb{R}_{\geq 0}$ be a distance function on Y.
166 We can use m to measure the extent to which f deviates from being $\bar{G}$-equivariant by computing

$$\int_{\mathcal{D}} \int_{g \in G} m(f(gx), g\hat{f}(x)) d\mu dx \tag{3}$$

167 where this time μ is the normalized Haar measure on G. Note that the argument $m(f(gx), g\hat{f}(x))$
168 measures the extent to which (1) fails to hold across distribution $\mathcal{D}$, except that $gf(x)$ is replaced by
169 $g\hat{f}(x)$. We use $\hat{f}(x)$ because it averages over all values in the orbit of x (under G) that should map to
170 $f(x)$. If f were genuinely G-equivariant, all these values $f(gx)$ would yield $f(x)$. This choice is
171 supported by the fact that it naturally interpolates between the two extreme cases: G acts trivially on
172 Y (invariance) and G acts faithfully on Y. In the former case $\hat{f}(x)$ is the average value of $f(gx)$ over
173 all of $g \in G$ and in the latter case $\hat{f}(x) = f(x)$.

174 **Proposition 3.2.** Let $f : X \to Y$ be a continuous function, G a group that acts linearly and faithfully
175 on both X and Y, and $m : Y \times Y \to \mathbb{R}_{\geq 0}$ a metric. Let $\mathcal{D}$ be a distribution on X. Then (3) is zero if
176 and only if f is G-equivariant almost surely, i.e., on a set of measure 1.

177 We provide a proof of Proposition 3.2 in Appendix A.7

178 To approximate (3) for real models and data where we always work with finite groups and finite
179 samples of $\mathcal{D}$, we define the G-EED of f with respect to m to be

$$\mathcal{E}(f, G) := \frac{1}{|D||G|} \sum_{x \in D} \sum_{g \in G} m(f(gx), g\hat{f}(x)). \tag{4}$$

180 Note that since G is a finite group (and hence discrete), the Haar measure turns into the usual counting
181 measure.

In the remainder of this section we describe some specific types of G-EED that may be relevant to computer vision tasks. By convention, when using a distance function m for which larger values of $m(x_1, x_2)$ indicates that x_1 and x_2 are "closer" (the opposite of a proper metric), we attach a negative sign to m. For example, rather than using cosine similarity, we use negative cosine similarity (e.g., 5). This way, larger values of G-EED consistently indicate less invariance, regardless of the m used. The diagram in Figure 1 provides a summary of the types of G-EED studied in this paper.

Figure 1: A diagram illustrating the different types of empirical equivariance deviation (EED) that we investigate in this paper.

The channelwise G-equivariance of convolutional layer activations: Throughout most layers of a CNN an individual image is represented as a 3-tensor. Let $f_\ell : X \to \mathbb{R}^{C_\ell \times H_\ell \times W_\ell}$ be the composition of the first ℓ layers of a CNN such that for input image $x \in X$, $f_\ell(x)$ is a $C_\ell \times H_\ell \times W_\ell$ tensor where the first dimension corresponds to the channels of the representation and the second and third dimensions correspond to the two spatial dimensions.

Suppose that G is a finite group that acts on images and other 2-tensors (e.g., rotations, translations, and reflections). To understand the extent to which the first ℓ layers of the network are G-equivariant, we can measure the G-EED of f_ℓ. Although there are numerous choices of m for (3) that could be used to measure the channelwise difference between $f_\ell(gx)$ and $gf_\ell(x)$, we choose the following: let $S : \mathbb{R}^{H_\ell \times W_\ell} \times \mathbb{R}^{H_\ell \times W_\ell} \to [0, 1]$ be the cosine similarity on individual channels treated as vectors in $\mathbb{R}^{H_\ell W_\ell}$. Write $[f_\ell(x)]_i$ for the ith channel of $f_\ell(x)$. Then we set

$$m(f_\ell(gx), g\hat{f}_\ell(x)) = -\frac{1}{C} \sum_{i=1}^{C} S([f_\ell(gx)]_i, g[\hat{f}_\ell(x)]_i).$$

That is, let m be the negative of the average cosine similarity between individual channels of $f_\ell(gx)$ and $g\hat{f}_\ell(x)$. This gives:

$$\mathcal{E}_{\text{channel}}(f, G, \ell) := \frac{1}{|D||G|} \sum_{x \in D} \sum_{g \in G} m(f_\ell(gx), g\hat{f}_\ell(x)) \tag{5}$$

Note that since rotation, translation, and reflection groups all act faithfully on $\mathbb{R}^{H_\ell \times W_\ell}$, for these specific G, $\hat{f} = f$. We call this version of G-EED *channelwise G-EED*. This metric assumes that G acts on each channel in a 3-tensor independently. It does not account for the more complicated setting where the action of G either permutes or mixes channels of $\mathbb{R}^{C_\ell \times H_\ell \times W_\ell}$ in a non-trivial way. In this work we always assume that the action of G on channels of $\mathbb{R}^{C_\ell \times H_\ell \times W_\ell}$ is identical as the action of G on X (up to differences in spatial scale). So if $G = C_8$ and G rotates the spatial dimension of input images, we assume G rotates each individual channel of hidden representations as well.

Invariance of latent space representations: Consider a model f consisting of feature extractor $f_1 : X \to \mathbb{R}^k$ and classifier $f_2 : \mathbb{R}^k \to \mathbb{R}^n$. If G is some group that acts on X, we can ask whether f_1 extracts G-invariant features. Define M to be either the average ℓ_2-distance or cosine similarity between distinct points in the set $f_1(D)$. By setting m to be the ℓ_2-distance (respectively cosine similarity), we calculate the *latent space G-EED* as

$$\mathcal{E}_{\text{latent}}(f, G) := \frac{1}{M} \frac{1}{|D||G|} \sum_{x \in D} \sum_{g \in G} m(f_1(gx), \hat{f}_1(x)). \tag{6}$$

Note that because in this setting G acts trivially on the latent space $\mathbb{R}^k$ (because of the invariance assumption), $\hat{f}_1(x) = \frac{1}{|G|} \sum_{g \in G} f_1(gx)$. We describe why the normalization term M is necessary in Section A.8 of the Appendix. See also Figure 15. As we show in Section 4.1, it is often useful to consider latent space G-EED with respect to both Euclidean distance and negative cosine similarity.

Invariance at the softmax layer of classifiers:

While the two examples above focused on calculating invariance and equivariance at different intermediate layers of computer vision models, invariance of classification models is most commonly considered with respect to the final softmax output. In this paper we choose to use KL-divergence for m because it is a distance function designed to handle probability distributions, which softmax outputs approximate. In particular,

$$\mathcal{E}_{\text{softmax}}(f, G) := \frac{1}{|D||G|} \sum_{x \in D} \sum_{g \in G} D_{KL}\big(f(gx), \hat{f}(x)\big).$$

We call this metric the *softmax G-EED*. Note that like all the metrics described in this section, softmax G-EED strictly measures invariance and is frequently not in line with task performance.

4 Understanding invariance and equivariance in deep learning

To prototype G-EED we experiment with the finite cyclic group C_8 that acts on images by $45°$ rotations. This symmetry is relevant to datasets where imagery does not have a preferred orientation. The datasets we use include *Rotated MNIST* which consists of randomly rotated MNIST digits from classes 0-8 and *xView Maritime*, a chipped version of the xView object detector overhead dataset composed of the nine maritime classes. We chose xView Maritime because it is a more real-world dataset that has an obvious symmetry (rotation) that is not hardcoded into standard CNNs. We describe these and other datasets we use in detail in Section A.2.

To reduce the computational burden, when calculating (4) we only used 50 randomly chosen examples from the corresponding dataset. We found that evaluating at more points did not substantially change the results. When not otherwise stated all invariance and equivariance measurements were calculated using points from the test set, not the training set. The normalization constant for latent space G-EED is calculated over 200 randomly chosen points.

4.1 Do networks trained with augmentation learn equivariant layers?

In this section we apply our metrics to standard CNNs and C_8-rotation equivariant, steerable CNNs (C_8-CNN) [46] to compare the invariance or equivariance of a model trained with augmentation with the invariance or equivariance of a model that is explicitly designed to learn invariance through progressive equivariant layers and pooling. We train 10 copies of each model type for 2,000 iterations on rotated MNIST. We apply random rotation augmentation to the models during training and all achieve an accuracy of over 98% on the test set. By design, for any $1 \le k \le 6$, the first k-blocks of one of the C_8-CNN models will be approximately rotation equivariant. The standard wisdom is that, with pooling, this will lead to an invariant representation in the latent space.

Despite the fact that both families of models achieve similar performance, we note that their invariance and equivariance properties differ significantly. The channelwise C_8-EED of the composition of the first k blocks (where $1 \le k \le 6$) of the C_8-CNN is significantly higher than that of the CNN, indicating that (as claimed) the C_8-CNN is more equivariant with respect to individual channel rotations of $45°$ in both input and hidden representations (see Figure 6 for examples of output at blocks 2 (left) and 5 (right)). Beyond that we see that equivariance decays for both models as input travels through additional blocks. This is particularly true for the C_8-CNN. We conjecture that this is likely caused by the accumulation of interpolation artifacts associated with rotation. Perhaps even more interesting is the fact that for no layer of either model do the channelwise C_8-EED values increase beyond a small jump at the beginning of training. This suggests that layerwise equivariance may not always be aligned with the learning objective and that learned invariance does not arise through the naive form of learned equivariance.

Both in terms of the Euclidean distance version of latent space C_8-EED and softmax C_8-EED, the C_8-CNNs show more invariance than the conventional CNNs (see Figure 2) but the difference was

less dramatic than it was for channelwise C_8-EED. This suggests that the CNNs likely caught up in terms of C_8-invariance using mechanisms distinct from layerwise C_8-equivariance. Notable also is the fact that unlike channelwise C_8-EED, which did not indicate increased C_8-equivariance over the course of training, both latent space and softmax C_8-EED decreased with training (suggesting learned invariance).

Most surprisingly, in Figure 9 we see that the C_8-CNNs are less invariant than the conventional CNNs with respect to the cosine similarity version of latent space C_8-EED. We conjecture two possible reasons for this. The first is based on the fact that C_8-CNNs are designed to be equivariant **on the nose**, **not up to scaling**. The structural constraint of exact equivariance may actually be misaligned with cosine similarity where vector magnitude no longer matters. From this perspective, projective representation theory, where symmetries are only taken up to scaling, might be a profitable direction of future research in equivariant architectures. The second possible explanation arises from Figure 8 which shows that in terms of absolute cosine similarity (that is, without the normalization term M in (6)), the C_8-CNN is more invariant. It may be that while C_8-CNNs indeed cluster orbits of points under the C_8 action closer together, the conventional CNNs are better at spreading other points further away in the latent space.

Figure 2: The latent space C_8-EED (left) and softmax C_8-EED (right) for conventional and C_8-equivariant CNNs (C_8-CNNs) [46] with respect to the rotated MNIST dataset. Both plots include 95% confidence intervals. Lower values for both plots indicate more C_8-invariance.

Summary: Equivariant architectures and nonequivariant architectures capture invariance in distinct ways. Nonequivariant networks do not learn layerwise equivariance (at least with respect to the naive C_8 action given by rotating individual channels in a hidden representation). Rather they achieve their learned invariance via some other mechanism. The level of invariance measured in the latent space depends on the underlying metric m which is used.

4.2 Does learned invariance hold for out-of-distribution data?

It was noted in Lyle et al. [34] that while augmentation may be satisfactory for many tasks, there is a risk that learned invariance will not extend to out-of-distribution (OOD) data. We investigate this question using G-EED metrics, studying the conventional CNN and C_8-equivariant CNN from Section 4.1 and a conventional CNN with untrained weights that can be used for comparison. Note that because rotation invariance is at some level hard coded into the architecture of the C_8-CNN, our default assumption is that the C_8-CNN models will tend to be more invariant on OOD data than models with learned augmentation. Images of example OOD data as well as dataset descriptions can be found in Appendix A.2.

The left plot in Figure 3 shows the latent space C_8-EED for the three model families that we tested. We can see that random weights extract significantly less invariant latent space representations compared to both the augmentation-trained CNNs and C_8-CNNs. Although this difference is not surprising for the C_8-CNNs, for the standard CNNs it indicates that augmentation does learn some rotation-invariant features that generalize to OOD data. Furthermore, while C_8-CNNs do exhibit more latent space invariance than the augmentation-trained CNNs, the difference is insignificant compared to the difference between augmentation-trained CNNs and CNNs with random weights. Note that in these OOD experiments, the normalization term M in (6) is calculated using the OOD

data (rather than the training or test set). This choice was made when considering situations in which a frozen network is used in combination with metric learning methods, as in Snell et al. [43], to solve a task with data drawn from a shifted distribution.

Figure 3: The latent space C_8-EED (left) and softmax C_8-EED (right) for conventional untrained CNNs, conventional CNNs trained on MNIST, and C_8-equivariant CNN (C_8-CNN) [46] trained on MNIST with respect to a range of in- and out-of-distribution datasets. Both plots include 95% confidence intervals.

As a showcase of how a single model can display different types of invariance, the CNNs with random weights are far more invariant in terms of softmax C_8-EED than the trained C_8-CNN, which is more invariant than the trained CNN (right plot, Figure 3). We suspect that invariance of the CNNs with random weights arises from the fact that an untrained network tends to be insensitive to input. This observation is useful to keep in mind, especially as the concept of invariance is frequently treated as a net benefit to any model. Invariance is useful when it is aligned with other metrics more directly related to the task the model was designed for.

Summary: Our experiments suggest that augmentation trained networks do learn invariance that mildly generalizes to OOD data. A single models can display differing kinds of invariance (an untrained network does not not extract invariant features but through insensitivity may make invariant predictions). In cases where invariance is critical and OOD data is expected, equivariant architectures may be a safer choice than training with augmentation.

4.3 How does the use of pretrained weights affect invariance and equivariance?

It has become standard practice in computer vision to initialize a model using weights trained on a large, diverse image dataset such as ImageNet [12]. It is reasonable to ask how such a strategy affects the invariance and equivariance of the resulting models. We choose four different image classifier architectures: ResNet50 [20], AlexNet [29], DenseNet121 [21], and LeViT192 [18]. For each of these architectures, we initialized five models with random weights and five models with weights from either the Torchvision package [35] (ResNet50, AlexNet, and DenseNet) or Timm [49] (LeViT192). We then trained all of these models on the xView Maritime training set. Next, we evaluated the latent space C_8-EED and softmax C_8-EED on the xView Maritime test set. It is important to note that pretrained weights, which were generated by training on ImageNet, might not be expected to have learned to extract fully rotationally invariant features. Indeed, the objects found in ImageNet mostly have a preferred orientation at which they generally are seen (there are very few instances of upside-down dogs or vehicles in ImageNet).

The results of our experiments are shown in Figure 4. Figure 4 shows the latent space C_8-EED for all eight model types every 200 iterations. We see that models trained from scratch extract more invariant features in their latent space. Moreover, while the invariance of models trained from scratch tends to decrease slightly over the course of training (latent space C_8-EED increases), the invariance of models trained using pretrained weights tends to increase slightly over the course of training. This may relate to ImageNet's lack of object classes that appear at a wide range of orientations. The models with pretrained weights may need to learn additional rotation invariance over the course

of training. Contrast that with the weights trained from scratch that may learn rotation invariant features quickly which are later discarded in favor of less rotationally invariant features that better optimize the cross-entropy loss function used to train these networks. This, along with the fact that models using pretrained weights tend to have slightly higher accuracy, points to a potential tradeoff between invariance and task performance. Whether the robustness of the features captured by the pretrained networks is related to the fact that they are less invariant requires further exploration. We also calculated the latent space D_8-EED (where D_8 is the order 16 dihedral group) for these same models and dataset. The results are recorded in Figure 10. We find the patterns to be fairly similar.

On the other hand, Figure 17 in the Appendix shows that the invariance properties of pretrained networks vs. networks trained from stratch is somewhat more ambiguous when considering softmax C_8-EED.

Figure 4: The latent space C_8-EED measured every 200 training iterations (for a total of 10,000 iterations) for a range of model architectures that were initialized with either random or pretrained weights generated using ImageNet.

Summary: Our experiments make it clear that networks with pretrained weights incorporate invariance differently than networks trained from scratch. Further research will be required to fully understand these differences.

5   Limitations and Conclusion

Although the G-EED family of metrics that we introduce is flexible in many ways, it is not capable of capturing notions of invariance that do not have a known underlying symmetry group (e.g., changes in image background), do not come from the action of a group (e.g., scaling corresponding to a semigroup action), or (for the purpose of measuring equivariance of internal representations) do not have a known action on the latent space of a model (e.g., changes in color). An important next step would be to bring our metrics to these broader notions of invariance and equivariance. It would be particularly valuable if our metrics could be modified so that they can measure equivariance without explicitly specifying a group action in a hidden layer. This would enable us to measure G-EED for emergent types of learned equivariance where the action of G on the output space is not specified by the user.

In this paper we described a novel family of metrics meant to measure equivariance in deep learning models. We use these metrics to suggest answers to questions related to the extent to which neural networks are or are not invariant or equivariant to different types of transformations. Surprisingly, while invariance and equivariance are fundamental topics within machine learning, this is one of the first works (to our knowledge) that tries to measure these properties empirically in modern neural networks. We hope that this work will open a conversation on this important topic that will ultimately lead to a better understanding of how deep learning is able to achieve the results that it does.

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A Appendix

A.1 Experimental Details

All our models were trained on an Nvidia A100 using the Adam optimizer. Batch size, learning rate (LR), and weight decay hyperparameters are summarized in the table below. Recall from Sections 4.1 through 4.3 that we train the CNN and C_8-CNN (architecture description below) on rotated MNIST and train AlexNet, ResNet50, DenseNet121, and LeViT192 on Maritime xView. Hyperparameters were chosen based on an informal search. Running our experiments with a more comprehensive hyperparameter search would be a worthwhile future exercise since it might yield insight into how different hyperparameters affect model invariance and equivariance.

The standard CNN and C_8-CNN used in Section 4.1 consist of 6 convolutional blocks, each containing a standard convolutional layer, a batch norm, a ReLU nonlinearity, and a pooling layer. The C_8-CNN models have an analogous 6 block structure with the difference that each block uses C_8-rotation equivariant, steerable convolutional layers and a so-called inner batch norm (a batch norm adapted for equivariant frameworks [46]). Both model types have a final linear layer.

Table 1: Experimental hyperparameters.

	Batch size	LR	Weight Decay
CNN	64	5×10^{-4}	1×10^{-5}
C_8-CNN	64	5×10^{-4}	1×10^{-5}
AlexNet	64	5×10^{-5}	1×10^{-5}
ResNet50	64	5×10^{-4}	1×10^{-5}
DenseNet121	64	1×10^{-5}	1×10^{-5}
LeViT192	64	5×10^{-5}	1×10^{-5}

A.2 Dataset Details

The datasets used in our experiments include (i) *rotated MNIST*, which consists of images from MNIST rotated by random angles [13] (MNIST is covered by a Creative Commons Attribution-Share Alike 3.0 license) and (ii) *xView maritime*, a classification dataset we constructed by cropping the bounding boxes of all maritime vessel classes found in xView [31], an overhead imaging dataset (xView is covered by an Attribution-Noncommercial-ShareAlike 4.0 International (CC BY-NC-SA 4.0) license). In our version of rotated MNIST we excluded the class 9 so that we could remove the drop in model accuracy resulting from the similarity of a 9 and an upside-down 6. We apply a circular mask to all images before using them as input to a model so that invariance is not broken by the artifacts introduced by rotating a rectangular image by θ degrees where $\theta \neq 0°, 90°, 180°, 270°$. See the bottom right image in Figure 5 for an example of this.

Below we describe our OOD datasets for Section 4.2.

- **MNIST Train:** The original MNIST training images.

- **CIFAR10:** Grayscale versions of the CIFAR10 images [28] (CIFAR10 is covered under an MIT license).

- **MNIST (Noisy) 1-6:** MNIST images perturbed by noise randomly sampled uniformly from intervals (1) $[0, 0.2]$, (2) $[0, 0.4]$, (3) $[0, 0.6]$, (4) $[0, 0.8]$, (5) $[0, 1.0]$, and (6) $[0, 1.2]$. Notice that any of these noise perturbations can push pixels outside of image bounds. We generally assume that images with more noise are farther OOD.

- **MNIST (blurry):** MNIST images with Gaussian blur applied.

- **Omniglot:** Another image classification dataset that contains characters [30] (Omniglot is covered under an MIT license).

- **Inverted MNIST:** MNIST where each pixel has had the transformation $f(x) = 1 - x$ applied to it. This inverts the intensity of pixels to make the MNIST dataset look more like Omniglot (the background has high intensity and the digits have low intensity).

Figure 5: Examples of the OOD datasets that we used to evaluate our models. From left to right: MNIST train, MNIST (noisy) 1–6, MNIST (blurry), omniglot, inverted MNIST, and CIFAR10 (grayscale).

A.3 How does invariance in a model's latent space change when augmentation is or is not used?

As in Section 4.3, we focus on the case where $G = C_8$, the group generated by $45°$ rotations, and the dataset is xView Maritime. We trained 5 ResNet50s, 5 AlexNets, and 5 DenseNet121s with and without rotation augmentation respectively. We then measured latent space C_8-EED in all models. Our results can be found in Figure 11. We find that models trained without augmentation indeed had consistently lower C_8-EED both when we used our standard Euclidean distance metric and when we used the cosine similarity version.

A.4 The invariance of supervised and self-supervised models

In an additional experiment, we compared the invariance of supervised models to the invariance of self-supervised models. To do this we evaluated four different convolutional neural networks in one of the simplest possible settings where G is the order 2 group of reflections across the vertical axis. The models we chose to test were a standard ResNet50 (we used the Torchvision pretrained weights) [20; 35], a Big Transfer ResNetV2 [26] (with weights from 'PyTorch Image Models' [49]), a ResNet50 trained using the self-supervised method DINO (we used the author's pretrained weights) [3], and a ResNet50 trained using the self-supervised method SimCLR [6] (we used weights from [45]). Note that the first two models utilized supervised training and the second two utilized self-supervised training techniques. Further, SimCLR is trained with a contrastive loss that directly optimizes for invariance of input to specific transformations. On the other hand, DINO uses 'knowledge distillation', without a contrastive loss. We choose to concentrate on latent space G-EED in this experiment.

Our results can be found in Figure 12. Note that since all of these models have a 2048-dimensional latent space, we can directly compare them. This is something we could not do in Section 4.3. We see that in terms of both versions of latent space G-EED (that which uses Euclidean distance and that which uses cosine similarity), the model trained using SimCLR has significantly more invariance. This is not surprising given that the contrastive loss that SimCLR uses explicitly optimizes for similarity between an image and its reflection. DINO, which is also trained in a self-supervised manner, but which does not explicitly use the contrastive loss is less invariant (how it compares to the two supervised models depends on which metric is used). This suggests that use of contrastive loss can boost the invariance properties of a model but that self-supervision alone may not always yield invariance properties different from supervised training. This is an area that could benefit from further, more comprehensive investigation.

A.5 Does learned equivariance involve re-ordering of tensor channels?

Suppose that the function $f_\ell : X \to \mathbb{R}^{C_\ell \times H_\ell \times W_\ell}$ corresponds to the first ℓ layers of a network, terminating with a 3-tensor which has C_ℓ channels of height H_ℓ and width W_ℓ. Suppose that G is a group that acts both on the input space X and the hidden space $\mathbb{R}^{C_\ell \times H_\ell \times W_\ell}$. The channelwise G-EED metric that we proposed in this paper, assumes that when we compare channels from $f_\ell(gx)$ with channels $gf_\ell(x)$, we should assume the trivial bijection. That is, we should compare the first channel of $f_\ell(gx)$, $[f_\ell(gx)]_1$, with the first channel of $gf_\ell(x)$, $g[f_\ell(x)]_1$, the second channel $[f_\ell(gx)]_2$ with the second channel $g[f_\ell(x)]_2$, etc.

Figure 6: The channelwise C_8-EED for the composition of various layers in 10 conventional CNNs and 10 C_8-equivariant CNNs (C_8-CNN) [46] trained on the rotated MNIST dataset. Both plots include 95% confidence intervals. Smaller values indicate more C_8-equivariance.

On the other hand, in many equivariant CNN's, the group action of g on $f_\ell(x)$ not only changes individual channels, it also permutes their order. It is reasonable to ask whether CNNs trained with augmentation might learn some similar "emergent" structure not only within individual channels, but also among them. The channelwise G-EED metric would likely not detect this kind of equivariance. In this section we examine this possibility. Though we do not disprove its existence, we run several preliminary experiments that suggest that this is not likely. This is an area that would benefit from additional study.

In our preliminary investigation, we focus on the filters at each layer (rather than input and output). We chose to do this based off of the observation that in equivariant CNNs that utilize the regular

Figure 7: **(Left)** The cosine similarity version of latent space C_8-EED for 10 conventional CNNs and 10 C_8-CNNs all trained on rotated MNIST. Surprisingly, the C_8-CNNs are **less** invariant with respect to this metric. We speculate as to why this might be in Section 4.1. **(Right)** One of our hypotheses is driven by plotting the unnormaized version of this metric which suggests that C_8-CNNs clusters points in a single C_8 orbit closer than the CNNs, but do not scatter other points as far as the CNNs do.

Figure 8: The unnormalized cosine similarity version of latent space C_8-EED, for 10 conventional CNNs and 10 C_8-CNNs all trained on rotated MNIST. This plot suggests that the higher invariance that we see for the conventional CNNs compared to the C_8-CNNs (Figure 9) is a result of the fact that the conventional CNNs push images from different rotational orbits apart rather than them being able to pull elements of the same orbit closer together.

representation and which are designed to display the phenomenon we are looking for, filters come in entire orbits. That is, if w is a filter in a layer, then so is each element in the orbit Gw (i.e., the orbit of w under the action of G). In Figure 13 for example, four filters of a C_4-equivariant convolutional layer [46] are displayed. The filters represent an orbit under the action of all 90-degree rotations (e.g., C_4).

As a first step towards identifying structured equivariance in augmentation trained CNNs, we compared all channels of each pair of filters at a given convolutional layer of an AlexNet CNN. However, comparing all the possible pairings is combinatorially prohibitive, even for simple architectures like AlexNet. In Figure 14, we plot the metric

$$\min_{\substack{j \neq i; k \\ g \in C_4}} ||g(w_{\ell,i,t}) - w_{\ell,j,k}||_{\ell_2}, \tag{7}$$

where $w_{\ell,i,t}$ is the height H'_ℓ and weight W'_ℓ 2-tensor obtained by taking channel t from filter i in layer ℓ and $g(w_{\ell,i,t})$ is the action of group element g on $w_{\ell,i,t}$. It this case simply rotation by a multiple of $90°$. We report the average of this metric over all convolutional layers of four different AlexNet models trained on MNIST: AlexNet trained from scratch without rotation augmentation, AlexNet trained rotation augmentation but no pretraining, AlexNet with both pretraining and rotation augmentation, and finally Alex with C_8-equivariant layers [46]. Random i and t are selected for each computation, and for computational simplicity we only evaluated on the subgroup C_4 of C_8 generated by 90-degree rotations.

Figure 9: The cosine similarity version of latent space C_8-EED (**normalized on the left**, **unnormalized on the right**) for conventional untrained CNNs, conventional CNNs trained on MNIST, and C_8-equivariant CNNs (C_8-CNN) [46] trained on MNIST with respect to a range of in- and out-of-distribution datasets. Both plots include 95% confidence intervals. **Lower values indications more C_8-invariance.** As can be seen, without normalization, the trained conventional CNNs and the C_8-CNNs are often comparable. On the other hand, after normalization the conventional CNNs show much lower latent space C_8-EEG, indicating more C_8-invariance. The differences between these two plots seems to indicate that the conventional CNNs have learned to better separate orbits of points rather than learning to cluster orbits together more tightly.

Figure 10: The latent space D_8-EED measured every 200 training iterations (for a total of $10,000$ iterations) for a range of model architectures that were initialized with either random or pretrained weights generated using ImageNet. Note that D_8 is the dihedral group of order 16 generated by a $45°$ angle and a reflection across an axis.

A network where some filters are rotations of others would be expected to achieve a value of 0 for (7). Indeed, we can see that this is what happens to the C_8-equivariant network. We see that the other networks do not achieve zero. Indeed, with the exception of the pretrained AlexNet, for which (7) increases slightly over training, the other non-equivariant networks do not change significantly at all. This indicates that this form of emergent equivariance does not emerge in this example.

Figure 11: Latent space G-EED on xView Maritime for models trained with and without rotation augmentation. **(Left)** The standard latent space G-EED metric (**smaller means more invariant to reflection**). **(Right)** The alternative version of latent space C_8-EED where cosine similarity is used instead of Euclidean distance (**larger means more invariant to reflection**). Note that different models are not necessarily comparable since their latent spaces can have different dimension.

Figure 12: Latent space G-EED for two supervised and two self-supervised models where G is the order 2 group of reflections across the vertical axis. BiT and ResNet50 were both trained in a supervised manner and DINO and SimCLR were both trained in a self-supervised manner. SimCLR is the only model trained with contrastive loss. All models use some version of the ResNet50 architecture. **(Left)** The standard latent space G-EED metric. **(Right)** G-EED where cosine similarity is used instead of Euclidean distance.

A.6   A Proof of Proposition 3.1

Proof. 1. To prove this, consider the function $f : \mathbb{R}^2 \to \mathbb{R}$ defined such that for $(x, y) \in \mathbb{R}^2$

$$f(x, y) = \frac{x + y}{2}.$$

The order 2 cyclic group $\mathbb{Z}_2 = \{1, \sigma\}$ acts on $\mathbb{R}^2$ by permuting coordinates. That is, the only nonidentity element σ acts on $\mathbb{R}^2$ by sending $(x, y) \mapsto (y, x)$. It is clear that f is $\mathbb{Z}_2$-invariant.

However, note that if $f_1 : \mathbb{R}^2 \to \mathbb{R}^2$ is defined by $f_1(x, y) = (2x, y)$ and $f_2 : \mathbb{R}^2 \to \mathbb{R}$ is defined by

$$f_2(x, y) = \frac{x + 2y}{4},$$

then $f = f_2 \circ f_1$. But neither f_1 nor f_2 is $\mathbb{Z}_2$-equivariant to the actions described above.

2. This proof follows easily from the definitions. Suppose that f_1 is G-invariant, then for any $x \in X$ and $g \in G$, $f_1(gx) = f_1(x)$. Hence

$$f(gx) = f_2(f_1(gx)) = f_2(f_1(x)) = f(x).$$

$\square$

Figure 13: Four 7×7 filters from a randomly initialized C_4-equivariant convolutional layer. Note that each is a 90-degree rotation of the others.

Figure 14: The average minimum ℓ_2 norm differences, (7), between pairs of individual channels of filters from each convolutional layer of the AlexNets, plotted against training iteration. Augmented training does not appear to cause at least 90-degree rotational symmetry to occur.

A.7 A Proof of Proposition 3.2

Proof. First note that for fixed x and g, $m(f(gx), g\hat{f}(x)) = 0$ if and only if $f(gx) = gf(x)$. This follows from the fact that since G acts faithfully on Y, $\hat{f}(x) = f(x)$. First assume that $m(f(gx), g\hat{f}(x)) = 0$. Then, since m is a metric, $f(gx) = g\hat{f}(x) = gf(x)$ giving the desired result. Next, if $f(gx) = gf(x) = g\hat{f}(x)$, then it again follows that $m(f(gx), g\hat{f}(x)) = 0$.

Next we recall the basic fact [16, proposition 2.16] from measure theory, which states that if $h : W \to [0, \infty]$ is a non-negative measurable function on measure space (W, ν), then

$$\int_W h = 0 \Leftrightarrow h = 0 \text{ almost everywhere.} \tag{8}$$

Recall that

$$\hat{f}(x) = \int_{g \in \ker(\phi_Y)} f(gx) d\mu_{\ker(\phi_Y)}$$

where ϕ_Y is the representation of G on Y and $\mu_{\ker(\phi_Y)}$ is the normalized Haar measure on the subgroup $\ker(\phi_Y) \subset G$. Let $W = X \times G \times \ker(\phi_Y)$ with $\xi = \nu \times \mu \times \mu_{\ker(\phi_Y)}$ the product measure on W generated by Haar measure μ on G, $\mu_{\ker(\phi_Y)}$, and the probability measure ν associated with $\mathcal{D}$. Note that f is measurable by virtue of being continuous, G acts linearly and hence is measurable, and m is measurable by virtue of being a metric. It follows that the function $h : X \times G \times G \to [0, \infty]$

670 defined by

$$h(x, g_1, g_2) = m(f(g_1 x), g_1 f(g_2 x))$$

671 is measurable. The result then follows from the observation that m is non-negative (and hence h is)
672 and from (8). That is, if (3) is zero, then since $m(f(gx), g\hat{f}(x))$ is non-negative, then (8) tells us that
673 $m(f(gx), g\hat{f}(x)))$ is zero almost-everywhere with respect to measure ξ. On the other hand, (8) also
674 says that if $m(f(gx), g\hat{f}(x))$ is zero almost everywhere (including the case where this term is zero
675 everywhere), then (3) is equal to zero. □

A.8 The Reason for Normalization of Latent Space G-EED

677 We normalize $\mathcal{E}_{\text{latent}}(f, G)$ by M because when we use ℓ_2-distance to compute G-EED without
678 normalization, it is sensitive to scaling in a way that is unrelated to downstream task performance. To
679 illustrate, note that by scaling f_1 by $c > 1$, the unnormalized latent space G-EED increases, indicating
680 a decrease in G-invariance. More precisely, if $f_1' = cf_1$, then $\mathcal{E}(f_1', G) = c\mathcal{E}(f_1, G)$. However,
681 if we set $f_2' = \frac{1}{c} f_2$, then $f_2' \circ f_1' = f = f_2 \circ f_1$. Thus, f_1 can be made to have arbitrarily large
682 unnormalized latent space G-EED while the total model f remains constant. A different but equally
683 illustrative example is visualized in Figure 15. Two feature extractors have identical unnormalized
684 latent space C_8-EED for a single rotation orbit of an image of a 4 (average distance between blue
685 points and their centroid), but the second feature extractor closely clusters points in the orbit relative
686 to other instances from MNIST, while the first feature extractor does not. We would argue that in
687 most cases the second feature extractor should be called *more invariant* with respect to this particular
688 task. Normalization mitigates this issue, giving a more reasonable notion of latent space invariance in
689 the context of machine learning.

Figure 15: This illustration shows why it is important to normalize the latent space G-EED by the
average distance between random pairs from the dataset. The set $\mathcal{O}$ (blue) is the orbit of an image
of a '4' under the rotation action of C_8. Two feature extractors f^1 and f^2 map $\mathcal{O}$ as well as other
unrelated images (red) from MNIST [13] to a latent space. While points from $f^1(\mathcal{O})$ and $f^2(\mathcal{O})$ both
have the same average distance to their centroid, $f^2(\mathcal{O})$ clusters closely together relative to other
points from the dataset. $f^1(\mathcal{O})$ is mixed with instances not belonging to $f^1(\mathcal{O})$. We would argue that
f^2 extracts more invariant features.

A.9 Channelwise C_8-EED for out-of-distribution datasets

691 In this section we provide Figure 16, which shows the channelwise C_8-EED for collections of: CNN
692 models with random weights, CNN models that have been trained on MNIST, and C_8-CNN models
693 that have been trained on MNIST.

694 In Figure 16 we show the channelwise C_8-EED at layers 2 and 5 for each of the model types.
695 Unsurprisingly, the C_8-CNN has high C_8-equivariance for all layers, whereas both the trained and
696 untrained CNNs have substantially lower C_8-equivariance. Across layers, the channelwise C_8-EED
697 remains fairly constant across datasets for the untrained models. However, the channelwise C_8-EED

for early layers of the trained CNNs differs across datasets (with equivariance on OOD datasets generally being less than the equivariance on the training set MNIST). In later layers, however, the difference in C_8-equivariance between MNIST and an OOD dataset is negligible (Figure 16, right). This suggests that CNNs do learn some minimal amount of equivariance at early layers, but this equivariance either dissipates or becomes undetectable at later layers.

Figure 16: The channelwise C_8-EED for the first two (left) and first five (right) convolutional blocks of a CNN with random weights, a CNN with weights trained on MNIST, and a C_8-CNN with weights trained on MNIST. Error bars indicated 95% confidence intervals.

Figure 17: The softmax C_8-EED after $10,000$ iterations of training on xView maritime for a range of model architectures initialized with either random or pretrained weights generated using ImageNet. The 95% confidence intervals are represented by the black bars.