# Symmetries in PAC-Bayesian Learning

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#### Abstract

Symmetries are known to improve the empirical performance of machine learning models, yet theoretical guarantees explaining these gains remain limited. Prior work has focused mainly on compact group symmetries and often assumes that the data distribution itself is invariant, an assumption rarely satisfied in real-world applications. In this work, we extend generalization guarantees to the broader setting of non-compact symmetries, such as translations and to non-invariant data distributions. Building on the PAC-Bayes framework, we adapt and tighten existing bounds, demonstrating the approach on McAllester's PAC-Bayes bound while showing that it applies to a wide range of PAC-Bayes bounds. We validate our theory with experiments on a rotated MNIST dataset with a non-uniform rotation group, where the derived guarantees not only hold but also improve upon prior results. These findings provide theoretical evidence that, for symmetric data, symmetric models are preferable beyond the narrow setting of compact groups and invariant distributions, opening the way to a more general understanding of symmetries in machine learning.

# 1 INTRODUCTION

Many real-world machine learning tasks exhibit inherent symmetric structures. For instance, in image classification, semantic labels remain unchanged under transformations such as rotations, reflections, or translations. Models that explicitly capture such symmetries typically outperform those that do not, as demonstrated empirically in prior work [6]. Early theoretical frameworks as, for example, in [20] and [11] have analyzed the advantages of incorporating symmetry into models, focusing on compact symmetry groups and data distributions that are invariant under these transformations. However, the assumptions of compact symmetries and invariant data distributions may not hold in many practical scenarios. Real-world data often exhibit more complex or non-compact symmetries. For example, the non-compact group of translations is an important class of symmetries that achieved a tremendous boost in performance through convolutional neural networks in domains such as image recognition [3]. Further the underlying distributions may vary under these transformations, illustrated by the example of rotations and the fact that a filled cup cannot appear upside-down in the real world.

In this work, we analyze models under general non-compact and non-uniform symmetry using a PAC-Bayesian Learning approach. Our framework delivers the theoretical foundations and guarantees for the, in practice, oftentimes reported and improved performance of models that exploit symmetry of the data. Exemplarily, our theoretical findings are supported by a numerical experiment that evaluates the PAC-Bayesian bound explicitly.

To the best of our knowledge, since the group of translations is non-compact, we provide the first PAC-Bayesian generalization bounds that explain the practical benefit and success of convolutional neural networks, which are translation invariant.

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#### 1.1 Related Work

The PAC-Bayes framework provides a powerful tool for deriving generalization guarantees. Early work by McAllester [24] laid the foundations for PAC-Bayes bounds, which were later refined to produce sharper and more robust guarantees for supervised classification tasks by Catoni [5]. Several well-known results provide concrete bounds e.g. [26, 17, 12, 22], and more recent work has explored non-vacuous or compression-based bounds for deep neural networks [2, 30, 9]. For an accessible overview of and introduction to PAC-Bayes theory, we refer the reader to [1].

Beyond purely theoretical guarantees, symmetries in machine learning models have been shown to confer practical benefits. Group-equivariant convolutional networks (G-CNNs) [6, 7] generalize standard convolutional layers to exploit symmetries in the data, leading to improved sample efficiency and robustness even when the data distribution is not strictly invariant. Steerable CNNs [8, 29] extend this approach by allowing more flexible equivariant mappings, and practical implementations [28, 4, 25] demonstrate the relevance of symmetries not only in computer vision but also in domains like physics, where symmetries arise naturally.

Several recent works provide theoretical analyses of symmetries in machine learning. [19, 20] established PAC-Bayesian generalization results for models with finite or compact group symmetries. [11, 10] studied the benefits of symmetry in compact groups from both the classical PAC and generalization perspectives, providing strict generalization benefits. [16] further formalized the necessity of convolutional structure for equivariance under compact groups. Together, these results provide a strong theoretical foundation for understanding the advantage of symmetric models under idealized conditions.

In contrast to prior analyses, our work extends these guarantees to non-compact symmetries such as translations, and to non-invariant data distributions, conditions that are more representative of practical scenarios. Within the PAC-Bayes framework, we adapt and tighten existing bounds, providing theoretical evidence that symmetry can improve generalization beyond the commonly assumed compact and invariant settings.

#### 1.2 Preliminaries and Notations

Let  $(\Omega, \mathcal{F}, \mathbb{P})$  denote the underlying probability space, which is assumed to be rich enough for the following analysis. Let X and Y be real-valued random variables. We write  $X \stackrel{d}{=} Y$  to indicate that X and Y are equal in distribution, meaning that their probability laws coincide  $\mathbb{P}(X \leq t) = \mathbb{P}(Y \leq t)$  for all  $t \in \mathbb{R}$ . We consider two standard Borel spaces  $(\mathcal{X}, \mathcal{X})$  as the input space and  $(\mathcal{Y}, \mathcal{Y})$  as the output space, where  $\mathcal{Y} \subset \mathbb{R}$ . Throughout,  $(\mathcal{G}, \cdot)$  will be an arbitrary topological group, whose Borel  $\sigma$ -algebra makes it a standard Borel space. The group  $\mathcal{G}$  acts measurably on the input space  $\mathcal{X}$  via the map  $\varphi \colon \mathcal{G} \times \mathcal{X} \to \mathcal{X}$  and on the output space  $\mathcal{Y}$  via  $\psi \colon \mathcal{G} \times \mathcal{Y} \to \mathcal{Y}$ . For convenience, we adopt the shorthand notation  $g \cdot x := \varphi(g, x)$  and  $g \cdot y := \psi(g, y)$ . Although the same symbol · is used for both actions, it is important to note that they may represent distinct group actions on  $\mathcal{X}$  and  $\mathcal{Y}$ , the intended meaning will be clear from context. In the following we denote the set of measurable functions by  $\mathcal{M}(\mathcal{X}, \mathcal{Y}) := \{f : \mathcal{X} \to \mathcal{Y} : f \text{ is measurable}\}$ , equipped with the evaluation  $\sigma$ -algebra  $\mathcal{M}$ . Let the hypothesis class  $\mathcal{H} \subset \mathcal{M}(\mathcal{X}, \mathcal{Y})$  be a subset of the measurable functions, and assume that it is a Polish space. Each element  $f \in \mathcal{H}$  is called a hypothesis function. A hypothesis function  $f \in \mathcal{H}$  is said to be equivariant, if  $f(g \cdot x) = g \cdot f(x)$  holds for all  $g \in \mathcal{G}$  and  $x \in \mathcal{X}$ . An equivariant hypothesis function  $f \in \mathcal{H}$ is called invariant if the group acts trivially on the output space  $\mathcal{Y}$ , meaning  $g \cdot y = y$  for all  $g \in \mathcal{G}$  and  $y \in \mathcal{Y}$ . In this case, the equivariance condition reduces to  $f(x) = f(g \cdot x)$  for all  $g \in \mathcal{G}$  and  $x \in \mathcal{X}$  so that invariance can be seen as a special case of equivariance where the output remains unchanged under the group action. In the following we will focus on the equivariant case, which also captures the invariant case. We denote by  $\mathcal{X}_{\varphi}$  a set of representatives of the quotient  $\mathcal{X}/\mathcal{G}$ , that is a set containing exactly one representative from each orbit. Let X be a random element taking values in the input space  $\mathcal X$  and Y a random element in the output space on  $\mathcal{Y}$ . We define a loss function as a measurable function  $\ell \colon \mathcal{Y} \times \mathcal{Y} \to [0, \infty)$ . Given a loss function, the (expected) risk  $\mathcal{R}_{\ell}$  is defined as

$$\mathcal{R}_{\ell} \colon \mathcal{H} \to [0, \infty), \quad \mathcal{R}_{\ell}(f) := \mathbb{E}[\ell(f(X), Y)].$$
 (1)

The empirical risk  $\hat{\mathcal{R}}_{\ell}$  of a measurable function f and a set of points  $\{(x_i, y_i)\}_{i=1}^n \in (\mathcal{X} \times \mathcal{Y})^n$  is given by

$$\hat{\mathcal{R}}_{\ell} \colon \mathcal{H} \times \bigcup_{n \in \mathbb{N}} (\mathcal{X} \times \mathcal{Y})^n \to [0, \infty) \,, \qquad \hat{\mathcal{R}}_{\ell} \left( f, \{ x_i, y_i \}_{i=1}^n \right) = \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i) \,. \tag{2}$$

To simplify notation for integration, we adopt the following shorthand for integrals, given a probability distribution  $\mathbb{Q}$  on a measurable space  $(\mathcal{E}, \mathcal{E})$  and an integrable function  $f: \mathcal{E} \to \mathbb{R}$ , we write

$$\mathbb{Q}[f] := \int_{\mathcal{E}} f(x) \, \mathbb{Q}(dx) \,. \tag{3}$$

Furthermore, let  $\mu$  and  $\nu$  be a probability measures on a measurable space  $(\mathcal{T}, \mathfrak{I})$ . We denote absolute continuity of  $\nu$  with respect to  $\mu$  by  $\nu \ll \mu$ . Let  $\pi \colon \mathcal{T} \to \mathcal{S}$  be a measurable function, where  $(\mathcal{S}, \mathcal{S})$  is another measurable space, then  $\pi_*\mu$  denotes the pushforward measure of  $\mu$  under  $\pi$ , defined by  $\pi_*\mu(B) = \mu(\pi^{-1}(B))$  for all measurable  $B \subset \mathcal{S}$ . A measurable space  $(\mathcal{T}, \mathcal{I})$  is called a standard Borel space if it is Borel isomorphic to a Polish space equipped with its Borel  $\sigma$ -algebra. That is, there exists a Polish space  $(\mathcal{Z}, \mathcal{B}(\mathcal{Z}))$  and a bijection  $\phi \colon \mathcal{T} \to \mathcal{Z}$  such that both  $\phi$  and  $\phi^{-1}$  are measurable. Lastly, we define the Kullback–Leibler (KL) divergence between two probability distributions  $\mu$  and  $\nu$  on a measurable space  $(\mathcal{S}, \mathcal{S})$  as

$$D_{\mathrm{KL}}(\mu \| \nu) := \begin{cases} \int_{\mathcal{S}} \log \left( \frac{d\mu}{d\nu}(s) \right) \, \mu(ds), & \quad \text{if } \mu \ll \nu \; ; \\ \infty, & \quad \text{otherwise} \, , \end{cases}$$

where  $\frac{d\mu}{d\nu}$  denotes the Radon-Nikodym derivative.

Having introduced the necessary notation, we now present the Disintegration Theorem and a well-known standard PAC-Bayesian bound due to McAllester. The Disintegration Theorem provides a way to decompose a joint probability measure into its marginal and a probability kernel. This result is fundamental for defining conditional distributions on general measurable spaces and underlies many constructions in probability theory and statistical learning.

**Theorem 1.1.** [13, Theorem 3.4] Let (S, S) and (T, T) be measurable spaces, where T is Borel. Let  $\mu$  be a probability measure on  $S \times T$ . Then  $\mu = \mu_S \otimes \kappa$ , where  $\mu_S \equiv \mu(\cdot \times T)$  is the marginal and  $\kappa : S \to T$  is a probability kernel. Further,  $\kappa$  is unique  $\mu_S$  a.e.

A probability kernel from (S, S) to (T, T) is a mapping  $\kappa : S \times T \to [0, 1]$  such that  $\kappa(s, \cdot)$  is a probability measure on (T, T) for each  $s \in S$ , and  $\kappa(\cdot, B)$  is S-measurable for each  $B \in T$ . Intuitively,  $\kappa(s, \cdot)$  describes a conditional distribution given s.

The PAC-Bayesian bound due to McAllester will serve as a baseline example to demonstrate how incorporating symmetries can lead to improved generalization guarantees. While our focus is on this particular result, the method we develop for exploiting symmetry applies analogously to a broader class of PAC-Bayesian bounds.

**Theorem 1.2.** [23] For any measurable loss function  $\ell$  and any distribution  $\mathbb{Q}$  on  $\mathcal{H}$ 

$$\mathbb{Q}[\mathcal{R}_{\ell}] \leq \mathbb{Q}[\hat{\mathcal{R}}_{\ell}(\cdot, S_n)] + \sqrt{\frac{D_{\mathrm{KL}}(\mathbb{Q}||\mathbb{P}_H) + \log\frac{1}{\delta} + \log n + 2}{2n - 1}}$$

holds with probability of at least  $1 - \delta$ , where  $S_n = \{X_i, Y_i\}_{i=1}^n$  are n i.i.d. copies of (X, Y).

As a technical tool, we next recall a result from prior work by [20] that establishes a relationship between the KL divergence of two measures and that of their pushforwards under measurable maps.

**Lemma 1.3.** [20] Suppose that (S, S) and (T, T) are two measurable spaces and T is standard Borel. Let  $\mu$  and  $\nu$  be two probability measures on (S, S) with  $\mu \ll \nu$  and  $\alpha \colon (S, S) \to (T, T)$  is a measurable map. Then

$$D_{\mathrm{KL}}(\mu \| \nu) = D_{\mathrm{KL}}(\alpha_* \mu \| \alpha_* \nu) + \int_{\mathcal{S}} \log \left( \frac{\frac{d\mu}{d\nu}(s)}{\frac{d\alpha_* \mu}{d\alpha_* \nu}(\alpha(s))} \right) \mu(ds), \tag{4}$$

where  $\frac{d\mu}{d\nu}$  and  $\frac{d\alpha_*\mu}{d\alpha_*\nu}$  are the Radon-Nikodym derivatives. In particular, it holds that

$$D_{\mathrm{KL}}(\mu \| \nu) \ge D_{\mathrm{KL}}(\alpha_* \mu \| \alpha_* \nu). \tag{5}$$

# 2 SYMMETRY IN HYPOTHESIS CLASS

In this section, we improve the PAC-Bayesian bound of McAllester in Theorem 1.2 by exploiting symmetries in the class of hypothesis functions. While for illustrative purpose, we focus on the formulation of McAllester, the approach extends to other PAC-Bayesian bounds as, for example, the well known bounds form [21], [27] or [5]. This first main result relies on a precise control of the effect of equivariance for the KL divergence between two measures. For this purpose, we introduce an averaging operator that maps arbitrary measurable functions to equivariant ones and apply the KL decomposition from Lemma 1.3 to the averaging operator. While this seems to be formally trivial, the detailed derivation of the conditions of the Lemma 1.3 is not and is postponed to the Appendix B for the reader's convenience.

Before introducing the averaging operator, we require additional assumptions to ensure that it is well-defined. Since  $\varphi$  defines the group action on the input space, it is surjective. Restricting  $\varphi$  to a set of representatives for the group orbits  $\mathcal{X}_{\varphi} \subset \mathcal{X}$  modulo the stabilizers stab $(x_{\varphi}) \subset \mathcal{G}$ , it becomes injective. Consequently the map

$$\overline{\varphi}_{|\mathcal{G}\times\mathcal{X}_{\varphi}}\colon (\mathcal{G}\times\mathcal{X}_{\varphi})/\!\sim\,\to\,\mathcal{X}$$

is a bijection, where two pairs are consider to be equivalent  $(g_1, x_1) \sim (g_2, x_2)$  if and only if  $x_1 = x_2$  and  $g_1 \cdot x_1 = g_2 \cdot x_2$ . The quotient space can also be consider as the disjoint union  $\dot{\cup}_{x_{\varphi} \in \mathcal{X}_{\varphi}} \mathcal{G}/\operatorname{stab}(x_{\varphi})$ , where  $\operatorname{stab}(x_{\varphi})$  denotes the stabilizer subgroup. The map  $\overline{\varphi}_{|\mathcal{G} \times \mathcal{X}_{\varphi}}$  is measurable when the quotient is equipped with the corresponding quotient  $\sigma$ -algebra. For simplicity, we assume in the following, that the action of  $\mathcal{G}$  on  $\mathcal{X}$  is free. For free actions on  $\mathcal{X}$ , the restricted map  $\varphi_{|\mathcal{G} \times \mathcal{X}_{\varphi}} : \mathcal{G} \times \mathcal{X}_{\varphi} \to \mathcal{X}$  is a bijection. The inverse is expressed in the terms of the projections  $\pi_{\mathcal{X}_{\varphi}} : \mathcal{X} \to \mathcal{X}_{\varphi}$  and  $\pi_{\mathcal{G}} : \mathcal{X} \to \mathcal{G}$  and is given by  $\varphi^{-1}(x) = (\pi_{\mathcal{X}_{\varphi}}, \pi_{\mathcal{G}})$ . The inverse  $\varphi^{-1}$  of the measurable map  $\varphi_{|\mathcal{G} \times \mathcal{X}_{\varphi}}$  between standard Borel spaces is measurable by [14, Corollary 15.2].

**Assumption 2.1.** 1. The group  $\mathcal{G}$  acts measurably on the input space  $\mathcal{X}$  via the map  $\varphi \colon \mathcal{G} \times \mathcal{X} \to \mathcal{X}$  and on the output space  $\mathcal{Y}$  via  $\psi \colon \mathcal{G} \times \mathcal{Y} \to \mathcal{Y}$ .

2. The action of  $\mathcal{G}$  on  $\mathcal{X}$  is free, i.e., the stabilizers are trivial  $\mathrm{stab}(x) = \{e_{\mathcal{G}}\}\$ for all  $x \in \mathcal{X}$ .

The following averaging operator turns an arbitrary hypothesis function into an equivariant one by integrating the evaluation of the hypothesis function over the groups' orbit with respect to the conditional distribution of the group given the representative of the respective orbit.

**Definition 2.2.** The averaging operator  $\mathcal{Q}: \mathcal{M}(\mathcal{X}, \mathcal{Y}) \to \mathcal{M}(\mathcal{X}, \mathcal{Y})$  is defined by

$$\mathcal{Q}(f)(x) := \pi_{\mathcal{G}}(x) \cdot \int_{\mathcal{G}} g^{-1} \cdot f\left(g \cdot \pi_{\mathcal{X}_{\varphi}}(x)\right) \, \kappa(\pi_{\mathcal{X}_{\varphi}}(x), dg) \,,$$

where  $\kappa \colon \mathcal{X}_{\varphi} \to \mathcal{G}$  is the probability kernel from the Disintegration Theorem 1.1.

Remark 2.3. The name "averaging operator" comes from the special case

$$Q_{\text{old}}(f)(x) = \int_{\mathcal{G}} g^{-1} \cdot f(g \cdot x) \,\lambda(dg) \,, \tag{6}$$

which appears in prior work, for example, [20] and [11]. In these works, the group  $\mathcal{G}$  is assumed to be compact and the random element X is assumed to be  $\mathcal{G}$ -invariant, i.e.,  $\mathbb{P}_X(B) = \mathbb{P}_X(g \cdot B)$  for all  $g \in \mathcal{G}$  and measurable  $B \subset \mathcal{X}$ . Under these assumptions, X admits a factorization of the form  $X \stackrel{d}{=} \varphi(G, X_{\varphi})$ , where  $X_{\varphi}$  is a random element on the representatives  $\mathcal{X}_{\varphi}$  and G is an independent random element distributed on the group  $\mathcal{G}$ . Additionally, the  $\mathcal{G}$ -invariance assumption yields that the random element G is uniformly distributed, i.e.,  $\mathbb{P}_G = \lambda$  the normalized Haar measure. This implies that the conditional distribution given by the probability kernel  $\kappa(\pi_{\mathcal{X}_{\varphi}}(x), \cdot)$  is  $\mathbb{P}_X$ -almost surely equal to the Haar measure  $\lambda$  for any  $x \in \mathcal{X}$ . Moreover, since  $\mathcal{Q}(f)$  is equivariant, as we will prove in the Appendix B, the averaging operator introduced in Definition 2.2 reduces to the standard averaging operator (6). Our formulation removes the restriction to compact groups and the distribution of G no longer needs to be invariant. This broadens the applicability to important non-compact groups, such as the group of translations.

In the Appendix B, we provide the details for showing that the averaging operator is well-defined, i.e., it maps measurable functions to equivariant measurable functions, and acts like a projection onto the respective subset

of equivariant functions. This justifies the application of Lemma 1.3 to the averaging operator. In order to study a restricted class of hypothesis functions  $\mathcal{H}$ , e.g., neural networks with a certain architecture, we assume that the hypothesis class is closed under the averaging operator, which is a reasonable assumption in practice, as we are typically interested in the equivariant versions of a given model, rather than arbitrary equivariant functions.

**Assumption 2.4.** The hypothesis class  $\mathcal{H}$  is closed under the averaging operator  $\mathcal{Q}$ , i.e., for all  $f \in \mathcal{H}$ ,  $\mathcal{Q}(f) \in \mathcal{H}$ .

The following KL decomposition separates the divergence between two probability measures into two components: the divergence between their equivariant portions and a remainder term capturing the non-equivariant "orthogonal" component. The remainder quantifies the portion of the KL divergence lost when projecting the measures onto the space of equivariant functions, corresponding to differences that are not preserved under the symmetry.

**Theorem 2.5.** Suppose Assumptions 2.1 and 2.4 hold. Let  $\mu$  and  $\nu$  be two probability measures on  $(\mathcal{H}, \mathcal{H})$  with  $\mu \ll \nu$ . Then

$$D_{\mathrm{KL}}(\mu \| \nu) = D_{\mathrm{KL}}(\mathcal{Q}_* \mu \| \mathcal{Q}_* \nu) + \int_{\mathcal{H}} \log \left( \frac{\frac{d\mu}{d\nu}(f)}{\frac{d\mathcal{Q}_* \mu}{d\mathcal{Q}_* \nu}(\mathcal{Q}(f))} \right) \mu(df), \tag{7}$$

where  $\frac{d\mu}{d\nu}$  and  $\frac{dQ_*\mu}{dQ_*\nu}$  are the Radon-Nikodym derivatives. In particular,

$$D_{\mathrm{KL}}(\mu \| \nu) \ge D_{\mathrm{KL}}(\mathcal{Q}_* \mu \| \mathcal{Q}_* \nu). \tag{8}$$

*Proof.* The statement follows directly from Lemma 1.3 and the measurability of the average operator.  $\Box$ 

We illustrate Theorem 2.5 for a toy example in the Appendix C.

As a simple consequence, if the second term in the decomposition is strictly positive, the KL divergence between the pushforward measures is strictly smaller than that between the original measures. This observation unlocks the potential for improved PAC-Bayesian generalization bounds, as we exploit in the following sections.

#### 2.1 PAC-Bayesian Bound

In Theorem 2.5, we showed that averaging each hypothesis function to their equivariant counterparts reduces the KL divergence of measures in the hypothesis class. This directly leads to a smaller generalization gap in McAllester's PAC-Bayesian bound (cf. Theorem 1.2), which we record in the following theorem.

**Theorem 2.6.** Suppose Assumptions 2.1 and 2.4 hold. For any measurable loss function  $\ell$  and any distribution  $\mathbb{Q}$  on  $\mathcal{H}$ 

$$Q_* \mathbb{Q}[\mathcal{R}_{\ell}] \leq Q_* \mathbb{Q}[\hat{\mathcal{R}}_{\ell}(\cdot, S_n)] + \sqrt{\frac{D_{\mathrm{KL}}(\mathcal{Q}_* \mathbb{Q} \| \mathcal{Q}_* \mathbb{P}_H) + \log \frac{1}{\delta} + \log n + 2}{2n - 1}}$$
(9)

holds with probability of at least  $1 - \delta$ .

Clearly, a similar argument applies to other PAC-Bayesian bound.

Remark 2.7. As discussed before, the generalization gap is reduced when restricting the hypothesis class to the subset of equivariant functions. Consequently, the empirical risk becomes a better approximation of the true risk within this subset. However, it is important to note that the true or empirical risk may not be smaller in absolute terms. In fact, both risks may remain large or even increase under the equivariant constraint. The apparent improvement merely reflects a tighter coupling between empirical and true risk. This issue is addressed in Section 3, where the data distribution is assumed to exhibit the same symmetries as the model class.

# 3 SYMMETRY ON DATA

In the previous discussion, we analyzed the impact of enforcing equivariance in the hypothesis class, observing a reduction in the generalization gap and an improved alignment between empirical and true risk. However, without considering the symmetry properties of the data itself, this structural constraint may not yield practical benefits in terms of generalization performance. In practice, data often exhibit symmetries, and hypothesis classes are designed to exploit these properties. In this chapter, we tackle this problem under the assumption that the data distribution exhibits symmetry, and that the hypothesis class is constructed to respect this symmetry.

To make this setting precise, we now introduce a set of assumptions that formalize the symmetry properties of the data-generating process and the loss function. These assumptions provide the foundation for analyzing the behavior of equivariant models in symmetric environments.

**Assumption 3.1.** Let  $f^* : \mathcal{X} \times \mathcal{E} \to \mathcal{Y}$  be a measurable function an consider

$$Y = f^*(X, \Xi), \tag{10}$$

where  $\Xi$  is a random element taking values in a measurable space  $(\mathcal{E}, \mathcal{E})$ , referred to as noise. The random element  $\Xi$  is assumed to be independent of X. Moreover, the function  $f^*$  is  $\mathcal{G}$ -equivariant in the first argument, meaning that for all  $g \in \mathcal{G}$ ,  $x \in \mathcal{X}$  and  $\xi \in \mathcal{E}$ ,  $f^*(g \cdot x, \xi) = g \cdot (f^*(x, \xi))$ .

**Remark 3.2.** Actually, it is sufficient to require  $\mathcal{G}$ -equivariance of  $f^*$  only on the support of X. Since X almost surely takes values in  $\operatorname{supp}(X)$ , the behavior of  $f^*$  outside this set is irrelevant for the distribution of Y defined in (10). This could be of interest, for example, under physical constraints of certain configurations (e.g. a filled upside down cup cannot occur).

**Assumption 3.3.** We assume that the loss function  $\ell \colon \mathcal{Y} \times \mathcal{Y} \to [0, \infty)$  is convex in its first argument and  $\mathcal{G}$ -invariant, i.e., for all  $g \in \mathcal{G}$ ,  $y, \hat{y} \in \mathcal{Y}$ , it holds that  $\ell(g \cdot y, g \cdot \hat{y}) = \ell(y, \hat{y})$ .

Building upon the previous assumptions, the following proposition demonstrates that averaging a hypothesis function over a group does not increase the true risk.

**Proposition 3.4.** Suppose Assumptions 2.1, 3.1 and 3.3 hold. Then for all  $f \in \mathcal{H}$ , we have that

$$\mathcal{R}_{\ell}(\mathcal{Q}(f)) \leq \mathcal{R}_{\ell}(f)$$
.

In particular, for a distribution  $\mathbb{Q}$  over the hypothesis class  $\mathcal{H}$ , it holds that

$$Q_*\mathbb{Q}[\mathcal{R}_\ell] \leq \mathbb{Q}[\mathcal{R}_\ell]$$
.

*Proof.* The proof can be found in Section A.1.

The preceding Proposition 3.4 demonstrates that, when both the data distribution and the hypothesis class exhibit the same symmetry, the true risk of the symmetrized (i.e., averaged) hypothesis is not greater than that of an unsymmetrized one. This implies that equivariant hypotheses approximate the underlying target function at least as well as their non-equivariant counterparts. Combined with the result from Theorem 2.6, restricting to equivariant functions not only tightens the generalization bound but also leads to truly improved generalization performance.

#### 3.1 Evaluating Risk on Representatives

For the remainder of this section, our goal is to move beyond evaluating the empirical risk over the full data distribution and instead focus on samples drawn only from a set of representatives. To this end, we first observe that, in distribution, the loss of an equivariant function evaluated on the full distribution (X,Y) coincides with the loss evaluated on the distribution of representatives  $(X_{\varphi},Y_{\varphi})$ , where  $X_{\varphi}=\pi_{\mathcal{X}_{\varphi}}(X)$  and  $Y_{\varphi}=f^{*}(X_{\varphi},\Xi)$ .

**Lemma 3.5.** Suppose Assumptions 2.1 and 3.1 hold. Let  $f \in \mathcal{H}$  be  $\mathcal{G}$ -equivariant. Then

$$\ell(f(X), Y) \stackrel{d}{=} \ell(f(X_{\varphi}), Y_{\varphi}).$$

*Proof.* The proof is found in Section A.2.

Clearly, this result suggests a similar identity for the true and empirical risk. For this sake, for an equivariant hypothesis function f, we introduce the risk on the representatives  $\mathcal{R}_{\ell\varphi}(f) := \mathbb{E}[\ell(f(X_{\varphi}), f^*(X_{\varphi}, \Xi)]]$ , where the data set  $S_{n\varphi} = \{X_{\varphi_i}, Y_{\varphi_i}\}_{i=1}^n$  consists of n i.i.d. copies of  $(X_{\varphi}, Y_{\varphi})$ .

Corollary 3.6. Suppose Assumptions 2.1 and 3.1 hold. Then, for an equivariant hypothesis function  $f \in \mathcal{H}$ , it holds that

$$\mathcal{R}_{\ell}(f) = \mathcal{R}_{\ell\varphi}(f)$$
 and  $\hat{\mathcal{R}}_{\ell}(f, S_n) \stackrel{d}{=} \hat{\mathcal{R}}_{\ell}(f, S_{n\varphi})$ .

In particular, for a distribution  $\mathbb{Q}$  over the subset of equivariant hypothesis functions, we have

$$\mathbb{Q}[\mathcal{R}_{\ell}] = \mathbb{Q}[\mathcal{R}_{\ell\varphi}] \quad \text{and} \quad \mathbb{Q}[\hat{\mathcal{R}}_{\ell}(\cdot, S_n)] \stackrel{d}{=} \mathbb{Q}[\hat{\mathcal{R}}_{\ell}(\cdot, S_{n\varphi})].$$

*Proof.* This is a direct consequence of Lemma 3.5.

The following main result is a refinement of the cAllester's PAC-Bayesian boun, in which the true risk is upper-bounded by the empirical risk computed solely from samples drawn from a set of orbit representatives.

**Theorem 3.7.** Suppose Assumptions 2.1, 2.4 and 3.1, 3.3 hold. For any measurable loss function  $\ell$  and any distribution  $\mathbb Q$  on  $\mathcal H$ 

$$Q_* \mathbb{Q}[\mathcal{R}_\ell] \le Q_* \mathbb{Q}[\hat{\mathcal{R}}_\ell(\cdot, S_{n\varphi})] + \sqrt{\frac{D_{\mathrm{KL}}(Q_* \mathbb{Q} \| Q_* \mathbb{P}_H) + \log \frac{1}{\delta} + \log n + 2}{2n - 1}}$$
(11)

holds with probability of at least  $1 - \delta$ , where  $S_n = \{X_i, Y_i\}_{i=1}^n$  are n i.i.d. copies of (X, Y).

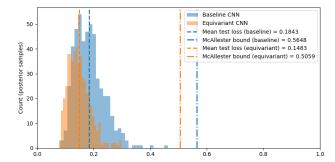
*Proof.* Combining Theorem 2.6 with Corollary 3.6 yields the result.

As a consequence, by exploiting symmetry, we obtain a tighter generalization bound, where the true risk can be controlled using empirical risk evaluated solely on a set of representatives. This has the important practical implication that training need only be performed on a reduced set of inputs, without compromising generalization performance on the full input space.

Moreover, unlike previous works, our analysis is not restricted to symmetries induced by compact groups or to data distributions that are invariant under the group action. Instead, we allow for a more general setting where the data distribution no longer need to be invariant and the group can be non-compact.

# 4 NUMERICAL ANALYSIS

The main objective of the following experiment is to provide evidence via our PAC-Bayesian generalization bound for the in practice observed and intuitively well-known fact that using equivariant hypotheses functions for symmetric data improves the generalization performance as compared to models that do not exploit such symmetry. Moreover, while previous approaches require the usage of compact symmetry groups and a uniform distribution of the data with respect to the same symmetry, we consider two problems that violate those assumptions. First, a rotation group with restricted support and second, the rotation group with restricted support combined with the translation group. This setting violates the invariance assumptions made in earlier work, causing existing guarantees to be inapplicable. Our approach, however, provides theoretical guarantees and is directly applicable in this more general scenario.



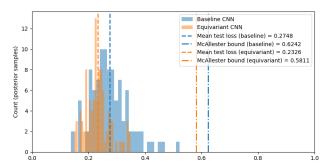


Figure 1: The figure displays the distribution of the test errors for the baseline CNN and the equivariant CNN on two datasets: the rotated MNIST (left) and the rotated and translated MNIST (right). Our PAC-Bayesian bound (Theorem 3.7) is visualized with a vertical dash-dotted line labeled as McAllester bound. The figure highlights two key observations. First, the equivariant CNN outperforms the baseline CNN in terms of empirical accuracy on rotated MNIST. Second, and more importantly from a theoretical perspective, the equivariant network also enjoys a strictly smaller generalization bound that is closer to the test error.

Data Generation. We build a rotated version of MNIST from the original training and test partitions by rotating each image by an angle  $\theta$  sampled uniformly from the interval  $(-90^{\circ}, 90^{\circ})$ . We restrict rotations to  $(-90^{\circ}, 90^{\circ})$  (unlike, for example, [18]), because this range models realistic digit appearances, small tilts and moderate rotations, while excluding extreme upside-down orientations that rarely occur in practice and may cause an unresolvable ambiguity, e.g., rotating the digit '6' by 180° exactly matches the digit '9'. As a consequence, the resulting dataset is not rotation-invariant in distribution, which further motivates our theoretical analysis of equivariant models beyond the classical setting of invariant data distributions.

**Models.** As a baseline we use a small convolutional network with two convolutional blocks, each consisting of a convolutional layer followed by max pooling, and two fully connected layers. This architecture does not incorporate any rotation-equivariance. Both convolutional layers use kernels of size  $5 \times 5$ , stride one, and zero-padding of size 2. For the equivariant network we employ a two-layer equivariant CNN implemented with the e2cnn library [28]. The overall capacity of this network is matched to that of the baseline CNN by using regular representation fields. This ensures that the effective number of channels, and hence the parameter count and model capacity, remain comparable between the baseline and the equivariant model, since it creates multiple rotated copies of each channel internally.

**Training.** For training, we split the generated MNIST dataset into  $N_{\rm train} = 40000$ ,  $N_{\rm val} = 10000$ , and  $N_{\rm prior} = 10000$  examples. We use the Adam optimizer by [15] for 20 epochs with a batch size of 128 and a learning rate of  $10^{-3}$  for minimizing the standard cross-entropy loss. Before the actual training, we first construct Gaussian priors by training the mean on the prior dataset and using a fixed standard deviation  $\sigma = 0.05$ , a choice that yielded stable and accurate results in practice. Then, we optimize the right-hand side of McAllester's PAC-Bayes bound for both the baseline CNN and the equivariant CNN. Model selection is based on validation accuracy.

Results. The results of our experiment are summarized in Figure 1, which displays the distribution of the test error for both the baseline CNN and the equivariant CNN. The histograms approximate the posterior expectation  $\mathbb{Q}[\mathcal{R}_\ell]$  by Monte Carlo sampling from the learned posterior distributions. Our PAC-Bayesian bound (Theorem 3.7) is visualized with a vertical dash-dotted line labeled as McAllester bound (since it is a generalization of this type of PAC bound) for  $\delta = 0.05$ . It guarantees an upper bound on the average (w.r.t. the posterior distribution) of the true risk (visualized as vertical dashed line). As shown in our main result, the bound for the equivariant model is smaller and tighter to the distribution of the true risk.

Based on the rotated MNIST dataset, we constructed another variant by additionally translating each image by a uniformly chosen number of pixels from -2, -1, 0, 1, 2 in both dimensions independently. We trained the same models on this dataset and observed similar performance, as shown in Figure 1.

These results highlight two key observations. First, the equivariant CNN outperforms the baseline CNN in terms of empirical accuracy on rotated MNIST. Second, and more importantly from a theoretical perspective, the equivariant network also enjoys a strictly smaller generalization bound that is closer to the true risk. This improvement stems from the reduced KL divergence of the equivariant posterior relative to the baseline, in line with the predictions of our theory. Prior analyses could not establish such an advantage for equivariant models in the presence of non-invariant data distributions; our framework overcomes this limitation and provides the first guarantees in this more realistic setting.

## 5 CONCLUSION

We have extended PAC-Bayes generalization guarantees to learning settings with non-compact symmetries and non-invariant data distributions, demonstrating both tighter bounds and improved performance on rotated MNIST for equivariant models. Our results provide theoretical support for the practical observation that symmetric models offer advantages beyond compact groups and invariant data distributions. This work broadens the theoretical foundations of symmetry in machine learning and suggests further exploration into richer classes of symmetries, more complex real-world data distributions, and alternative generalization bounds that do not rely on the KL divergence.

# A APPENDIX: COLLECTION OF PROOFS

#### A.1 Proof of Proposition 3.4

Let  $f \in \mathcal{H}$ . Due to the limitations of line space, we employ the notation from (3) for the following estimation, where the subscript at the bracket indicates the variable that acts as argument of the function inside the brackets. We aim to rewrite the risk

$$\mathcal{R}_{\ell}(f) = \mathbb{E}[\ell(f(X), Y)] = \mathbb{E}[\ell(f(X), f^*(X, \Xi)] = \int_{\mathcal{E}} \int_{\mathcal{X}} \ell(f(x), f^*(x, \xi)) \, \mathbb{P}_X(dx) \mathbb{P}_\Xi(d\xi) \,.$$

Since the calculation is only concerned with the inner integral, we derive the following identities  $\mathbb{P}_{\Xi}$ -a.e. for  $\xi \in \mathcal{E}$ . Using first the Disintegration Theorem 1.1 and, then, the  $\mathcal{G}$ -invariance together with notation (3), we obtain

$$\begin{split} \int_{\mathcal{X}} \ell \big( f(x), \, f^*(x, \, \xi) \big) \, \mathbb{P}_X(dx) &= \int_{\mathcal{X}_{\varphi}} \int_{\mathcal{G}} \ell \big( f(g \cdot x_{\varphi}), \, f^*(g \cdot x_{\varphi}, \, \xi) \big) \, \kappa(x_{\varphi}, \, dg) \mathbb{P}_{X_{\varphi}}(dx_{\varphi}) \\ &= \mathbb{P}_{X_{\varphi}} \Big[ \int_{\mathcal{G}} \ell \big( g^{-1} \cdot f(g \cdot x_{\varphi}), \, f^*(x_{\varphi}, \, \xi) \big) \, \kappa(x_{\varphi}, \, dg) \Big]_{x_{\varphi}} \, . \end{split}$$

Convexity of the loss function  $\ell$  in the first argument yields the lower bound:

$$\mathbb{P}_{X_{\varphi}}\left[\ell\left(\int_{\mathcal{G}}g^{-1}\cdot f(g\cdot x_{\varphi})\,\kappa(x_{\varphi},\,dg),\,f^{*}(x_{\varphi},\,\xi)\right)\right]_{x_{\varphi}},$$

which can be trivially reformulated and connected to the average operator  $\mathcal Q$  as follows

$$\mathbb{P}_{X_{\varphi}} \left[ \ell \left( h \cdot \int_{\mathcal{G}} g^{-1} \cdot f(g \cdot x_{\varphi}) \, \kappa(x_{\varphi}, dg), \, h \cdot f^{*}(x_{\varphi}, \xi) \right) \kappa(x_{\varphi}, dh) \right]_{x_{\varphi}} \\
= \mathbb{P}_{X_{\varphi}} \left[ \int_{\mathcal{G}} \ell \left( \mathcal{Q}(f)(h \cdot x_{\varphi}), \, f^{*}(h \cdot x_{\varphi}, \xi) \right) \, \kappa(x_{\varphi}, dh) \right]_{x_{\varphi}} \\
= \int_{\mathcal{X}} \ell \left( \mathcal{Q}(f)(x), \, f^{*}(x, \xi) \right) \, \mathbb{P}_{X}(dx),$$

where the last equality is again based on the Disintegration Theorem 1.1. Incorporating the integration over  $\xi$ , the last expression is exactly

$$\mathbb{E}[\ell(\mathcal{Q}(f)(X), f^*(X, \Xi)] = \mathcal{R}_{\ell}(\mathcal{Q}(f)),$$

which shows the first part of the statement. We proved that the true risk of a single hypothesis does not increase when averaged over the group. This result extends naturally to distributions over the hypothesis class.  $\Box$ 

#### A.2 Proof of Lemma 3.5

Let  $f \in \mathcal{H}$ . For the subsequent calculation, we continue to employ the notation established in (3). Let  $t \in \mathbb{R}$  and in the following, we will rewrite the probability of the loss

$$\mathbb{P}\big(\ell(f(X),Y) \le t\big) = \mathbb{P}\big(\ell(f(X),f^*(X,\Xi)) \le t\big) = \int_{\mathcal{E}} \int_{\mathcal{X}} \mathbf{1}_{\{\ell(f(X),f^*(X,\xi)) \le t\}} \, \mathbb{P}_X(dX) \mathbb{P}_\Xi(d\xi) \,,$$

Since the calculation once more focuses only on the inner integral, we establish the following identities, holding  $\mathbb{P}_{\Xi}$ -a.e. for  $\xi \in \mathcal{E}$ . Beginning with the Disintegration Theorem 1.1, and using the  $\mathcal{G}$ -equivariance of f and  $f^*$  along with the notation in (3), we obtain

$$\begin{split} \int_{\mathcal{X}} \mathbf{1}_{\{\ell(f(x),f^*(x,\xi)) \leq t\}} \, \mathbb{P}_X(dx) &= \int_{\mathcal{X}_\varphi} \int_{\mathcal{G}} \mathbf{1}_{\{\ell(f(g \cdot x_\varphi),f^*(g \cdot x_\varphi,\xi)) \leq t\}} \, \kappa(x_\varphi,dg) \mathbb{P}_{X_\varphi}(dx_\varphi) \\ &= \mathbb{P}_{X_\varphi} \left[ \int_{\mathcal{G}} \mathbf{1}_{\{\ell(g \cdot f(x_\varphi),g \cdot f^*(x_\varphi,\xi)) \leq t\}} \, \kappa(x_\varphi,dg) \right]_{x_\varphi}. \end{split}$$

The  $\mathcal{G}$ -invariance of the loss function  $\ell$  implies the reformulation

$$\mathbb{P}_{X_{\varphi}} \left[ \int_{\mathcal{G}} \mathbf{1}_{\{\ell(f(x_{\varphi}), f^*(x_{\varphi}, \xi)) \leq t\}} \, \kappa(x_{\varphi}, dg) \right]_{x_{\varphi}} = \mathbb{P}_{X_{\varphi}} \left[ \mathbf{1}_{\{\ell(f(x_{\varphi}), f^*(x_{\varphi}, \xi)) \leq t\}} \right]_{x_{\varphi}} = \mathbb{P}(\ell(f(X_{\varphi}), Y_{\varphi}) \leq t) .$$

Incorporating the integration over  $\xi$ , the last expression is

$$\mathbb{P}_{\Xi} \left[ \mathbb{P}_{X_{\varphi}} \left[ \mathbf{1}_{\{\ell(f(x_{\varphi}), f^*(x_{\varphi}, \xi)) \leq t\}} \right]_{x_{\varphi}} \right]_{\xi} = \mathbb{P} \left( \ell(f(X_{\varphi}), Y_{\varphi}) \leq t \right),$$

which concludes the proof.

# B APPENDIX: WELL-DEFINEDNESS AND PROPERTIES OF THE AVERAGING OPERATOR

This section provides additional technical details concerning the averaging operator introduced in the main paper. In particular, we establish that the operator is well-defined under the assumptions stated therein, and we derive several of its fundamental properties that are used throughout the theoretical analysis. While the main text focuses on its implications for the PAC-Bayes bounds, the proofs and auxiliary results presented here ensure the mathematical soundness of the operator's definition. We begin by formally verifying the well-definedness of the averaging operator. We then proceed to prove its key properties. These results serve to justify the operator's use within our framework and to support the theoretical claims referenced in the main text.

The following lemma proves, that the average operator is well defined, in the sense that, it actually maps into the set of measurable measurable functions.

**Lemma B.1.** Suppose Assumption 2.1 holds. Let  $f: \mathcal{X} \to \mathcal{Y}$  be a measurable function. Then  $\mathcal{Q}(f)$  is a measurable function.

Proof. We start with proving, that the  $\pi_{\mathcal{G}} \colon \mathcal{X} \to \mathcal{G}$  and  $\pi_{\mathcal{X}_{\varphi}} \colon \mathcal{X} \to \mathcal{X}_{\varphi}$  are measurable functions. First, note that we can rewrite  $\pi_{\mathcal{G}} = \tilde{\pi}_{\mathcal{G}} \circ \varphi^{-1}$ , where  $\tilde{\pi}_{\mathcal{G}} \colon \mathcal{G} \times \mathcal{X} \to \mathcal{G}$  is given by  $\tilde{\pi}_{\mathcal{G}}(g,x) := g$ . Since  $\varphi^{-1}$  is measurable and  $\mathcal{G} \times \mathcal{X}$  is equipped with the product  $\sigma$ -algebra,  $\tilde{\pi}_{\mathcal{G}}$  is measurable. Hence  $\pi_{\mathcal{G}}$  and analogously also  $\pi_{\mathcal{X}_{\varphi}}$  are measurable. Further  $\mathcal{G}$  acts measurably on both the input and output space. Therefore,  $\mathcal{G} \times \mathcal{X} \to \mathcal{Y}$  given by  $(g,x) \mapsto g^{-1} \cdot f(g \cdot \pi_{\mathcal{X}_{\varphi}}(x))$  is measurable. Finally, [13, Lemma 3.2] implies, that  $\mathcal{Q}(f)$  is measurable.

The purpose of the averaging operator is to transform an arbitrary hypothesis function into one that is equivariant with respect to the group action. The following proposition confirms that this transformation indeed yields an equivariant function.

**Proposition B.2.** Suppose Assumption 2.1 holds. Let  $f: \mathcal{X} \to \mathcal{Y}$  be a measurable function. Then  $\mathcal{Q}(f)$  is an equivariant function.

Proof. Let  $h \in \mathcal{G}$  and  $x \in \mathcal{X}$ . Since x and  $h \cdot x$  belong to the same orbit,  $\pi_{\mathcal{X}_{\varphi}}(h \cdot x) = \pi_{\mathcal{X}_{\varphi}}(x)$  holds. Furthermore for any  $z \in \mathcal{X}$ , the projections  $\pi_{\mathcal{G}}(z)$  and  $\pi_{\mathcal{X}_{\varphi}}(z)$  are the unique elements in  $\mathcal{G}$  and  $\mathcal{X}_{\varphi}$  respectively, such that  $z = \pi_{\mathcal{G}}(z) \cdot \pi_{\mathcal{X}_{\varphi}}(z)$ . Since  $h \cdot x = h \cdot (\pi_{\mathcal{G}}(x) \cdot \pi_{\mathcal{X}_{\varphi}}(x)) = (h\pi_{\mathcal{G}}(x)) \cdot \pi_{\mathcal{X}_{\varphi}}(x)$ , the projection onto the group  $\mathcal{G}$  commutes with the group action, i.e.  $\pi_{\mathcal{G}}(h \cdot x) = h\pi_{\mathcal{G}}(x)$ . Hence, we obtain

$$Q(f)(h \cdot x) = \pi_{\mathcal{G}}(h \cdot x) \cdot \int_{\mathcal{G}} g^{-1} \cdot f\left(g \cdot \pi_{\mathcal{X}_{\varphi}}(h \cdot x)\right) \, \kappa(\pi_{\mathcal{X}_{\varphi}}(h \cdot x), dg)$$

$$= h \cdot \left(\pi_{\mathcal{G}}(x) \cdot \int_{\mathcal{G}} g^{-1} \cdot f\left(g \cdot \pi_{\mathcal{X}_{\varphi}}(x)\right) \, \kappa(\pi_{\mathcal{X}_{\varphi}}(x), dg)\right)$$

$$= h \cdot Q(f)(x) \,.$$

The operator not only transforms hypothesis functions into equivariant functions but also provides a functional characterization of the equivariance.

**Lemma B.3.** Suppose Assumption 2.1 holds. A function f is equivariant if and only if Qf = f. Moreover, Q satisfies the idempotency condition  $Q^2 = Q$ , implying that it is a projection operator onto the respective subset of equivariant functions.

*Proof.* That Q(f) = f implies equivariance of the hypothesis function f is already proven by Proposition B.2. On the other hand if f is equivariant, we obtain for any  $x \in \mathcal{X}$ 

$$Q(f)(x) = \pi_{\mathcal{G}}(x) \cdot \int_{\mathcal{G}} g^{-1} \cdot f\left(g \cdot \pi_{\mathcal{X}_{\varphi}}(x)\right) \, \kappa(\pi_{\mathcal{X}_{\varphi}}(x), dg)$$

$$= \pi_{\mathcal{G}}(x) \cdot \int_{\mathcal{G}} f\left(\pi_{\mathcal{X}_{\varphi}}(x)\right) \, \kappa(\pi_{\mathcal{X}_{\varphi}}(x), dg)$$

$$= \pi_{\mathcal{G}}(x) \cdot f\left(\pi_{\mathcal{X}_{\varphi}}(x)\right) = f(x) \,.$$

In order to apply Lemma 1.3 from the main paper to the averaging operator, it is necessary to verify that the operator defines a measurable map. The lemma below confirms this property.

**Lemma B.4.** Suppose Assumptions 2.1 holds. The average operator  $Q: \mathcal{M}(\mathcal{X}, \mathcal{Y}) \to \mathcal{M}(\mathcal{X}, \mathcal{Y})$  is measurable.

*Proof.* Since the set of measurable functions  $\mathcal{M}(\mathcal{X}, \mathcal{Y})$  is equipped with the evaluation  $\sigma$ -algebra  $\mathcal{M}$ , proving that  $\mathcal{Q}$  is measurable is equivalent to prove, that the map  $f \mapsto \mathcal{Q}f(x)$  is measurable for all  $x \in \mathcal{X}$ . To this end, we fix  $x \in \mathcal{X}$  and define

$$F_x \colon \mathcal{M}(\mathcal{X}, \mathcal{Y}) \times \mathcal{G} \to \mathcal{Y}, \quad F_x(f, g) := g^{-1} \cdot f(g \cdot x)$$

where  $\mathcal{M}(\mathcal{X}, \mathcal{Y}) \times \mathcal{G}$  is equipped with the product  $\sigma$ -algebra  $\mathcal{M} \otimes \mathcal{B}(\mathcal{G})$ , and  $\mathcal{B}(\mathcal{G})$  denotes the Borel  $\sigma$ -algebra on the group. F is measurable, because the group  $\mathcal{G}$  acts measurably on both the input space  $\mathcal{X}$  and the output space  $\mathcal{Y}$ , the map  $f \mapsto f(z)$  is measurably for all  $z \in \mathcal{X}$  and the composition of measurable functions is measurable. Applying Fubini's Theorem yields, that the map

$$f \mapsto \int_G F_x(f,g) \, \kappa(x,dg) = \int_{\mathcal{G}} g^{-1} \cdot f(g \cdot x) \, \kappa(x,dg)$$

is measurable. Since this holds for any  $x \in \mathcal{X}$ , it implies  $f \mapsto \mathcal{Q}f(x)$  is measurable and therefore  $\mathcal{Q}$  is measurable.  $\square$ 

Remark B.5. While we have shown that the averaging operator is measurable with respect to the evaluation  $\sigma$ -algebra, measurability also holds for other  $\sigma$ -algebras and function spaces. In particular, under additional assumptions, the operator is measurable with respect to the Borel  $\sigma$ -algebra induced by the  $L^p$ -norm on  $L^p(\mathcal{X}, \mathcal{Y})$ , since the averaging operator is a continuous linear map in this setting.

# C APPENDIX: EXAMPLE FOR GAUSSIAN KL DECOMPOSITION

In this section, we present an illustrative example that complements the theoretical discussion in the main paper. Specifically, we provide an explicit computation of the KL divergence between two Gaussian measures defined on a function space, as well as between their corresponding pushforward measures restricted to the subset of equivariant functions. This example serves to concretely demonstrate the decomposition of the KL divergence established in the main text and to clarify how the abstract results apply in a tractable Gaussian setting.

**Example C.1** (Gaussian KL decomposition). Let the hypothesis space be the linear maps from  $\mathbb{R}^2$  to  $\mathbb{R}$ ,  $\mathcal{H} = \mathcal{L}(\mathbb{R}^2 \to \mathbb{R}) \cong \mathbb{R}^2$ . Let  $\mathcal{G} = S_2$  denote the group be the symmetric group on two elements, acting on the input space  $\mathbb{R}^2$  by permuting its coordinates. Explicitly, for  $(x, y) \in \mathbb{R}^2$  and  $\sigma \in S_2$ , the action is given by

$$\sigma \cdot (x, y) = \begin{cases} (x, y) & \text{if } \sigma = e, \\ (y, x) & \text{else.} \end{cases}$$

We equip the output space  $\mathbb{R}$  with the trivial (identity) group action. In this setting, the space of equivariant functions is  $\mathcal{U} = \{ f \in \mathcal{L}(\mathbb{R}^2, \mathbb{R}) : f(x, y) = f(y, x), \ \forall x, y \in \mathbb{R} \}$ . Since the output is invariant under the group action, the equivariant functions are, in fact, invariant with respect to the action of  $S_2$  on the input space. In the following we identify each linear map  $f \in \mathcal{L}(\mathbb{R}^2, \mathbb{R})$  with its matrix representation  $w \in \mathbb{R}^2$  given the standard basis,  $f(x) = w^{\top}x$ . Therefore  $\mathcal{U}$  is a one-dimensional subspace corresponding to the diagonal line in  $\mathbb{R}^2$ . The average operator  $\mathcal{Q}: \mathcal{L}(\mathbb{R}^2, \mathbb{R}) \to \mathcal{U}$  is given by the orthogonal projection

$$Q(w) = \left(\frac{w_1 + w_2}{2}, \frac{w_1 + w_2}{2}\right)^{\top}.$$

Next, let  $\mu = \mathcal{N}(0, I_2)$  and  $\nu = \mathcal{N}(m, I_2)$  be Gaussian probability distributions on  $\mathbb{R}^2$  with  $m = (1, 0)^{\top}$ . We first compute the KL divergence directly:

$$D_{\mathrm{KL}}(\nu \| \mu) = \frac{1}{2} \left( \| m \|^2 + \mathrm{tr}(I_2^{-1} I_2) - 2 - \log \det(I_2^{-1} I_2) \right) = \frac{1}{2}.$$

Next, we compute the pushforward distributions under the linear operator QQ. Since Q is linear, the pushforward measures are given by

$$Q_*\mu = \mathcal{N}(0,\Sigma), \quad Q_*\nu = \mathcal{N}(Q(m),\Sigma),$$

where the covariance matrix  $\Sigma$  and the mean  $\mathcal{Q}(m)$  are given by

$$\Sigma = M_{\mathcal{Q}} I_2 M_{\mathcal{Q}}^\top = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} , \quad \mathcal{Q}(m) = \left(\frac{1}{2}, \frac{1}{2}\right) .$$

Here,  $M_{\mathcal{Q}} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$  denotes the matrix representation of  $\mathcal{Q}$  with respect to the standard basis. We now restrict to the subspace  $\mathcal{U}$ , and compute the KL divergence:

$$D_{\mathrm{KL}}(\mathcal{Q}_*\nu\|\mathcal{Q}_*\mu) = \frac{1}{2}\left(\left(\frac{1}{\sqrt{2}}\right)^2\right) = \frac{1}{4}.$$

To compute the conditional KL divergence, observe that the conditional distributions  $\kappa_{\mu}$  and  $\kappa_{\nu}$  are Gaussians in the orthogonal direction  $\mathcal{U}^{\perp} = \{(x, -x)\}$  with mean 0 and  $1/\sqrt{2}$  respectively, and unit variance. Thus,

$$D_{\mathrm{KL}}(\kappa_{\nu}(u,\cdot)||\kappa_{\mu}(u,\cdot)) = \frac{1}{2} \left( \left(\frac{1}{\sqrt{2}}\right)^2 \right) = \frac{1}{4},$$

for all  $u \in \mathcal{U}$ . Therefore,

$$\int_{\mathcal{U}} D_{\mathrm{KL}}(\kappa_{\nu}(u,\cdot) \| \kappa_{\mu}(u,\cdot)) \, \mathcal{Q}_* \nu(du) = \frac{1}{4} \, .$$

By Corollary 2.5 in the main paper, we confirm:

$$D_{\mathrm{KL}}(\nu \| \mu) = D_{\mathrm{KL}}(\mathcal{Q}_* \nu \| \mathcal{Q}_* \mu) + \int_{\mathcal{U}} D_{\mathrm{KL}}(\kappa_{\nu}(u, \cdot) \| \kappa_{\mu}(u, \cdot)) \, \mathcal{Q}_* \nu(du) = \frac{1}{4} + \frac{1}{4} = \frac{1}{2} \,.$$

Since in this example the conditional KL divergence is strictly positive, the KL divergence for the projected distributions is strictly smaller than the KL divergence of the initial distributions.

The reduction of the KL divergence established in the previous example has direct implications for the complexity term appearing in PAC-Bayesian generalization bounds. In particular, since the KL term forms the principal component of the bound's data-independent complexity measure, its decomposition and reduction naturally lead to tighter guarantees. To make this connection explicit, we next illustrate how the reduced KL divergence translates into an improved bound in the setting of McAllester's PAC-Bayes formulation, which serves as the reference bound throughout the main paper.

**Example C.2.** Consider the same setting as in Example C.1. In this setting, the generalization bound from (9) becomes strictly tighter in the equivariant case. As shown in the previous Example C.1, the KL divergence halves for the equivariant case. Consequently,

$$\sqrt{\frac{D_{\mathrm{KL}}(\mathcal{Q}_*\mathbb{Q}\|\mathcal{Q}_*\mathbb{P}_H) + \log\frac{1}{\delta} + \log n + 2}{2n-1}} < \sqrt{\frac{D_{\mathrm{KL}}(\mathbb{Q}\|\mathbb{P}_H) + \log\frac{1}{\delta} + \log n + 2}{2n-1}}.$$

This explicit relation illustrates how enforcing equivariance not only reduces the divergence term but also strictly tightens the overall PAC-Bayes bound.

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