Distributional Generalization: A New Kind of Generalization

Preetum Nakkiran 1  Yamini Bansal 1

Abstract

We discover a new set of empirical properties of interpolating classifiers, including neural networks, kernel machines and decision trees. Informally, the output distribution of an interpolating classifier matches the distribution of true labels, when conditioned on certain subgroups of the input space. For example, if we mislabel 30% of images in the subgroup dogs as cats in the train set of CIFAR-10, then a ResNet trained to interpolation will in fact mislabel roughly 30% of dogs as cats on the test set as well, while leaving other classes unaffected. These behaviors are not captured by classical generalization, which would only consider the average error over the inputs, and not where these errors occur. We introduce and experimentally validate a formal conjecture that specifies the subgroups for which we expect this distributional closeness. Further, we show that these properties can be seen as a new form of generalization, which advances our understanding of the implicit bias of interpolating methods.

1. Introduction

In learning theory, when we study how well a classifier “generalizes”, we usually consider a single metric – its test error (Shalev-Shwartz & Ben-David, 2014). However, there could be many different classifiers with the same test error that differ substantially in, say, the subgroups of inputs on which they make errors or in the features they use to attain this performance. Reducing classifiers to a single number misses these rich aspects of their behavior.

In this work, we propose formally studying the entire joint distribution of classifier inputs and outputs. That is, the distribution $(x, f(x))$ for samples from the distribution $x \sim D$ for a classifier $f(x)$. This distribution reveals many structural properties of the classifier beyond test error (such as where the errors occur). In fact, we discover new behaviors of modern classifiers that can only be understood in this framework. As an example, consider the following experiment (Figure 1).

**Experiment 1.** Consider a binary classification version of CIFAR-10, where CIFAR-10 images $x$ have binary labels Animal/Object. Take 50K samples from this distribution as a train set, but apply the following label noise: flip the label of cats to Object with probability 30%. Now train a WideResNet $f$ to 0 train error on this train set. How does the trained classifier behave on test samples? Options below:

(1) The test error is low across all classes, since there is only 3% overall label noise in the train set.

(2) Test error is “spread” across the animal class. After all, the classifier is not explicitly told what a cat or a dog is, just that they are all animals.

(3) The classifier misclassifies roughly 30% of test cats as “objects”, but all other animals are largely unaffected.

The reality is closest to option (3) as shown in Figure 1. The left panel shows the joint density of train inputs $x$ with train labels Animal/Object. Since the classifier is interpolating, the classifier outputs on the train set are identical to the left panel. The right panel shows the classifier predictions $f(x)$ on test inputs $x$.

There are several notable things about this experiment. First, the error is localized to cats in the test set as it was in the train set, even though no explicit cat labels were provided. The interpolating model is thus sensitive to subgroup-structures in the distribution. Second, the amount of error on the cat class is close to the noise applied on the train set. Thus, the behavior of the classifier on the train set generalizes to the test set in a stronger sense than just average error. Specifically, when conditioned on a subgroup (cat), the distribution of the true labels is close to that of the classifier outputs. Third, this is not the behavior of the Bayes-optimal classifier, which would always output the maximum-likelihood label instead of reproducing the noise in the distribution. The network is thus behaving poorly from the perspective of Bayes-optimality, but behaving well in a certain distributional sense (which we will formalize soon).

Now, consider a seemingly unrelated experimental obser-
Distributional Generalization

Figure 1. The setup and result of Experiment 1. The CIFAR-10 train set is labeled as either Animals or Objects, with label noise affecting only cats. A WideResNet-28-10 is then trained to 0 train error on this train set, and evaluated on the test set. Full experimental details in Appendix D.2

1.1. Distributional Generalization

Informally, Distributional Generalization states that the outputs of classifiers $f$ on their train sets and test sets are close as distributions (as opposed to close in just error). That is, the following joint distributions\(^1\) are close:

\[
(x, f(x))_{x \sim \text{TestSet}} \approx (x, f(x))_{x \sim \text{TrainSet}}
\]

The remainder of this paper is devoted to making the above statement precise, and empirically checking its validity on real-world tasks. Specifically, we want to formally define the notion of approximation ($\approx$), and understand how it depends on the problem parameters (the type of classifier, number of train samples, etc). We focus primarily on interpolating methods, where we formalize Equation (1) through our Feature Calibration Conjecture.

\(^1\)These distributions also include the randomness in sampling the train and test sets, and in training the classifier, as we define more precisely in Section 3.

1.2. Our Contributions and Organization

In this work, we discover new empirical properties of interpolating classifiers, which are not captured in the classical framework of generalization. We then propose formal conjectures to characterize these behaviors.

- In Section 3, we introduce a formal “Feature Calibration” conjecture, which unifies our experimental observations. Roughly, Feature Calibration says that the outputs of classifiers match the statistics of their training distribution when conditioned on certain subgroups.
- In Section 4, we experimentally stress test our Feature Calibration conjecture across various settings in machine learning, including neural networks, kernel machines, and decision trees. This highlights the universality of our results across machine learning.
- In Section 5, we relate our results to classical generalization, by defining a new notion of Distributional Generalization which subsumes both classical generalization and our new conjectures.
- Finally, in Section 5.2 we informally discuss how Distributional Generalization can be applied even for non-interpolating methods.

Our results, thus, extend our understanding of the implicit bias of interpolating methods, and introduce a new type of generalization exhibited across many methods in machine learning.

1.3. Related Work and Significance

Our work has connections to, and implications for many existing research programs in deep learning, described below.

Implicit Bias and Overparameterization. There has been a long line of recent work towards understanding overparameterized and interpolating methods, since these pose challenges for classical theories of generalization (e.g. Zhang et al. (2016); Belkin et al. (2018a;b; 2019); Liang & Rakhlin


Distributional Generalization

(2018); Nakkiran et al. (2020); Schapire et al. (1998); Breiman (1995); Soudry et al. (2018); Gunasekar et al. (2018)). The “implicit bias” program here aims to answer: *Among all models with 0 train error, which model is actually optimal classifiers— is unique to our work as far as we know,* and highlights the broad implications of our results.

**Locality and Manifold Learning.** Our intuition for the behaviors in this work is that they arise due to some form of “locality” of the trained classifiers, in an appropriate embedding space. For example, the behavior observed in Experiment 1 would be consistent with that of a 1-Nearest-Neighbor classifier in an embedding that separates the CIFAR-10 classes well. This intuition that classifiers learn good embeddings is present in various forms in the literature, for example: the so-called “manifold hypothesis,” that natural data lie on a low-dimensional manifold (e.g. Narayanan & Mitter (2010); Sharma & Kaplan (2020)), as well as works on local stiffness of the loss landscape (Fort et al., 2019), and works showing that overparameterized neural networks can learn hidden low-dimensional structure in high-dimensional settings (Gerace et al., 2020; Bach, 2017; Chizat & Bach, 2020). It is open to more formally understand connections between our work and the above.

**Other Related Works.** Our conjectures also describe neural networks under label noise, which has been empirically and theoretically studied in the past (Zhang et al., 2016; Belkin et al., 2018b; Rolnick et al., 2017; Natarajan et al., 2013; Thulasidasan et al., 2019; Ziyin et al., 2020; Chatterji & Long, 2020), though not formally characterized. We include a full discussion of related works in Appendix B.

2. Preliminaries

**Notation.** We consider joint distributions \( \mathcal{D} \) on \( x \in \mathcal{X} \) and discrete \( y \in \mathcal{Y} = [k] \). Let \( S = \{ (x_i, y_i) \}_{i=1}^n \sim \mathcal{D}^n \) denote a train set of \( n \) iid samples from \( \mathcal{D} \). Let \( \mathcal{A} \) denote the training procedure (including architecture and training algorithm for neural networks), and let \( f \leftarrow \text{Train}_{\mathcal{A}}(S) \) denote training a classifier \( f \) on train-set \( S \) using procedure \( \mathcal{A} \). We consider classifiers which output hard decisions \( f : \mathcal{X} \to \mathcal{Y} \). Let \( \text{NN}_S(y)(x) = y_i \) denote the nearest-neighbor to \( x \) in train-set \( S \), with respect to a distance metric \( d \). Our theorems will apply to any distance metric, and so we leave this unspecified. Let \( \text{NN}_S(y)(x) \) denote the nearest-neighbor estimator itself, that is, \( \text{NN}_S(y)(x) \) := \( y_i \) where \( x_i = \text{NN}_S(x) \).

**Experimental Setup.** Briefly, we train all classifiers to interpolation (to 0 train error). Neural networks (MLPs and ResNets (He et al., 2016)) are trained with SGD. Interpolating decision trees are trained using the growth rule from Random Forests (Breiman, 2001). For kernel classification, we consider kernel regression on one-hot labels and kernel SVM, with small or 0 of regularization (which is often optimal Shankar et al. (2020)). Full experimental details are provided in Appendix C.

**Distributional Closeness.** We consider the following notion of closeness for two probability distributions: For two distributions \( P,Q \) over \( \mathcal{X} \times \mathcal{Y} \), let a “test” (or “distin-
that these definitions, crucially, involve randomness from sampling the train set, training the classifier, and sampling a test point).

3.2. Feature Calibration

We now formally describe the Feature Calibration Conjecture. At a high level, we argue that the distributions $D_{\epsilon}$ and $\mathcal{D}$ are statistically close for interpolating classifiers if we first “coarsen” the domain of $x$ by some partition $L : \mathcal{X} \rightarrow [M]$ into $M$ parts. That is, for certain partitions $L$, the following distributions are statistically close:

$$
(L(x), f(x))_{x \sim D} \approx_{\epsilon} (L(x), y)_{x \sim \mathcal{D}}
$$

We think of $L$ as defining subgroups over the domain---for example, $L(x) \in \{\text{dog}, \text{cat}, \text{horse} \ldots\}$. Then, the above statistical closeness is essentially equivalent to requiring that for all subgroups $\ell \in [M]$, the conditional distribution of classifier output on the subgroup—$p(f(x)|L(x) = \ell)$—is close to the true conditional distribution: $p(y|L(x) = \ell)$. The crux of our conjecture lies in defining exactly which subgroups $L$ satisfy this distributional closeness, and quantifying the $\epsilon$ approximation. This is subtle, since it must depend on almost all parameters of the problem. For example, consider a modification to Experiment 1, where we use a fully-connected network (MLP) instead of a ResNet. An MLP cannot properly distinguish cats even when it is actually provided the real CIFAR-10 labels, and so (informally) it has no hope of behaving differently on cats in the setting of Experiment 1, where the cats are not labeled explicitly (See Figure D.2 for results with MLPs). Similarly, if we train the ResNet with very few samples from the distribution, the network will be unable to recognize cats. Thus, the allowable partitions must depend on the classifier family and the training method, including the number of samples.

We conjecture that allowable partitions are those which can themselves be learnt to good test performance with an identical training procedure, but trained with the labels of the partition $L$ instead of $y$. To formalize this, we define a distinguishable feature: a partition of the domain $\mathcal{X}$ that is learnable for a given training procedure. Thus, in Experiment 1, the partition into CIFAR-10 classes would be a distinguishable feature for ResNets (trained with SGD with 50K or more samples), but not for MLPs. The definition below depends on the training procedure $\mathcal{A}$, the data distribution $\mathcal{D}$, number of train samples $n$, and an approximation parameter $\epsilon$ (which we think of as $\epsilon \approx 0$).

**Definition 1 (($\epsilon, \mathcal{A}, \mathcal{D}, n$)-Distinguishable Feature).** For a distribution $\mathcal{D}$ over $\mathcal{X} \times \mathcal{Y}$, number of samples $n$, training procedure $\mathcal{A}$, and small $\epsilon \geq 0$, an ($\epsilon, \mathcal{A}, \mathcal{D}, n$)-distinguishable feature is a partition $L : \mathcal{X} \rightarrow [M]$ of the domain $\mathcal{X}$ into $M$ parts, such that training a model using $\mathcal{A}$ on $n$ samples labeled by $L$ works to classify $L$ with high
Conjecture 1 (Feature Calibration). For all natural distributions \( D \), number of samples \( n \), interpolating training procedures \( A \), and \( \varepsilon \geq 0 \), the following distributions are statistically close for all \((\varepsilon, A, D, n)\)-distinguishable features \( L \):

\[
\Pr_{f \sim \text{Train}_A(D^n)} \left[ \left( L(x), f(x) \right) \approx_{\varepsilon} \left( L(x), y \right) \right]_{x,y \sim D} 
\]

or equivalently:

\[
\left( L(x), \hat{y} \right) \approx_{\varepsilon} \left( L(x), y \right) 
\]

This claims that the TV distance between the LHS and RHS of Equation (4) is at most \( \varepsilon \), where \( \varepsilon \) is the error of the distinguishable feature (in Definition 1). We claim that this holds for all distinguishable features \( L \) “automatically” – we simply train a classifier, without specifying any particular partition. The formal statements of Definition 1 and Conjecture 1 may seem somewhat arbitrary, involving many quantifiers over \((\varepsilon, A, D, n)\). However, we believe these statements are natural: In addition to extensive empirical evidence in Section 4, we also prove that Conjecture 1 is formally true as stated for 1-Nearest-Neighbor classifiers in Theorem 1.

3.3. Feature Calibration for 1-Nearest-Neighbors

Here we prove that the 1-Nearest-Neighbor classifier formally satisfies Conjecture 1, under mild assumptions. Although the classifiers we empirically test are far more complex than 1-Nearest-Neighbors, we view this theorem as support for our (somewhat involved) formalism of Conjecture 1. Indeed, without Theorem 1 below, it is unclear if our statement of Conjecture 1 can ever be satisfied by any classifier, or if it is simply too strong to be true.

This theorem applies generically to a wide class of distributions, with no assumptions on the ambient dimension of inputs or the underlying metric. The only assumption is a weak regularity condition: sampling the nearest-neighbor train point to a random test point should yield (close to) a uniformly random test point.

Theorem 1. Let \( D \) be a distribution over \( X \times Y \), and let \( n \in \mathbb{N} \) be the number of train samples. Assume the following regularity condition holds: Sampling the nearest-neighbor train point to a random test point yields (close to) a uniformly random test point. That is, suppose that for some small \( \delta \geq 0 \), the distributions: \( \{ \text{NN}_S(x) \} \approx_{\delta} \{ x \} \). Then, Conjecture 1 holds. That is, for all \((\varepsilon, \text{NN}, D, n)\)-distinguishable partitions \( L \), the following distributions are statistically close:

\[
\{(y, L(x)) \} \approx_{\varepsilon + \delta} \{(y, \text{NN}_S(x)) \}
\]

The proof of Theorem 1 is straightforward, and provided in Appendix E. Proving this conjecture for more complex models is an important direction for future work.

3.4. Limitations: Natural Distributions

Technically, Conjecture 1 is not fully specified, since it does not specify exactly which classifiers or distributions obey the conjecture. We do not claim that all classifiers and distributions satisfy our conjectures, since it is always possible to construct pathological examples. Nevertheless, we claim our conjectures hold in all “natural” settings, which informally means settings with real data and classifiers that are actually used in practice.

The problem of understanding what separates “natural distributions” from artificial ones is not unique to our work, and lies at the hard of deep learning theory. Many theoretical works handle this by considering simplified distributional assumptions (e.g. smoothness, well-separatedness, gaussianity), which are mathematically tractable, but untested in practice (Arora et al., 2019; Li et al., 2019; Allen-Zhu et al., 2018). In contrast, we do not make untestable mathematical assumptions. This benefit of realism comes at the cost of mathematical formalism. We hope that as the theory of deep learning evolves, we will better understand how to formalize the notion of “natural” in our conjectures.

4. Experiments: Feature Calibration

We now give empirical evidence for our conjecture in a variety of settings in machine learning, including neural networks, kernel machines, and decision trees. While testing all possible distinguishable features for a given setting is computationally intractable, we can check if the conjecture holds for partitions we know to be distinguishable. We begin by considering the simplest possible distinguishable feature,
Distributional Generalization

Figure 2. Feature Calibration. (A) Random confusion matrix on CIFAR-10, with a WideResNet28-10 trained to interpolation. Left: Joint density of labels $y$ and original class $L$ on the train set. Right: Joint density of classifier predictions $f(x)$ and original class $L$ on the test set. These two joint densities are close, as predicted by Conjecture 1. (B) Constant partition: The CIFAR-10 train set is class-rebalanced according to the left panel distribution. The center and right panels show that both ResNets and MLPs have the correct marginal distribution of outputs, even though the MLP has high test error.

and progressively consider more complex ones. Each of the experimental settings below highlights a different aspect of interpolating classifiers, which may be of independent theoretical or practical interest. Selected experiments are summarized here, with full details and further experiments in Appendix D.

Constant Partition: Consider the trivially-distinguishable constant feature: $L(x) = 0$ everywhere. For this feature, Conjecture 1 reduces to the statement that the marginal distribution of class labels for any interpolating classifier is close to the true marginals $p(y)$. To test this, we construct a variant of CIFAR-10 with class-imbalance and train classifiers with varying levels of test errors to interpolation on it. As shown in Figure 2B, the marginals of the classifier outputs are close to the true marginals, even for a classifier that only achieves 37% test error.

Coarse Partition: Consider AlexNet trained on ILSVRC-2012 ImageNet (Russakovsky et al., 2015), a 1000-class image classification problem with 116 varieties of dogs. The network achieves only 56.5% accuracy on the test set. But it will at least classify most dogs as dogs (with 98.4% accuracy), making $L(x) \in \{\text{dog, not-dog}\}$ a distinguishable feature. Moreover, as predicted by Conjecture 1, the network is calibrated with respect to dogs: 22.4% of all dogs in ImageNet are Terriers, and indeed the network classifies 20.9% of all dogs as Terriers (though it has 9% error on which specific dogs it classifies as Terriers). See Appendix D.5 for details.

Class Partition: We now consider settings where the class labels are themselves distinguishable features (e.g., CIFAR-10 classes are distinguishable by ResNets). Thus, this setting predicts the behavior of interpolating classifiers under structured label noise. As an example, we generate a random spare confusion matrix and apply this to the labels of CIFAR-10 as shown in Figure 2A. We find that a WideResNet trained to interpolation outputs the same confusion matrix on the test set as well (Figure 2B).

Now, to test that this phenomenon is indeed robust to the level of noise, we mislable class $0 \rightarrow 1$ with probability $p$ in the CIFAR-10 train set for varying levels of $p$. We then observe $\hat{p}$, the fraction of samples mislabeled by this network from $0 \rightarrow 1$ in the test set (Figure 3A shows $p$ versus $\hat{p}$). The Bayes optimal classifier for this distribution behaves as a step function (in red), and a classifier that obeys Conjecture 1 exactly would follow the diagonal (in green). The actual experiment (in blue) is close to the behavior predicted by Conjecture 1. This experiment shows a contrast with classical learning theory. While most existing theory focuses on whether classifiers converge to the Bayes optimal solution, we show that interpolating classifiers behave “optimally” in a different sense: they match the distribution of their train set. We discuss this more formally in Section 5. Appendix D.4 includes experiments for more distributions and other classifiers such as Decision Trees.

Multiple features: Conjecture 1 states that the network should be automatically calibrated for all distinguishable features, without any explicit labels for them. To do this, we use the CelebA dataset (Liu et al., 2015), containing images with many binary attributes per image (“male”, “blond hair”, etc). We train a ResNet-50 to classify one of the hard attributes (accuracy 80%) and confirm that the Feature Calibration holds for all the other attributes (Figure 3) that are themselves distinguishable. See Appendix D.5 for details.

Quantitative predictions: We now test the quantitative predictions made by Conjecture 1. This conjecture states that the TV-distance between the joint distributions $(L(x), f(x))$ and $(L(x), y)$ is at most $\varepsilon$, where $\varepsilon$ is the error of the training procedure in learning $L$ (see Definition 1). To test this, we consider binary task similar to Experiment 1 where (Ship, Plane) are labeled as class 0 and (Cat, Dog) are labeled as class 1, with $p = 0.3$ fraction of cats mislabeled to class 0. Then, we train a convolutional network to interpolation on this task. To vary the error $\varepsilon$ on these distinguishable
features systematically, we train networks with varying number of train samples. Networks with fewer samples have larger \( \varepsilon \) since they are worse at classifying the distinguishable features of (Ship, Plane, Cat, Dog). Then, we use the same setup to train networks on the binary task and measure the TV-distance between \( (L(x), f(x)) \) and \( (L(x), y) \) in this task. The results are shown in Figure 3C. As predicted, the TV distance on the binary task is upper bounded by \( \varepsilon \) error on the 4-way classification task.

**Note about Proper Scoring Rules:** If the loss function used in training is a strictly-proper scoring rule such as cross-entropy, then we may expect that in the limit of a large-capacity network and infinite data, training on samples \( \{(x_i, y_i)\} \) will yield a good density estimate of \( p(y|x) \) at the softmax layer. However, this is not what is happening in our experiments: First, our experiments consider the hard-decisions, not the softmax outputs. Second, we observe Conjecture 1 even in settings without proper scoring rules (kernel SVM and decision trees).

5. Distributional Generalization

In order to relate our results to the classical theory of generalization, we now propose a formal notion of “Distributional Generalization”, which subsumes both Feature Calibration and classical generalization. In fact, we will also give preliminary evidence that this new notion can apply even for non-interpolating methods, unlike Feature Calibration.

A trained model \( f \) obeys classical generalization (with respect to test error) if its error on the train set is close to its error on the test distribution. We first rewrite this using our definitions below.

**Classical Generalization (informal):** Let \( f \) be a trained classifier. Then \( f \) generalizes if:

\[
\mathbb{E}_{x \sim \text{TrainSet}} \left[ \mathbb{I} \{ \hat{y} \neq y(x) \} \right] \approx \mathbb{E}_{x \sim \text{TestSet}} \left[ \mathbb{I} \{ \hat{y} \neq y(x) \} \right]
\]  

(6)

Above, \( y(x) \) is the true class of \( x \) and \( \hat{y} \) is the predicted class. The LHS of Equation 6 is the train error of \( f \), and the RHS is the test error. Using our definitions of \( \mathcal{D}_{tr}, \mathcal{D}_{te} \) from Section 3.1, and defining \( T_{err}(x, \hat{y}) := \mathbb{I} \{ \hat{y} \neq y(x) \} \), we can write Equation 6 equivalently:

\[
\mathbb{E}_{x, \hat{y} \sim \mathcal{D}_{tr}} \left[ T_{err}(x, \hat{y}) \right] \approx \mathbb{E}_{x, \hat{y} \sim \mathcal{D}_{te}} \left[ T_{err}(x, \hat{y}) \right]
\]  

(7)

That is, classical generalization states that a certain function \( T_{err} \) has similar expectations on both the Train Distribution \( \mathcal{D}_{tr} \) and Test Distribution \( \mathcal{D}_{te} \). We can now introduce Distributional Generalization, which is a property of trained classifiers. It is parameterized by a set of bounded functions ("tests"): \( \mathcal{T} \subseteq \{ T : \mathcal{X} \times \mathcal{Y} \rightarrow [0, 1] \} \).

**Distributional Generalization: Let \( f \) be a trained classifier. Then \( f \) satisfies Distributional Generalization with respect to tests \( \mathcal{T} \) if:**

\[
\forall T \in \mathcal{T} : \mathbb{E}_{x, \hat{y} \sim \mathcal{D}_{tr}} \left[ T(x, \hat{y}) \right] \approx \mathbb{E}_{x, \hat{y} \sim \mathcal{D}_{te}} \left[ T(x, \hat{y}) \right]
\]  

(8)

or equivalently: \( \mathcal{D}_{tr} \approx_{\mathcal{T}} \mathcal{D}_{te} \).

This states that the train and test distribution have similar expectations for all functions in the family \( \mathcal{T} \). For the singleton set \( \mathcal{T} = \{ T_{err} \} \), this is equivalent to classical generalization, but it may hold for much larger sets \( \mathcal{T} \).

This definition of Distributional Generalization, like the definition of classical generalization, is just defining an object—not stating when or how it is satisfied. Feature Calibration turns this into a concrete conjecture, by proposing exactly how Distributional Generalization applies in a given setting.
5.1. Feature Calibration as Distributional Generalization

Here we show that our Feature Calibration Conjecture is a special case of Distributional Generalization, for a certain family of tests $T$. Informally, for a given setting, the family $T$ is all tests which take input $(x, y)$, but only depend on $x$ via a distinguishable feature (Definition 1). For example, a test of the form $T(x, y) = g(L(x), y)$ where $L$ is a distinguishable feature, and $g$ is arbitrary. Formally, for a given problem setting, suppose $L$ is the set of $(\epsilon, A, D, n)$-distinguishable features. Then Conjecture 1 states that for all $L \in L$, we have $L(x), f(x) \approx \epsilon (L(x), y)$. This is equivalent to the statement

$$D_{te} \approx_{\epsilon} T \approx D$$

(9)

where $T$ is the set of functions $T := \{T : T(x, y) = g(L(x), y), L \in L, g : \mathcal{X} \times \mathcal{Y} \to [0, 1]\}$. For interpolating classifiers, we have $D \equiv D_{tr}$, and so Equation (9) is equivalent to $D_{te} \approx_{\epsilon} T D_{tr}$, which is a statement of Distributional Generalization. Since any classifier family will contain a large number of distinguishable features, the set $L$ may be very large. Hence, the distributions $D_{tr}$ and $D_{te}$ can be thought of as being close as distributions.

5.2. Beyond Interpolating Methods

The previous sections have focused on interpolating classifiers, which fit their train sets exactly. Here we informally discuss how to extend our results beyond interpolating methods. We stress that the discussion in this section is not as precise as in previous sections, and is only meant to suggest that our abstraction of Distributional Generalization can be useful in other settings.

For non-interpolating classifiers, we may still expect that they behave similarly on their test and train sets – that is, $D_{te} \approx_{\epsilon} T D_{tr}$, for some family of tests $T$. For example, the following is a possible generalization of Feature Calibration to non-interpolating methods.

**Conjecture 2** (Generalized Feature Calibration, informal). For trained classifiers $f$, the following distributions are statistically close for any partitions $L$ of the domain:

$$\forall L \in L : (L(x), f(x)) \approx_{\epsilon} (L(x), y)$$

(10)

We leave unspecified the exact set of partitions $L$ for which this holds, since we do not yet understand the appropriate notion of “distinguishable feature” in this setting. However, we give experimental evidence suggesting some refinement of Conjecture 2 is true. In Figure 4 we train Gaussian kernel regression on MNIST, with label noise determined by a random sparse confusion matrix. We vary the $\ell_2$ regularization, and plot the confusion matrix of predictions on the train and test sets. With higher regularization, the kernel no longer interpolates the train set, but the test and train confusion matrices remain close. That is, regularization prevents the kernel from fitting the noise on both the train and test sets in a similar way. Full experimental details are given in Appendix C, including an analogous experiment for neural networks on CIFAR-10, with early-stopping in place of regularization (Figure 14). These experiments suggest that Distributional Generalization is a meaningful notion even for non-interpolating classifiers.

6. Conclusion

This work initiates the study of a new kind of generalization—Distributional Generalization— which considers the entire input-output behavior of classifiers, instead of just their test error. We presented both new empirical behaviors, and new formal conjectures which characterize these behaviors. Roughly, our conjecture states that the outputs of interpolating classifiers on the test set are “close in distribution” to their outputs on the train set. These results build a deeper understanding of models used in practice, and also guide us towards theories of overparameterization, implicit bias, and interpolation which better capture practice. We hope our results inspire further work on this important set of properties across machine learning.
ACKNOWLEDGEMENTS

We especially thank Jacob Steinhardt and Boaz Barak for useful discussions during this work. We thank Vaishaal Shankar for providing the Myrtle10 kernel, the ImageNet classifiers, and advice regarding UCI tasks. We thank Guy Gur-Ari for noting the connection to existing work on networks picking up fine-structural aspects of distributions. We also thank a number of people for reviewing early drafts or providing valuable comments, including: Collin Burns, Mihaela Curmei, Benjamin L. Edelman, Sara Fridovich-Keil, Boriana Gjura, Wenshuo Guo, Thibaut Horel, Meena Jagadeesan, Dimitris Kalimeris, Gal Kaplun, Song Mei, Aditi Raghunathan, Ludwig Schmidt, Ilya Sutskever, Yaodong Yu, Kelly W. Zhang, Ruiqi Zhong.

Work supported in part by the Simons Investigator Awards of Boaz Barak and Madhu Sudan, and NSF Awards under grants CCF 1565264, CCF 1715187 and IIS 1409097. Computational resources supported in part by a gift from Oracle, and Microsoft Azure credits (via Harvard Data Science Initiative). P.N. supported in part by a Google PhD Fellowship. Y.B is partially supported by MIT-IBM Watson AI Lab.

References


Nagarajan, V. and Kolter, J. Z. Uniform convergence may be unable to explain generalization in deep learning, 2019.


A. Author Contributions

PN designed the initial neural network experiments which initiated this study. PN and YB brainstormed the formalization of the experimental observations and PN devised the final version of the definitions, conjectures, and their framing as a version of generalization. YB designed the experiments to stress test the Feature Calibration Conjecture under various settings and conducted the final experiments that appear in the Feature Calibration section. PN discovered and investigated the Agreement Property and did the Student-Teacher section. PN did the kernel and decision tree experiments, literature review, and nearest-neighbor proofs. Both authors wrote the paper.

B. Full Related Work

Our work is inspired by the broader study of interpolating and overparameterized methods in machine learning; a partial list of works in this theme includes Zhang et al. (2016); Belkin et al. (2018a;b; 2019); Liang & Rakhlin (2018); Nakkiran et al. (2020); Mei & Montanari (2019); Schapire et al. (1998); Breiman (1995); Ghorbani et al. (2019); Hastie et al. (2019); Bartlett et al. (2020); Advani & Saxe (2017); Geiger et al. (2019); Gerace et al. (2020); Chizat & Bach (2020); Goldt et al. (2019); Arora et al. (2019); Allen-Zhu et al. (2019); Neşhobur et al. (2018); Dziugaite & Roy (2017); Muthukumar et al. (2020); Neal et al. (2018).

Interpolating Methods. Many of the best-performing techniques on high-dimensional tasks are interpolating methods, which fit their train samples to 0 train error. This includes neural-networks and kernels on images (He et al., 2016; Shankar et al., 2020), and random forests on tabular data (Fernández-Delgado et al., 2014). Interpolating methods have been extensively studied both recently and in the past, since we do not theoretically understand their practical success (Schapire et al., 1998; Schapire, 1999; Breiman, 1995; Zhang et al., 2016; Belkin et al., 2018a;b; 2019; Liang & Rakhlin, 2018; Mei & Montanari, 2019; Hastie et al., 2019; Nakkiran et al., 2020). In particular, much of the classical work in statistical learning theory (uniform convergence, VC-dimension, Rademacher complexity, regularization, stability) fails to explain the success of interpolating methods (Zhang et al., 2016; Belkin et al., 2018a;b; Nagarajan & Kolter, 2019). The few techniques which do apply to interpolating methods (e.g. margin theory (Schapire et al., 1998)) remain vacuous on modern neural-networks and kernels.

Decision Trees. In a similar vein to our work, Wyner et al. (2017); Olson & Wyner (2018) investigate decision trees, and show that random forests are equivalent to a Nadaraya–Watson smoother (Nadaraya, 1964; Watson, 1964) with a certain smoothing kernel. Decision trees (Breiman et al., 1984) are often intuitively thought of as “adaptive nearest-neighbors,” since they are explicitly a spatial-partitioning method (Hastie et al., 2009). Thus, it may not be surprising that decision trees behave similarly to 1-Nearest-Neighbors. Wyner et al. (2017); Olson & Wyner (2018) took steps towards characterizing and understanding this behavior – in particular, Olson & Wyner (2018) defines an equivalent smoothing kernel corresponding to a random forest, and empirically investigates the quality of the conditional density estimate. Our work presents a formal characterization of the quality of this conditional density estimate (Conjecture 1), which is a novel characterization even for decision trees, as far as we know.

Kernel Smoothing. The term kernel regression is sometimes used in the literature to refer to kernel smoothers, such as the Nadaraya–Watson kernel smoother (Nadaraya,
1964; Watson, 1964). But in this work we use the term “kernel regression” to refer only to regression in a Reproducing Kernel Hilbert Space, as described in the experimental details.

Label Noise. Our conjectures also describe the behavior of neural networks under label noise, which has been empirically and theoretically studied in the past, though not formally characterized before (Zhang et al., 2016; Belkin et al., 2018b; Rolnick et al., 2017; Natarajan et al., 2013; Thulasidasan et al., 2019; Ziyin et al., 2020; Chatterji & Long, 2020). Prior works have noticed that vanilla interpolating networks are sensitive to label noise (e.g. Figure 1 in Zhang et al. (2016), and Belkin et al. (2018b)), and there are many works on making networks more robust to label noise via modifications to the training procedure or objective (Rolnick et al., 2017; Natarajan et al., 2013; Thulasidasan et al., 2019; Ziyin et al., 2020). In contrast, we claim this sensitivity to label noise is not necessarily a problem to be fixed, but rather a consequence of a stronger property: distributional generalization.

Conditional Density Estimation. Our density calibration property is similar to the guarantees of a conditional density estimator. More specifically, Conjecture 1 states that an interpolating classifier samples from a distribution approximating the conditional density of $p(y|x)$ in a certain sense. Conditional density estimation has been well-studied in classical nonparametric statistics (e.g. the Nadaraya–Watson kernel smoother (Nadaraya, 1964; Watson, 1964)). However, these classical methods behave poorly in high-dimensions, both in theory and in practice. There are some attempts to extend these classical methods to modern high-dimensional problems via augmenting estimators with neural networks (e.g. Rothfuss et al., 2019). Random forests have also been known to exhibit properties similar to conditional density estimators. This has been formalized in various ways, often only with asymptotic guarantees (Meinshausen, 2006; Pospisil & Lee, 2018; Athey et al., 2019).

No prior work that we are aware of attempts to characterize the quality of the resulting density estimate via testable assumptions, as we do with our formulation of Conjecture 1. Finally, our motivation is not to design good conditional density estimators, but rather to study properties of interpolating classifiers — which we find happen to share properties of density estimators.

Feature Calibration (Conjecture 1) is also related to the concepts of calibration and multicalibration (Guo et al., 2017; Niculescu-Mizil & Caruana, 2005; Hébert-Johnson et al., 2018). In our framework, calibration is implied by Feature Calibration for a specific set of partitions $L$ (determined by level sets of the classifier’s confidence). However, we are not concerned with a specific set of partitions (or “subgroups” in the algorithmic fairness literature) but we generally aim to characterize for which partitions Feature Calibration holds. Moreover, we consider only hard-classification decisions and not confidences, and we study only standard learning algorithms which are not given any distinguished set of subgroups/partitions in advance. Our notion of distributional generalization is also related to the notion of “distributional subgroup overfitting” introduced recently by Yaghini et al. (2019) to study algorithmic fairness. This can be seen as studying distributional generalization for a specific family of tests (determined by distinguished subgroups in the population).

Locality and Manifold Learning. Our intuition for the behaviors in this work is that they arise due to some form of “locality” of the trained classifiers, in an appropriate space. This intuition is present in various forms in the literature, for example: the so-called called “manifold hypothesis,” that natural data lie on a low-dimensional manifold (e.g. Narayanan & Mitter (2010); Sharma & Kaplan (2020)), as well as works on local stiffness of the loss landscape (Fort et al., 2019), and works showing that overparameterized neural networks can learn hidden low-dimensional structure in high-dimensional settings (Gerace et al., 2020; Bach, 2017; Chizat & Bach, 2020). It is open to more formally understand connections between our work and the above.

C. Experimental Details

Here we describe general background, and experimental details common to all sections. Then we provide section-specific details below.

C.1. Datasets

We consider the image datasets CIFAR-10 and CIFAR-100 (Krizhevsky et al., 2009), MNIST (LeCun et al., 1998), Fashion-MNIST (Xiao et al., 2017), CelebA (Liu et al., 2015), and ImageNet (Russakovsky et al., 2015). We normalize images to $x \in [0, 1]^{C \times W \times H}$.

We also consider tabular datasets from the UCI repository (Dua & Graff, 2017). For UCI data, we consider the 121 classification tasks as standardized in Fernández-Delgado et al. (2014). Some of these tasks have very few examples, so we restrict to the 92 classification tasks from Fernández-Delgado et al. (2014) which have at least 200 total examples.

C.2. Models

We consider neural-networks, kernel methods, and decision trees.
C.2.1. Decision Trees

We train interpolating decision trees using a growth rule from Random Forests (Breiman, 2001; Ho, 1995): selecting a split based on a random \( \sqrt{d} \) subset of \( d \) features, splitting based on Gini impurity, and growing trees until all leaves have a single sample. This is as implemented by Scikit-learn (Pedregosa et al., 2011) defaults with RandomForestClassifier (\( n_{\text{ estimators}} = 1 \), bootstrap=False).

C.2.2. Kernels

Throughout this work we consider classification via kernel regression and kernel SVM. For \( M \)-class classification via kernel regression, we follow the methodology in e.g. Rahimi & Recht (2008); Belkin et al. (2018b); Shankar et al. (2020). We solve the following convex problem for training:

\[
\alpha^* := \arg\min_{\alpha \in \mathbb{R}^{N \times M}} \|K\alpha - y\|_2^2 + \lambda \alpha^T K\alpha
\]

where \( K_{ij} = k(x_i, x_j) \) is the kernel matrix of the training points for a kernel function \( k, y \in \mathbb{R}^{N \times M} \) is the one-hot encoding of the train labels, and \( \lambda \geq 0 \) is the regularization parameter. The solution can be written

\[
\alpha^* = (K + \lambda I)^{-1} y
\]

which we solve numerically using SciPy linalg.solve (Virtanen et al., 2020). We use the explicit form of all kernels involved. That is, we do not use random-feature approximations (Rahimi & Recht, 2008), though we expect they would behave similarly.

The kernel predictions on test points are then given by

\[
\begin{align*}
g_\alpha(x) &:= \sum_{i \in [N]} \alpha_i k(x, x) \\
f_\alpha(x) &:= \arg\max_{j \in [M]} g_\alpha(x)_j
\end{align*}
\]

where \( g(x) \in \mathbb{R}^M \) are the kernel regressor outputs, and \( g(x) \in [M] \) is the thresholded classification decision. This is equivalent to training \( M \) separate binary regressors (one for each label), and taking the argmax for classification. We usually consider unregularized regression (\( \lambda = 0 \)), except in Section 5.2.

For kernel SVM, we use the implementation provided by Scikit-learn (Pedregosa et al., 2011) sklearn.svm.SVC with a precomputed kernel, for inverse-regularization parameter \( C \geq 0 \) (larger \( C \) corresponds to smaller regularization).

Types of Kernels. We use the following kernel functions \( k: \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R} \geq 0 \).

- **Gaussian Kernel (RBF):**
  \[
k(x_i, x_j) = \exp\left(-\frac{||x_i - x_j||^2}{\sigma^2}\right).
  \]

- **Laplace Kernel:**
  \[
k(x_i, x_j) = \exp\left(-\frac{||x_i - x_j||}{\sigma}\right).
  \]

- **Myrtle10 Kernel:** This is the compositional kernel introduced by Shankar et al. (2020). We use their exact kernel for CIFAR-10.

For the Gaussian and Laplace kernels, we parameterize bandwidth by \( \sigma := \bar{\sigma}/\sqrt{d} \). We use the following bandwidths, found by cross-validation to maximize the unregularized test accuracy:

- **MNIST:** \( \sigma = 0.15 \) for RBF kernel.
- **Fashion-MNIST:** \( \sigma = 0.1 \) for RBF kernel, \( \sigma = 1.0 \) for Laplace kernel.
- **CIFAR-10:** Myrtle10 Kernel from Shankar et al. (2020), and \( \sigma = 0.1 \) for RBF kernel.

C.2.3. Neural Networks

We use 4 different neural networks in our experiments. We use a multi-layer perceptron, and three different Residual networks.

**MLP:** We use a Multi-layer perceptron or a fully connected network with 3 hidden layers with 512 neurons in each layer. A hidden layer is followed by a BatchNormalization layer and ReLU activation function.

**WideResNet:** We use the standard WideResNet-28-10 described in Zagoruyko & Komodakis (2016). Our code is based on this repository.

**ResNet50:** We use a standard ResNet-50 from the PyTorch library (Paszke et al., 2017).

**ResNet18:** We use a modification of ResNet18 (He et al., 2016) adapted to CIFAR-10 image sizes. Our code is based on this repository.

For Experiment 1 and Section 4, the hyperparameters used to train the above networks are given in Table 1.
<table>
<thead>
<tr>
<th>Hyperparameter</th>
<th>MLP</th>
<th>ResNet18</th>
<th>WideResNet</th>
<th>ResNet50</th>
</tr>
</thead>
<tbody>
<tr>
<td>Batchsize</td>
<td>128</td>
<td>128</td>
<td>128</td>
<td>32</td>
</tr>
<tr>
<td>Epochs</td>
<td>820</td>
<td>200</td>
<td>200</td>
<td>50</td>
</tr>
<tr>
<td>Optimizer</td>
<td>Adam ($\beta_1 = 0.9, \beta_2 = 0.999$)</td>
<td>SGD + Momentum (0.9)</td>
<td>SGD + Momentum (0.9)</td>
<td>SGD</td>
</tr>
<tr>
<td>Learning rate (LR) schedule</td>
<td>Constant LR = 0.001</td>
<td>Initial LR = 0.05 scale by 0.1 at epochs (80, 120)</td>
<td>Initial LR = 0.1 scale by 0.2 at epochs (80, 120, 160)</td>
<td>Initial LR = 0.001, scale by 0.1 if training loss stagnant for 2000 gradient steps</td>
</tr>
<tr>
<td>Data Augmentation</td>
<td>Random flips + RandomCrop(32, padding=4)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CIFAR-10 Error</td>
<td>$\sim 37%$</td>
<td>$\sim 8%$</td>
<td>$\sim 4%$</td>
<td>N/A</td>
</tr>
</tbody>
</table>

*Table 1. Hyperparameters used to train the neural networks and their errors on the unmodified CIFAR-10 dataset*
D. Feature Calibration: Appendix

D.1. A guide to reading the plots

All the experiments in support of Conjecture 1 involve various quantities which we enumerate here

1. Inputs $x$: Each experiment involves inputs from a standard dataset like CIFAR-10 or MNIST. We use the standard train/test splits for every dataset.

2. Distinguishable feature $L(x)$: This feature depends only on input $x$. We consider various features like the original classes itself, a superset of classes (as in coarse partition) or some secondary attributes (like the binary attributes provided with CelebA)

3. Output labels $y$: The output label may be some modification of the original labels. For instance, by adding some type of label noise, or a constructed binary task as in Experiment 1

4. Classifier family $F$: We consider various types of classifiers like neural networks trained with gradient based methods, kernel and decision trees.

In each experiment, we are interested in two joint densities $(y, L(x))$, which depends on our dataset and task and is common across train and test, and $(f(x), L(x))$ which depends on the interpolating classifiers outputs on the test set. Since $y, L(x)$ and $f(x)$ are discrete, we will look at their discrete joint distributions. We sometimes refer to $(y, L(x))$ as the train joint density, as at interpolation $(y, L(x)) = (f(x), L(x))$ for all training inputs $x$. We also refer to $(f(x), L(x))$ as the test density, as we measure this only on the test set.

D.2. Experiment 1

Experimental details: We now provide further details for Experiment 1. We first construct a dataset from CIFAR-10 that obeys the joint density $(y, L(x))$ shown in Figure 1 left panel. We then train a WideResNet-28-10 (WRN-28-10) on this modified dataset to zero training error. The network is trained with the hyperparameters described in Table 1. We then observe the joint density $(f(x), L(x))$ on the test images and find that the two joint densities are close as shown in Figure 5.

We now consider a modification of this experiment as follows:

Experiment 2. Consider the following distribution over images $x$ and binary labels $y$. Sample $x$ as a uniformly random CIFAR-10 image, and sample the label as $p(y|x) = \text{Bernoulli}(\text{CIFAR-Class}(x)/10)$. That is, if the CIFAR-10 class of $x$ is $k \in \{0, 1, \ldots 9\}$, then the label is 1 with probability $(k/10)$ and 0 otherwise. Figure 5 shows this joint distribution of $(x, y)$.

As before, train a WideResNet to 0 training error on this distribution.

In this experiment too, we observe that the train and test joint densities are close as shown in Figure 5.

Now, we repeat the same experiment, but with an MLP instead of WRN-28-10. The training procedure is described in Table 1. This MLP has an error on 37% on the original CIFAR-10 dataset.

Since this MLP has poor accuracy on the original CIFAR-10 classification task, it does not form a distinguishable partition for it. As a result, the train and test joint densities (Figure 6) do not match as well as they did for WRN-28-10.

D.3. Constant Partition

Conjecture 1 states that the marginal distribution of class labels for any interpolating classifier $f(x)$ is close to the true marginals $p(y)$. To show this, we construct a dataset based on CIFAR-10 that has class-imbalance. For class $k \in \{0...9\}$, sample $(k + 1) \times 500$ images from that class. This will give us a dataset where classes will have marginal
distribution \( p(y = \ell) \propto \ell + 1 \) for classes \( \ell \in [10] \), as shown in Figure 2. We do this both for the training set and the test set, to keep the distribution \( D \) fixed.

We then train a variety of classifiers (MLPs, RBF Kernel, ResNets) to interpolation on this dataset, which have varying levels of test errors (9-41%). The class balance of classifier outputs on the (rebalanced) test set

D.4. Class Partition

D.4.1. Neural Networks and CIFAR-10

We now describe details for the experiments in Figures 2A and 3A. A WRN-28-10 achieves an error of 4% on CIFAR-10. Hence, the original labels in CIFAR-10 form a distinguishable partition for this dataset. To demonstrate that Conjecture 1 holds, we consider different structured label noise on the CIFAR-10 dataset. To do so, we apply a variety of confusion matrices to the data. That is, for a confusion matrix \( C : 10 \times 10 \) matrix, the element \( c_{ij} \) gives the joint density that a randomly sampled image had original label \( j \), but is flipped to class \( i \). For no noise, this would be an identity matrix.

We begin by a simple confusion matrix where we flip only one class 0 \( \rightarrow \) 1 with varying probability \( p \). Figure 7A shows one such confusion matrix for \( p = 0.4 \). We then train a WideResNet-28-10 to zero train error on this dataset. We use the hyperparameters described in C.2 We find that the classifier outputs on the test set closely track the confusion matrix that was applied to the distribution. Figure 7C shows that this is independent of the value of \( p \) and continues to hold for \( p = [0, 1] \).

We add label noise that takes class \( 0 \rightarrow 1 \) with probability \( p \). Figure 7A shows one such confusion matrix for \( p = 0.4 \). We then train a WideResNet-28-10 to zero train error on this dataset. We use the hyperparameters described in C.2 We find that the classifier outputs on the test set closely track the confusion matrix that was applied to the distribution. Figure 7C shows that this is independent of the value of \( p \) and continues to hold for \( p = [0, 1] \).

D.4.2. Decision Trees

Figure 8 shows a version of this experiment for decision trees on the molecular biology UCI task. The molecular biology task is a 3-way classification problem: to classify the type of a DNA splice junction (donor, acceptor, or neither), given the sequence of DNA (60 bases) surrounding the junction. We add varying amounts of label noise that flips class 2 to class 1 with a certain probability, and we observe that interpolating decision trees reproduce this same structured label noise on the test set.

Similar results hold for decision trees; here we show experiments on two UCI tasks: wine and mushroom.

The wine task is a 3-way classification problem: to identify the cultivar of a given wine (out of 3 cultivars), given 13 physical attributes describing the wine. Figure 9 shows an analogus experiment with label noise taking class 1 to class 2.

The mushroom task is a 2-way classification problem: to classify the type of edibility of a mushroom (edible vs poisonous) given 22 physical attributes (e.g. stalk color, odor, etc). Figure 10 shows an analogous experiment with label noise flipping class 0 to class 1.

D.5. Multiple Features

Conjecture 1 states that the network should be automatically calibrated for all distinguishable features, without any explicit labels for them. To verify this, we use the CelebA dataset (Liu et al., 2015), containing images with various labelled binary attributes per-image (“male”, “blond hair”, etc).
Figure 9. Decision trees on UCI (wine). We add label noise that takes class 1 to class 2 with probability $p \in [0, 0.5]$. Each column shows the test and train confusion matrices for a given $p$. Note that this decision trees achieve high accuracy on this task with no label noise (leftmost column). We plot the empirical joint density of the train set, and not the population joint density of the train distribution, and thus the top row exhibits some statistical error due to small-sample effects.

Figure 10. Decision trees on UCI (mushroom). We add label noise that takes class 0 to class 1 with probability $p \in [0, 0.5]$. Each column shows the test and train confusion matrices for a given $p$. Note that this decision trees achieve high accuracy on this task with no label noise (leftmost column).

e etc). Some of these attributes form a distinguishable feature for ResNet50 as they are learnable to high accuracy (Jahangideh et al., 2018). We pick one of hard attributes as the target classification task. We train a ResNet-50 to predict the attribute \{Attractive, Not Attractive\}. We choose this attribute because a ResNet-50 performs poorly on this task (test error $\sim 20\%$) and has good class balance. We choose an attribute with poor generalization because the conjecture would hold trivially for if the network generalizes well. We initialize the network with a pretrained ResNet-50 from the PyTorch library (Paszke et al., 2017) and use the hyperparameters described in Section C.2 to train on this attribute. We then check the train/test joint density with various other attributes like Male, Wearing Lipstick etc. Note that the network is not given any label information for these additional attributes, but is calibrated with respect to them. That is, the network says $\sim 30\%$ of images that have 'heavy makeup' will be classified as 'Attractive', even if the network makes mistakes on which particular inputs it chooses to do so. In this setting, the label distribution is deterministic, and not directly dependent on the distinguishable features, unlike the experiments considered before. Yet, as we see in Figure 11, the classifier outputs are correctly calibrated for each attribute. Loosely, this can be viewed as the network performing 1NN classification in a metric space that is well separated for each of these distinguishable features.

D.6. Coarse Partition

We now consider cases where the original classes do not form a distinguishable partition for the classifier in consideration. That is, the classifier is not powerful enough to obtain low error on the original dataset, but can perform well on a coarser division of the classes.

To verify this, we consider a division of the CIFAR-10 classes into Objects \{airplane, automobile, ship, truck\} vs Animals \{cat, deer, dog, frog\}. An MLP trained on this problem has low error ($\sim 8\%$), but the same network performs poorly on the full dataset ($\sim 37\%$ error). Hence, Object vs Animals forms a distinguishable partition with MLPs. In Figure 12a, we show the results of training an MLP on the original CIFAR-10 classes. We see that the network mostly classifies objects as objects and animals as animals, even when it might mislabel a dog for a cat.

We perform a similar experiment for the RBF kernel on Fashion-MNIST, with partition \{clothing, shoe, bag\}, in Figure 12b.

ImageNet experiment. In Table 2 we provide results of the terrier experiment in the body, for various ImageNet classifiers. We use publicly available pretrained ImageNet models from this repository, and use their evaluations on the ImageNet test set.

D.7. Discussion: Proper Scoring Rules

Here we distinguish the density-estimation of Conjecture 1 from another setting where density estimation occurs. If
Table 2. ImageNet classifiers are calibrated with respect to dogs: All classifiers predict terrier for roughly ~ 22% of all dogs (last row), though they may mistake which specific dogs are terriers.

(a) CIFAR10 + MLP

(b) Fashion-MNIST + RBF

Figure 12. Coarse partitions as distinguishable features: We consider a setting where the original classes are not distinguishable, but a superset of the classes are distinguishable.
Distributional Generalization

$\ell(\hat{p}, y)$ is a strictly-proper scoring rule\(^3\) on predicted distribution $\hat{p} \in \Delta(\mathcal{Y})$ and sample $y \in \mathcal{Y}$, then the population minimizer of $\ell(F(x), y)$ is exactly the conditional density $F(x) = p(y|x)$. That is,

$$p(y|x) = \arg\min_{F: \mathcal{X} \to \Delta(\mathcal{Y})} \mathbb{E}_{(x,y) \sim p} [\ell(F(x), y)]$$

This suggests that in the limit of large-capacity network and very large data (to approximate population quantities), training neural nets with cross-entropy loss on samples $(x,y)$ will yield a good density estimate of $p(y|x)$ at the softmax layer. However, this is not what is happening in our experiments. First, our experiments consider the hard-thresholded classifier, i.e. the argmax of the softmax layer. If the softmax layer itself was close to $p(y|x)$, then the classifier itself will be close to $\arg\max_y p(y|x)$ – that is, close to the optimal classifier. However, this is not the case (since the classifiers make significant errors). Second, we observe Conjecture 1 even in settings where we train with non-proper scoring rules (e.g. kernel regression, where the classifier does not output a probability).

E. Nearest-Neighbor Proofs

E.1. Feature Calibration Property

Proof of Theorem 1. Recall that $L$ being an $(\varepsilon, NN, D, n)$-distinguishable partition means that nearest-neighbors works to classify $L(x)$ from $x$:

$$\Pr_{\{x_i, y_i\}_i \sim D^n} [NN_S^{(y)}(x) = L(x)] \geq 1 - \varepsilon \quad (13)$$

Now, we have

$$\{(NN_S^{(y)}(x), L(x))\} \sim_{D^n} \{(\hat{y}_i, L(x))\} \sim_{D^n} \hat{x}_i, \hat{y}_i \sim_{NN_S(x)} x, y \sim D \quad (14)$$

$$\approx \varepsilon \{(\hat{y}_i, L(\hat{x}_i))\} \sim_{D^n} \hat{x}_i, \hat{y}_i \sim_{NN_S(x)} x, y \sim D \quad (15)$$

$$\approx \delta \{(\hat{y}_i, L(\hat{x}_i))\} \sim_{D^n} \hat{x}_i, \hat{y}_i \sim D \quad (16)$$

Line (15) is by distinguishability, since $\Pr[L(x) \neq L(\hat{x}_i)] \leq \varepsilon$. And Line (16) is by the regularity condition.

F. Non-interpolating Classifiers: Appendix

Here we give an additional example of distributional generalization: in kernel SVM (as opposed to kernel regression, in the main text).

---

\(^3\)See (Gneiting & Raftery, 2007) for a survey of proper scoring rules.
Figure 13. **Distributional Generalization.** Train (left) and test (right) confusion matrices for kernel SVM on MNIST with random sparse label noise. Each row corresponds to one value of inverse-regularization parameter $C$. All rows are trained on the same (noisy) train set.
Figure 14. **Distributional Generalization for WideResNet on CIFAR-10.** We apply label noise from a random sparse confusion to the CIFAR-10 train set. We then train a single WideResNet28-10, and measure its predictions on the train and test sets over increasing train time (SGD steps). The top row shows the confusion matrix of predictions $f(x)$ vs true labels $L(x)$ on the train set, and the bottom row shows the corresponding confusion matrix on the test set. As the network is trained for longer, it fits more of the noise on the train set, and this behavior is mirrored almost identically on the test set.