Generalization Bounds for Equivariant Networks

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Abstract

Equivariant networks capture the inductive bias about the symmetry of the learning task by building those symmetries into the model. In this paper, we study how equivariance relates to generalization error utilizing PAC Bayesian analysis for equivariant networks, where the transformation laws of feature spaces are determined by group representations. By using perturbation analysis of equivariant networks in Fourier domain for each layer, we derive norm-based PAC-Bayesian generalization bounds. The bound characterizes the impact of group size, and multiplicity and degree of irreducible representations on the generalization error and thereby provide a guideline for selecting them. In general, the bound indicates that using larger group size in the model improves the generalization error substantiated by extensive numerical experiments.

1 Introduction

Equivariant networks are widely believed to enjoy better generalization properties than their fully-connected counterparts by including an inductive bias about the invariance of the task. A canonical example is a convolutional layer for which the translation of the input image (over $\mathbb{R}^2$) leads to translation of convolutional features. This construction can be generalized to actions of other groups including rotation and permutation. Intuitively, the inductive bias about invariance and equivariance helps to focus on features that matter for the task, and thereby help the generalization. Recently, many works provide theoretical support for this claim mainly for general equivariant and invariant models. In this work, however, we focus on a class of equivariant neural networks built using representation theoretic tools. As in Shawe-Taylor and Wood [1996], Cohen and Welling [2016b], Weiler et al. [2018a], this approach can build general equivariant networks using irreducible representations of a group. An open question is about how to design feature spaces and combine representations. Besides, the question of impact of these choices on generalization remain. On the other hand, while it is rather well understood how to build a G equivariant model when G is finite, the choice of the group G to consider is not always obvious. Indeed, using a subgroup $H < G$ smaller than G is usually sufficient to achieve significant improvements over a non-equivariant baseline. Moreover, the symmetries G of the data are often continuous, which means G-equivariance can not be built into the model using a group convolution design as in Cohen and Welling [2016a]. In such cases, the most successful approaches approximate it with a discrete subgroup $H < G$, e.g. see Weiler and Cesa [2019] for the $G = O(2)$ case. In addition, the choice of the equivariance group H can affect either the complexity or the expressiveness of the model and, therefore, its generalization capability, depending on how the architecture is adapted. For instance, if one can not freely increase the model size, using a larger group H only increases the parameters sharing but reduces the expressiveness of the model. For this reason, using the whole group G might not be beneficial even when feasible. In that line, we consider how the choice of group size affects generalization.

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Contributions In this paper, we utilize PAC Bayes framework to derive generalization bounds on equivariant networks. Our focus is on equivariant networks built following Weiler et al. [2018a], Cohen and Welling [2016b].

We combine the representation theoretic framework of Weiler and Cesa [2019] with PAC-Bayes framework of Neyshabur et al. [2018] to get generalization bounds on equivariant networks as a function of irreducible representations (irreps) and their multiplicities. Different from previous PAC-Bayes analysis, we derive the perturbation analysis in Fourier domain. Without this approach, as we will show, the naive application of Neyshabur et al. [2018] lead to degenerate bounds. As part of the proof, we derive a tail bound on the spectral norm of random matrices characterized as direct sum of irreps. Note that for building equivariant networks, we need to work with real representations and not complex ones, which are conventionally studied in representation theory. The obtained generalization bound provide new insights about the effect of design choices on the generalization error verified via numerical results. To the best of our knowledge, this is the first generalization bound for equivariant networks with an explicit equivariant structure. We conduct extensive experiments to verify our theoretical insights, as well as some of the previous observations about neural networks.

2 Related Works

Equivariant networks. In machine learning, there has been many works on incorporating symmetries and invariances in neural network design. This class of models has been extensively studied from different perspectives Shawe-Taylor [1993, 1989], Kondor and Trivedi [2018], Cohen et al. [2018], Mallat [2012], Dieleman et al. [2016], Cohen and Welling [2016a,b], Worrall et al. [2017], Weiler et al. [2018b,a], Thomas et al. [2018], Bekkers et al. [2018], Weiler and Cesa [2019], Bekkers [2020], Defferrard et al. [2019], Finzi et al. [2020], Weiler et al. [2021], Cesa et al. [2022] to mention only some. Indeed, the most recent developments in the field of equivariant networks suggest a design which enforces equivariance not only at a global level Laptev et al. [2016] but also at each layer of the model. An interesting question is how a particular choice for designing equivariant networks affect its performance and in particular generalization. A related question is whether including this inductive bias helps the generalization. The authors in Sokolić et al. [2017a] consider general invariant classifiers and obtain robustness based generalization bounds, as in Sokolić et al. [2017b], assuming that data transformation changes the inputs drastically. For finite groups, they reported a scaling of generalization error with $1/\sqrt{|H|}$ where $|H|$ is the cardinality of underlying group. In Elesedy [2022], the gain of invariant or equivariant hypotheses was studied in PAC learning framework, where the gain in generalization is attributed to shrinking the hypothesis space to the space of orbit representatives. A similar argument can be found in Sannai et al. [2021] for permutation groups. The authors in Lyle et al. [2020] use PAC-Bayesian framework to study the effect of invariance on generalization, although do not obtain any explicit bound. Bietti and Mairal [2019] studies the stability of models equivariant to compact groups from a RKHS point of view, relating this stability to a Rademacher complexity of the model and a generalization bound. The authors in Elesedy and Zaidi [2021] provided the generalization gain of equivariant models more concretely and reported VC-dimension analysis. Subsequent works also considered the connection of invariance and generalization Zhu et al. [2021]. In contrast with these models, we consider the equivariant networks with representation theoretic construction. Beyond generalization, we are interested in getting design insights from the bound.

Generalization error for neural networks.

A more general study of generalization error in neural networks, however, has been ongoing for some time with huge body of works on the topic. We refer to some highlights here. A challenge for this problem was brought up in Zhang et al. [2017], where it was shown the generalization error can be arbitrarily large for neural networks, and therefore, any complexity measure for neural networks should be consistent with the above observation. As a result, uniform complexity measures like VC-dimension do not satisfy this requirement as they provide a uniform measure over the whole hypothesis space.

In this light, recent works related the generalization errors to quantities like margin and different norms of weights for example in, among others, Wei and Ma [2019], Sokolić et al. [2017b], Neyshabur et al. [2018], Arora et al. [2018], Bartlett et al. [2017], Golowich et al. [2018], Dziugaite and Roy [2018a], Long and Sedghi [2019], Vardi et al. [2022], Ledent et al. [2021] despite some of these

bounds being vacuous or dimension-dependent (see Jiang et al. [2020] for detailed experimental investigation and Nagarajan and Kolter [2019], Koehler et al. [2021], Negrea et al. [2021]). Class of convolutional neural networks are particularly relevant as they can be considered as a special case of equivariant models. These models are discussed in Pitas et al. [2019], Long and Sedghi [2019], Vardi et al. [2022], Ledent et al. [2021]. We choose PAC Bayesian framework for deriving generalization bounds. There are many works on PAC Bayesian bounds for neural networks Neyshabur et al. [2018], Biggs and Guedj [2022], Dziugaite and Roy [2018b,a], Dziugaite et al. [2020] ranging from randomized and deterministic bounds to choosing priors for non-vacuous bounds. Our method combines the machinery of Neyshabur et al. [2018] with representation theoretic tools.

3 Background

3.1 Preliminaries and notation

We fix some notations first. We consider a classification task with input space $\mathcal{X}$ and output space $\mathcal{Y}$. The input is assumed to be bounded in ℓ_2-norm by B. The data distribution, over $\mathcal{X} \times \mathcal{Y}$, is denoted by $\mathcal{D}$. The hypothesis space, $\mathcal{H}$, consists of all functions realized by a L-layer general neural network with 1-Lipschitz homogeneous activation functions[1]. The network function, $f_{\mathbb{W}}(\cdot)$ with fixed architecture, is specified by its parameters $\mathbb{W} := (\boldsymbol{W}_1, \ldots, \boldsymbol{W}_L)$. The operations on $\mathbb{W}$ are extended from the underlying vector spaces of weights. For any function $f(\cdot)$, the k'th component of the function is denoted by $f(\boldsymbol{x})[k]$ throughout the text. For a loss function $\mathtt{L} : \mathcal{H} \times \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$, the empirical loss is defined by $\hat{\mathcal{L}}(f) := \frac{1}{m}\sum_{i=1}^{m} \mathtt{L}(f, \boldsymbol{x}_i, y_i))$ and the true loss is defined by $\mathcal{L}(f) = \mathbb{E}_{(\boldsymbol{x},y)\sim\mathcal{D}}[\mathtt{L}(f, \boldsymbol{x}, y))]$. For classification, the margin loss is given by

$$\mathcal{L}_\gamma(f_{\mathbb{W}}) = \mathbb{P}_{(\boldsymbol{x},y)\sim\mathcal{D}}\left(f_{\mathbb{W}}(\boldsymbol{x})[y] \leq \gamma + \max_{j\neq y} f_{\mathbb{W}}(\boldsymbol{x})[j]\right). \tag{1}$$

The true loss of a given classifier is then given by $\mathcal{L}(f_{\mathbb{W}}) = \mathcal{L}_0(f_{\mathbb{W}})$. The empirical margin loss is similarly defined and denoted by $\hat{\mathcal{L}}_\gamma$.

In this work, we consider invariance with respect to transformations modeled as the action of a compact group G. See Supplementary A for a brief introduction to group theory and the concepts we will use throughout this paper.

3.2 Equivariant Neural networks

We provide a concise introduction to equivariant networks here with more details given in Supplementary B. Consider an Multi-Layer Perceptron (MLP) with L layers with the layer $l \in [L]$ given by the matrix $\boldsymbol{W}_l \in \mathbb{R}^{c_l \times c_{l-1}}$. The action of the group H on layer l is determined by the group representation ρ_l on $\mathbb{R}^{c_l}$, which is a homomorphism from H to $\mathrm{GL}(\mathbb{R}^{c_l})$ (see B for more details). A group element $h \in H$ linearly transforms the layer l by the matrix $\rho_l(h)$. The matrix $\boldsymbol{W}_l$ is equivariant w.r.t. the representations ρ_l and ρ_{l-1} acting on its input and output iff $\forall h \in H$, we have:

$$\boldsymbol{W}_l \rho_{l-1}(h) = \rho_l(h)\boldsymbol{W}_l \quad .$$

Representation theory provides a way of characterizing equivariant layers using Maschke's theorem and Schur's lemma. The key step is to start from characterizing the irreducible representations (irreps) $\{\psi\}$ of the group H. As we will see, irreps are closely related to generalization of Fourier analysis for functions defined on H. Maschke's theorem implies that the representation ρ_l decomposes into direct sum of irreps as $\rho_l = Q_l \left(\bigoplus_\psi \bigoplus_{i=1}^{m_{l,\psi}} \psi\right) Q_l^{-1}$, where $m_{l,\psi}$ is the number of times the irrep ψ is present in the representation ρ_l. Each ψ is a $\dim_\psi \times \dim_\psi$ matrix, and the direct sum is effectively a block diagonal matrix with irreps ψ on the diagonal. Through this decomposition, we can parameterize equivariant networks in terms of irreps, that is in Fourier space. Defining $\widehat{\boldsymbol{W}}_l = Q_l^{-1}\boldsymbol{W}_l Q_{l-1}$, the equivariance condition writes as

$$\widehat{\boldsymbol{W}}_l \left(\bigoplus_\psi \bigoplus_{i=1}^{m_{l-1,\psi}} \psi\right) = \left(\bigoplus_\psi \bigoplus_{i=1}^{m_{l,\psi}} \psi\right) \widehat{\boldsymbol{W}}_l.$$

[1]The function $\sigma(\cdot)$ is homogeneous if and only if for all $\boldsymbol{x}$ and $\lambda \in \mathbb{R}$, we have $\sigma(\lambda\boldsymbol{x}) = \lambda\sigma(\boldsymbol{x})$.

The block diagonal structure of $\left(\bigoplus_{\psi} \bigoplus_{i=1}^{m_{l,\psi}} \psi\right)$ induces a similar structure on $\widehat{\boldsymbol{W}}_l$. The block (j, i), denoted by $\widehat{\boldsymbol{W}}_l(\psi_2, j, \psi_1, i)$, relates ψ_1 to ψ_2 as:

$$\widehat{\boldsymbol{W}}_l(\psi_2, j, \psi_1, i)\psi_1 = \psi_2 \widehat{\boldsymbol{W}}_l(\psi_2, j, \psi_1, i).$$

Schur's lemma implies that if $\psi_1 \neq \psi_2$, the block needs to be zero to guarantee equivariance. Otherwise, it needs to have one of the three forms in Supplementary B, depending on the *type* of ψ_1. To simplify the notation, we write $\widehat{\boldsymbol{W}}_l(\psi, j, i)$ as $\widehat{\boldsymbol{W}}_l(\psi, j, \psi, i)$. As it is shown in Supplementary B, the matrix $\widehat{\boldsymbol{W}}_l(\psi, j, i)$ can be written as the linear sum

$$\widehat{\boldsymbol{W}}_l(\psi, j, i) = \sum_{k=1}^{c_\psi} \widehat{w_{l,i,j}}(\psi)_k \boldsymbol{B}_{l,\psi,i,j,k} \tag{2}$$

where $\{\widehat{w_{l,i,j}}(\psi)_k\}_{k=1}^{c_\psi}$ are learnable parameters with fixed matrices $\boldsymbol{B}_{l,\psi,i,j,k}$. The value of c_ψ is either 1,2 or 4. The structure of $\boldsymbol{B}_{l,\psi,i,j,k}$ changes according to each type c_ψ. In Supplementary B, we present a version Schur's lemma for real-valued representations rather than complex representations, which is amenable to neural network implementation. Each layer is parameterized by the set of parameters $\widehat{\boldsymbol{w}_{l,i,j}}$. For each layer, there will be $\sum_\psi m_{l,\psi} m_{l-1,\psi} c_\psi$ parameters with $\sum_\psi m_{l,\psi} \dim_\psi = c_l$. Note that, if $\boldsymbol{x}_l = \boldsymbol{W}_l \boldsymbol{x}_{l-1}$, then $\widehat{\boldsymbol{x}}_l = \widehat{\boldsymbol{W}}_l \widehat{\boldsymbol{x}}_{l-1}$, where $\widehat{\boldsymbol{x}}_l = Q_l^{-1} \boldsymbol{x}_l$. The non-linearities should satisfy equivariance condition to have full end-to-end equivariance.

An important question is which representation ρ_l of H should be used for each layer. For the input, the representation is fixed by the input space and its structure. However, the intermediate layers can choose ρ_l by selecting irreps and their multiplicity. We explain how this choice impacts generalization bounds.

4 PAC-Bayesian bound

We derive PAC-Bayes bounds for equivariant networks presented in the previous section. Althouth the proof follows a similar strategy as in Neyshabur et al. [2018], it differs in two important aspects. First, the weights of equivariant MLPs have specific structure requiring reworking proof steps. Second, we carry out the analysis in Fourier domain. In Supplementary E, we also show that naively applying norm-bounds of Neyshabur et al. [2018] cannot explain the generalization behaviour of equivariant networks.

4.1 PAC-Bayesian Bounds for Randomized Networks

The starting point is the PAC-Bayes theorem Langford and Shawe-taylor [2002], McAllester [1998], which provides a generalization bound on randomized classifiers. If the function is chosen randomly from a distribution Q, then the losses are defined as $\mathcal{L}(Q) = \mathbb{E}_{f\sim Q}\mathcal{L}(f)$ and $\hat{\mathcal{L}}(Q) = \mathbb{E}_{f\sim Q}\hat{\mathcal{L}}(f)$. We use the following version from Germain et al. [2009].

Lemma 4.1. *For any hypothesis space $\mathcal{H}$, let P be a probability distribution on $\mathcal{H}$. Then for all $\delta \in (0, 1]$, with probability $1 - \delta$, for all Q on $\mathcal{H}$, we have:*

$$\mathcal{L}(Q) \leq \hat{\mathcal{L}}(Q) + \sqrt{\frac{D(Q\|P) + \log(\xi(m)/\delta)}{2m}}. \tag{3}$$

where $\xi(m) := \sum_{k=0}^{m} \binom{m}{k} (k/m)^k (1 - k/m)^{m-k}$.

In PAC-Bayes vernacular, the distributions P and Q are *a* prior and posterior distribution on $\mathcal{H}$. This indicates that the distribution P and Q are chosen two independent dataset. Choosing an appropriate prior plays a central role in getting non-vacuous bounds. The lemma provides immediately a generalization bound for randomized equivariant classifiers. The hypothesis space is parametrized by all $\widehat{\boldsymbol{w}_{l,i,j}}$. We work with a prior distribution P chosen as zero-mean normal with covariance matrix $\sigma^2 \boldsymbol{I}$ over the parameters. The posterior Q is chosen as normal distribution with the final parameters $\widehat{\boldsymbol{w}_{l,i,j}}$ as mean value and the same covariance matrix $\sigma^2 \boldsymbol{I}$. The KL-divergence in the PAC-Bayesian theorem is then given by:

$$D(Q\|P) = \frac{\sum_{l,j,i} \|\widehat{\boldsymbol{w}_{l,i,j}}\|_2^2}{2\sigma^2}. \tag{4}$$

The generalization bound depends depends on thr sum of the norm of kernels. In the next step, we de-randomize the bound.

4.2 De-Randomization and Perturbation Bounds

Our de-randomization technique follows closely that of Neyshabur et al. [2018]. We provide the sketch of derivations here, and the full proof is relegated to the supplementary materials. To de-randomize the previous bound, a common step is to choose Q such that the probability of margin violation is controlled. Let $\mathcal{S}_{\mathbb{W}}$ be defined as:

$$\mathcal{S}_{\mathbb{W}} := \{h \in \mathcal{H} : \|h - f_{\mathbb{W}}\|_{\infty} \leq \gamma/4\}. \tag{5}$$

Any function on this set can change the margin of $f_{\mathbb{W}}$ at most by $\gamma/2$. Therefore, for any h, $\mathcal{L}(f_{\mathbb{W}}) \leq \mathcal{L}_{\gamma/2}(h)$, which implies $\mathcal{L}(f_{\mathbb{W}}) \leq \mathcal{L}_{\gamma/2}(Q)$ if Q is supported only on this set. Similarly $\hat{\mathcal{L}}_{\gamma/2}(Q) \leq \hat{\mathcal{L}}_{\gamma}(f_{\mathbb{W}})$. To choose Q, first, we characterize the output perturbation of equivariant networks for a given input perturbation. Next, we determine the variance σ such that the output perturbation is bounded by $\gamma/4$ with probability[2] $1/2$. The first step is the perturbation analysis.

Lemma 4.2 (Perturbation Bound)**.** *For a neural network $f_{\mathbb{W}}(\cdot)$ with input space of ℓ_2-norm bounded by B, and for any weight perturbations $\mathbb{U} = (\boldsymbol{U}_1, \ldots, \boldsymbol{U}_L)$, we have:*

$$\|f_{\mathbb{W}+\mathbb{U}}(\boldsymbol{x}) - f_{\mathbb{W}}(\boldsymbol{x})\|_2 \leq eB \left(\prod_{i=1}^{L} \|\boldsymbol{W}_i\|_2 \right) \sum_{i=1}^{L} \frac{\|\boldsymbol{U}_i\|_2}{\|\boldsymbol{W}_i\|_2}. \tag{6}$$

For equivariant networks, where the weights are parameterized as in eq. 2, the spectral norm of the perturbation $\boldsymbol{U}_l$ is bounded as

$$\|\boldsymbol{U}_l\|_2 \leq \sqrt{\max_{\psi} \max_{1 \leq i \leq m_{l-1,\psi}} m_{l-1,\psi} \frac{1}{\dim_{\psi}} \sum_{j=1}^{m_{l,\psi}} \left\| \widehat{\boldsymbol{U}_l}(\psi, j, i) \right\|_F^2} \tag{7}$$

The first inequality is already given in Neyshabur et al. [2015]. The inequality 18 will be shown in supplementary materials.

The perturbation bound already suggests the benefit of equivariant Kernels. As it will be shown in Supplementary materials, the equivariant kernels w.r.t. ψ satisfy

$$\|\boldsymbol{W}\|_2 = \frac{1}{\sqrt{\dim_{\psi}}} \|\boldsymbol{W}\|_F, \tag{8}$$

which is the smallest possible norm (compare with general relation for $\dim_{\psi} \times \dim_{\psi}$ matrices: $\|\boldsymbol{W}\|_2 \geq \frac{1}{\sqrt{\dim_{\psi}}} \|\boldsymbol{W}\|_F$). Therefore, the term $\frac{1}{\dim_{\psi}} \left\| \widehat{\boldsymbol{U}_l}(\psi, j, i) \right\|_F^2$ in the perturbation bound is already tight.

The perturbation bound helps defining a posterior Q by adding zero-mean Gaussian perturbations $\widehat{u_{l,i,j}}(\psi)_k$ of variance σ^2 to the learnable parameters $\widehat{w_{l,i,j}}(\psi)_k$. The output perturbation is given by the above theorem in terms of norm of $\boldsymbol{U}_i$. The following lemma controls the norm of this random matrix, and thereby the output perturbation.

Lemma 4.3. *Consider a random equivariant matrix $\boldsymbol{U}_l$ defined by i.i.d. Gaussian $N(0, \sigma^2)$ choice of $\widehat{u_{l,i,j}}(\psi)_k$ in eq. 2. We have:*

$$\mathbb{P}\left(\|\boldsymbol{U}_l\|_2 \geq \sigma \sqrt{\max_{\psi} (5 m_{l-1,\psi} m_{l,\psi} c_{\psi} t)} \right) \leq \left(\sum_{\psi} m_{l,\psi} \right) e^{-t} \tag{9}$$

The proof is given in supplementary materials. With Lemma 4.3, we can choose the variance σ^2 such that the output perturbation does not violate the intended margin. Using an union bound over all

[2] This value can be changed to any probability with proper adjustments. See the supplementary materials.

layers, one finds that by choosing $t = \log\left(2\sum_l \sum_\psi m_{l,\psi}\right)$, with probability at least $\frac{1}{2}$ the following inequality holds for every layer $l \in [L]$:

$$\|\boldsymbol{U}_l\|_2 < \sigma\sqrt{\max_\psi 5 m_{l-1,\psi} m_{l,\psi} c_\psi}\sqrt{\log\left(2\sum_l \sum_\psi m_{l,\psi}\right)} \tag{10}$$

We can use this bound jointly with the perturbation bound eq. 6 to choose σ such that the margin is below $\gamma/4$ with high probability. Note that σ is then chosen as a function of learned weights, which cannot be the case because of the nature of prior. A trick for circumventing this issue is to select many priors that can adequately cover the space of possible weights, and take the union bound over it. We present the details in the supplementary materials. The bound for equivariant networks is given below.

Theorem 4.4 (Homogeneous Bounds for Equivariant Networks)**.** *For any equivariant network, with probability $1-\delta$, we have:*

$$\mathcal{L}_{\mathcal{D}}(f_{\mathbb{W}}) \leq \hat{\mathcal{L}}_\gamma(f_{\mathbb{W}}) + \tag{11}$$

$$\sqrt{\frac{32e^4 B^2 \beta^{2L}}{\gamma^2 m \eta}\left(\sum_{l=1}^{L}\sqrt{M(l,\eta)}\right)^2\left(\sum_l \frac{\sum_{\psi,i,j}\left\|\widehat{\boldsymbol{W}}_l(\psi,i,j)\right\|_F^2 / \dim_\psi}{\|\boldsymbol{W}_l\|_2^2}\right) + \frac{\log(\xi(m)\frac{Lm^{1+1/2L}}{\delta})}{2\gamma^2 m}} \tag{12}$$

where $\beta = \left(\prod_l \|\boldsymbol{W}_l\|_2\right)^{1/L}$, and

$$M(l,\eta) := \log\left(\frac{\sum_{l=1}^{L}\sum_\psi m_{l,\psi}}{1-\eta}\right)\max_\psi\left(5 m_{l-1,\psi} m_{l,\psi} c_\psi\right). \tag{13}$$

The proof of the theorem is given in Supplementary C, where we also consider special cases of this generalization bound for group convolutional networks Cohen and Welling [2016a] where regular representations are used..

Discussions. The above generalization bound contains the term $M(l,\eta)$, which encodes the multiplicity and type of used irreps. Let the hidden layer dimension $c_l = \sum_\psi \dim_\psi m_{l,\psi}$ be fixed. For Abelian groups, all real irreps are 2-dimensional, therefore, we have:

$$M(l,\eta) = \log\left(\frac{\sum_{l=1}^{L} c_l}{2(1-\eta)}\right)\max_\psi\left(5 m_{l-1,\psi} m_{l,\psi} c_\psi\right).$$

The bound can be controlled further by appropriate choice of $m_{l-1,\psi}, m_{l,\psi}, c_\psi$, which favors smaller multiplicity and type c_ψ. Therefore using different irreps is better. For non-abelian cases, irreps can have larger $\dim_\psi$, which keeping the layer dimension c_l fixed, amounts to smaller multiplcity. This can improve the sum $\sum_{l=1}^{L}\sum_\psi m_{l,\psi}$ in $M(l,\eta)$ too. This also indicates a potential improved generalization for non-abelian groups. For dihedral groups, which is in general non-abelian, the real irreps are also two dimensional, however, of type $c_\psi = 1$. As we will see, they provide slightly better generalization compared to the cyclic groups. Note that for finite groups, there is a connection between irrep degrees and group order $|H| = \sum_\psi \dim_\psi^2 / c_\psi$. The impact of group size manifests itself in the whole generalization error term. We numerically verify this in the experimental results.

5 Experiments

We also validate the theoretical insights derived in the previous sections with an extensive experimental study. We include all details about the experiments together with the results found in Supplementary F. In particular, we use four different types of datasets, including natural images and synthetic data. In all experiments we consider data symmetries G which are subgroups of the

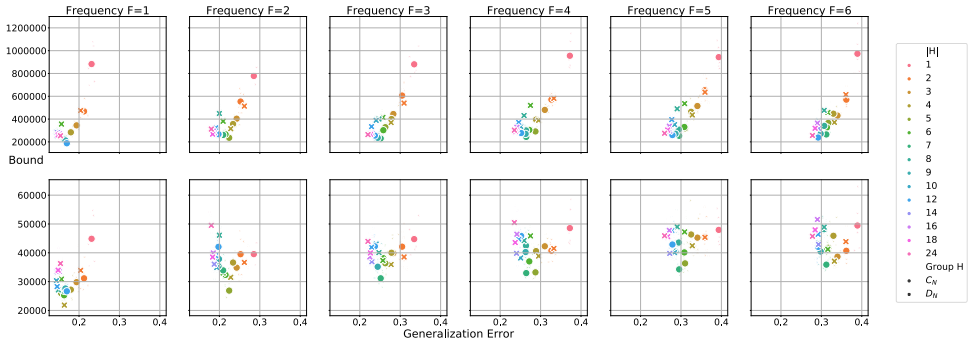


Figure 1: Comparison between the bound in Theorem 4.4 (1st row) and the one in Supplementary E (2nd row) on the synthetic $\mathrm{O}(2)$ datasets with different frequencies. The bound from Supplementary E clearly does not capture the effect of group equivariance.

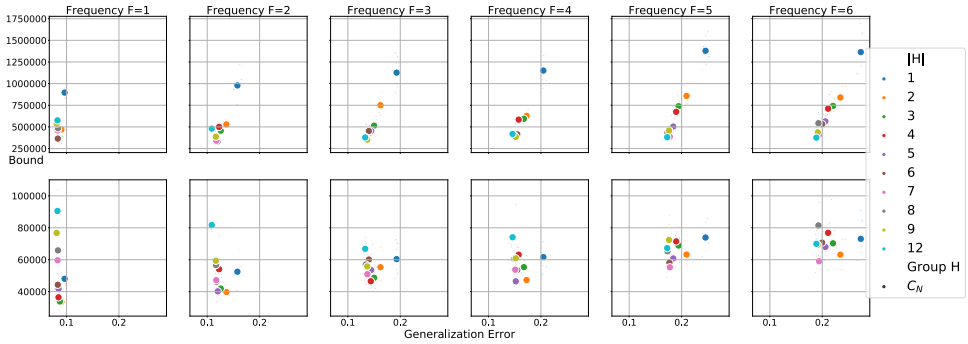
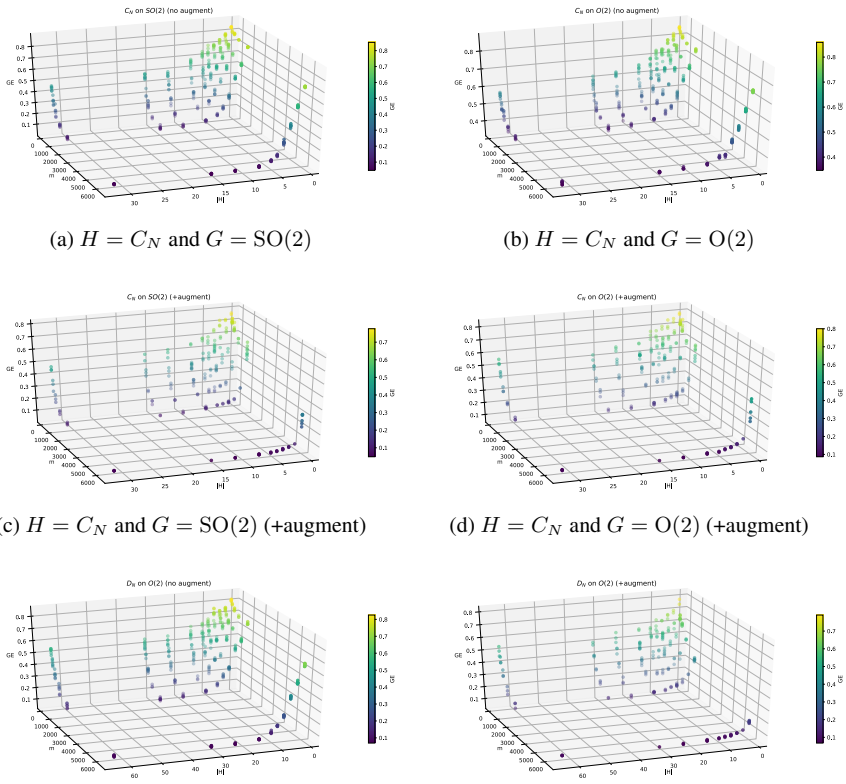


Figure 2: Comparison between Theorem 4.4 (1st row) and the one in Supplementary E (2nd row) on the synthetic $\mathrm{SO}(2)$ datasets.

group $\mathrm{O}(2)$ of planar rotations and reflections. This includes a number of finite/continuous and commutative/non-commutative groups, in particular C_N (N rotations), D_N (N rotations and reflections), $\mathrm{SO}(2)$ (continuous planar rotations) and $\mathrm{O}(2)$ itself (see Supplementary A). Moreover, all models are based on group convolution over a finite subgroup $H < G$. This means that the features at layer l have shape $|H| \times c_l^H$; see Section **??** and supplementary materials. For each layer l, we keep the total number of features (approximatively) constant when changing the group H. Models are trained until 99% of the training set is correctly classified with at least a margin γ. We used $\gamma = 10$ in the synthetic datasets and $\gamma = 2$ in the image ones.

First, we compare our result with the bound derived in Supplementary E using naive application of Neyshabur et al. [2018]. In Fig. 1 and Fig. 2 we compare these two bounds on 6 synthetic datasets with $\mathrm{O}(2)$ and $\mathrm{SO}(2)$ symmetries (one per column). Each dataset lives on high dimensional tori and $\mathrm{O}(2)$ (or $\mathrm{SO}(2)$) rotates the circles composing them, possibly with different frequencies; we consider different maximum frequencies $F \in \{1, 2, \dots, 6\}$ in the experiments; see Supplementary F for more details. The results in Fig. 1 and 2 indicate that the bound built using the strategy from Neyshabur et al. [2018] can not explain the effect of equivariance on generalization. Conversely, the bound in Theorem 4.4 which uses the parametrization in the Fourier domain correlates with the measured generalization error, suggesting that it can account for the effect of different groups on generalization. In addition, note that it also correlates with the saturation effect observed when using larger discrete groups H to approximate the continuous group $G = \mathrm{O}(2)$. Indeed, on low frequency datasets the bound tends to saturate faster as we increase the group size $|H|$. Conversely, on high frequency datasets, choosing a larger group H results in larger improvements in the estimated bound.

In Fig. 7 we perform a larger study on the transformed MNIST datasets to investigate the simultaneous effect of the group size $|H|$, data augmentation and training set size m. These figures highlight the



(a) $H = C_N$ and $G = \mathrm{SO}(2)$

(b) $H = C_N$ and $G = \mathrm{O}(2)$

(c) $H = C_N$ and $G = \mathrm{SO}(2)$ (+augment)

(d) $H = C_N$ and $G = \mathrm{O}(2)$ (+augment)

(e) $H = D_N$ and $G = \mathrm{O}(2)$)

(f) $H = D_N$ and $G = \mathrm{O}(2)$ (+augment)

Figure 3: Generalization Error (GE) of different H-equivariant models ($H = C_N$ or $H = D_N$) on different G-MNIST datasets ($G = \mathrm{SO}(2)$ or $G = \mathrm{O}(2)$) for different training set sizes m.

fact that the benefit of using a larger equivariance group H is greater on smaller datasets. Additionally, note that in these cases the effect of data augmentation alone is not particularly beneficial. Moreover, it can be seen that Dihedral groups provide slightly better generalization error.

6 Conclusion

We provided learning theoretic frameworks to study the effect of invariance and equivariance on the generalization error and provide guidelines for design choices. The obtained bounds provide useful insights and guidelines for understanding these architectures. As limitation of our work, we show experimentally in supplementary materials that the obtained bounds do not decrease with larger training sizes m as expected. Nevertheless, for a fixed training set, the trend of the generalization bound correlates with the generalization error.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes]
   (c) Did you discuss any potential negative societal impacts of your work? [Yes]
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes]
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [No] The code and the data are proprietary
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes]
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] We have scatter plots of points from each run.
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [No]
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5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
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