Does Learning Require Memorization?
A Short Tale about a Long Tail

Vitaly Feldman[*]
Google Research, Brain Team

Abstract

State-of-the-art results on image recognition tasks are achieved using over-parameterized learning algorithms that (nearly) perfectly fit the training set and are known to fit well even random labels. This tendency to memorize the labels of the training data is not explained by existing theoretical analyses. Memorization of the training data also presents significant privacy risks when the training data contains sensitive personal information and thus it is important to understand whether such memorization is necessary for accurate learning.

We provide a simple conceptual explanation and a theoretical model demonstrating that for natural data distributions memorization of labels is *necessary* for achieving close-to-optimal generalization error. The model is motivated and supported by the results of several recent empirical works. In our model, data is sampled from a mixture of subpopulations and the frequencies of these subpopulations are chosen from some prior. The model allows to quantify the effect of not fitting the training data on the generalization performance of the learned classifier and demonstrates that memorization is necessary whenever frequencies are long-tailed. Image and text data are known to follow such distributions and therefore our results establish a formal link between these empirical phenomena. Our results also have concrete implications for the cost of ensuring differential privacy in learning.

[*] Part of this work was done while the author was visiting the Simons Institute for the Theory of Computing.

1 Introduction

Understanding the generalization properties of learning systems based on deep neural networks (DNNs) is an area of great practical importance and significant theoretical interest. The main conceptual hurdle to adapting the classical approaches for analysis of generalization is the well-known fact that state-of-the-art approaches to training DNNs reach zero (or very low) training error even when the test error is relatively high. In fact, as highlighted in the influential work of Zhang et al. [ZBHRV17], low training error is achieved even when the labels are generated at random. The only way to fit an example whose label cannot be predicted based on the rest of the dataset is to effectively memorize it. In this work we will formalize and quantify this notion of memorization. For now we will informally say that a learning algorithm memorizes the label of some example (x, y) in its dataset S if the model output on S predicts y on x whereas when the learning algorithm is trained on S without (x, y) it is unlikely to predict y on x.

The classical approach to understanding generalization starts with the decomposition of the generalization error $\mathtt{err}_P(h)$ relative to the data distribution P into the empirical error on the training set S and generalization gap (or estimation error):

$$\mathtt{err}_P(h) = \mathtt{err}_S(h) + (\mathtt{err}_P(h) - \mathtt{err}_S(h)) .$$

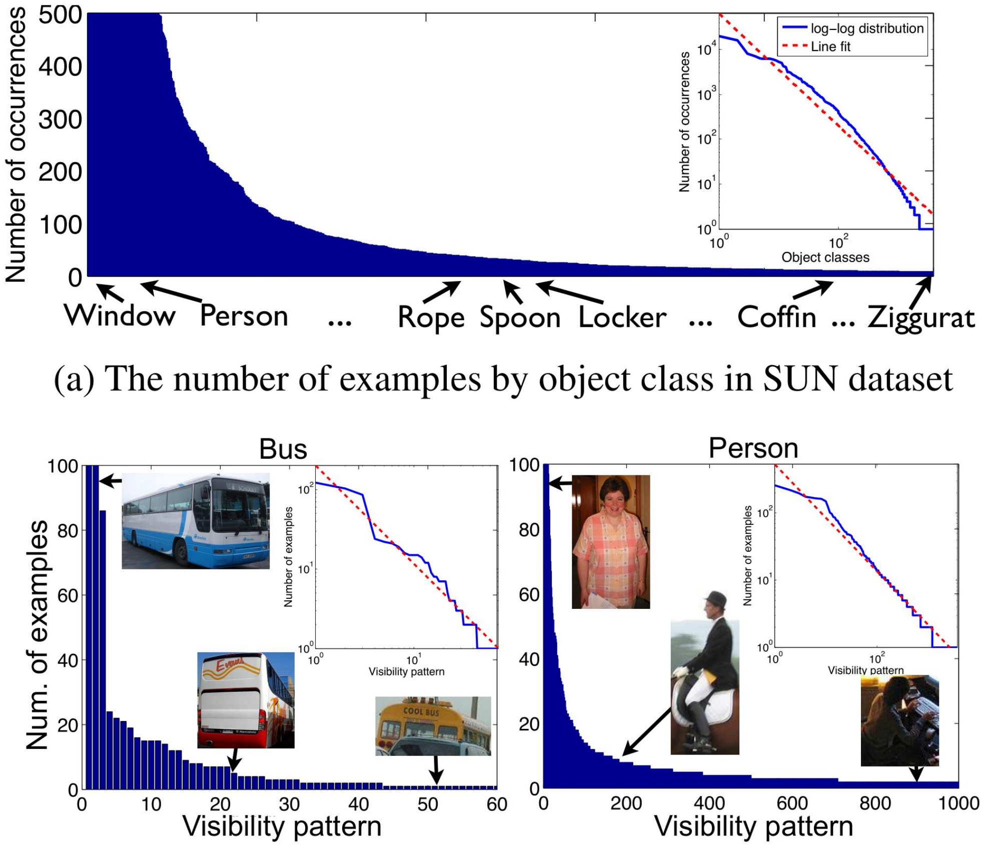
The generalization gap is then upper bounded via some proxy that measures the algorithm's ability to fit arbitrary labels, for example, model complexity or algorithmic stability. For each training example whose label is memorized by the algorithm, the capacity to fit needs to increase at least as much as the training error decreases. Further, a proxy used for theoretical analysis needs to be conservative and tend to grow faster than the actual increase in the algorithm's ability to fit. Thus standard theoretical analyses suggest that algorithms which memorize labels are balancing the empirical error and the ability to fit in a suboptimal way. In particular, they cannot explain why modern ML relies on such algorithms.

This captivating disconnect between the classical theory and modern ML practice has attracted significant amount of research and broad interest in recent years (see Sec. 1.3 for an overview). At the same time the phenomenon is far from new. Random forests [Bre01] and Adaboost [FS97] are known to achieve their optimal generalization error on many learning problems while fitting the training data perfectly [SFBL98; Sch13; WOBM17]. There is also recent evidence that this holds for kernel methods in certain regimes as well [ZBHRV17; BMM18; LR18].

1.1 Our contribution

We propose a conceptually simple explanation and supporting theory for why memorization of labels may be necessary to achieve close-to-optimal generalization error. It is based on the view that the primary hurdle to learning an accurate model is not the noise inherent in the labels but rather an insufficient amount of data to predict accurately on rare and atypical instances. Such instances are usually referred in practice as the "long tail" of the data distribution. It has been widely observed that modern datasets used for visual object recognition and text labeling follow the classical long-tailed distributions such as Zipf distribution (or more general power law distributions).

To formalize the notion of having a "long tail" we will model the data distribution of each class as a mixture of distinct subpopulations. For example, images of birds include numerous different species photographed from different perspectives and under different conditions (such as close-ups, in foliage and in the sky) [VHP17]. Naturally, the subpopulations may have different frequencies (which correspond to mixture coefficients). We model the informal notion of long-tailed data distributions as distributions in which the frequencies of subpopulations are long-tailed. The long-tailed nature of subpopulation frequencies is known



(a) The number of examples by object class in SUN dataset

(b) Distributions of the visibility patterns for bus and person

Figure 1: Long tail of class frequencies and subpopulation frequencies within classes. The figure is taken from [ZAR14] with the authors' permission.

in datasets for which additional human annotations are available. A detailed discussion of this phenomenon in the SUN object detection benchmark [XHEOT10] can be found in the work of Zhu et al. [ZAR14]. In Fig. 1 we include a plot from the work that demonstrates the long tail of the frequency distribution.

Additional evidence that classes can be viewed as long-tailed mixtures of subpopulations comes from extreme multiclass problem. Specifically, these problems often have more than $10,000$ fine-grained labels and the number of examples per class is long-tailed [BS17; WRH17; Kri+17; VHP17; CSSHB18; BS19a]. Observe that fine-grained labels in such problems correspond to subcategories of coarser classes (for example, different species of birds all correspond to the "bird" label in a coarse classification problem). We also remark that subpopulations do not have to directly correspond to human-definable categories. They are the artifacts of the representation used by the learning algorithm which are often relatively low-level.

It is natural to assume that before seeing the dataset the learning algorithm does not know the frequencies of subpopulations and may not be able to predict accurately on a subpopulation without observing any examples from it. A dataset of n samples from a long-tailed mixture distribution will have some subpopulations from which just a single one example was observed (and some subpopulations from which none at all). By our assumption, to fit such an example the learning algorithm will need to memorize the label. The question is whether this is necessary for achieving close-to-optimal generalization error. If the example comes from an extremely rare (or "outlier") subpopulation then memorizing it has no significant benefits. At the same time, it is possible that the example comes from a "borderline" subpopulation with frequency on the order of $1/n$. Fitting such an example is likely to improve the accuracy on the entire subpopulation and thus has a measurable effect on the generalization error.

The key point of this work is that based on observing a single sample from a subpopulation, it is impossible to distinguish samples from "borderline" populations from those in the "outlier" ones. Therefore an algorithm can only avoid the risk of missing "borderline" subpopulations by also memorizing examples from the "outlier" subpopulations. Importantly, in a long-tailed distribution of frequencies, the total weight of frequencies on the order of $1/n$ is significant enough that ignoring these subpopulations will hurt the generalization error substantially. Thus, for such distributions, an algorithm needs to be able to memorize the labels in order to achieve close-to-optimal generalization.

1.1.1 Overview

On a technical level our primary contribution is turning this intuitive but informal explanation into a formal model that allows to quantify the trade-offs involved. This model also allows to quantify the cost of ensuring differential privacy (and even weaker forms of stability) when learning from natural data distributions.

Our starting point is a simple model for classification problems that incorporates the long tail of frequencies in the data distribution. The goal of the model is to isolate the discussion of the effect of memorization on the accuracy from other aspects of modeling subpopulations. More formally, in our problem the domain X is unstructured and has size N (each point will correspond to a subpopulation in the more general model). As usual, we will assume that the labeling function belongs to some class of functions F known to the learning algorithm. We will be primarily interested in the setting where F is rich (or computationally hard) enough that for a significant fraction of the points the learning algorithm cannot predict the label of a point well without observing it in the dataset. In particular, fitting some of the examples will require memorizing their labels.

Nothing is known a priori about the frequency of any individual point aside from a prior distribution over the frequencies described by a list of N frequencies $\pi = (\pi_1, \dots, \pi_N)$. Our results are easiest to express when the objective of the learning algorithm is to minimize the expectation of the error over a random choice of the marginal distribution D over X from some distribution $\mathcal{D}$ (instead of the more usual worst-case error). In addition, for convenience of notation we will also measure the error with respect to a random choice of the labeling function from some distribution $\mathcal{F}$ over F. That is, the objective of a learning algorithm $\mathcal{A}$ is defined as:

$$\overline{\mathtt{err}}(\mathcal{D}, \mathcal{F}, \mathcal{A}) := \mathop{\mathbf{E}}_{D\sim\mathcal{D}, f\sim\mathcal{F}}\left[\mathop{\mathbf{E}}_{S\sim(D,F)^n,\ h=\mathcal{A}(S)}\left[\mathop{\mathbf{E}}_{x\sim D}[h(x)\neq f(x)]\right]\right].$$

Specifically, we consider the following distribution over marginal distributions on X: the frequency of each point in the domain is chosen randomly and independently from the prior π of individual frequencies and then normalized to 1. This process results in a distribution $\mathcal{D}$ over marginal distributions that is similar to choosing the frequencies of the elements to be a random permutation of the elements of π. Models measuring the worst-case error over all the permutations of a list of frequencies underlie the recent breakthroughs in the analysis of density estimation algorithms [OS15; VV16]. We believe that our results can be extended to this worst-case model as well and leave such an extension for future work. (The extension to measuring the worst-case error over the choice of $f \in F$, on the other hand, is straightforward).

Our main result (Thm. 2.3) directly relates the number of points that an algorithm does not fit to the sub-optimality (or excess error) of the algorithm via a quantity that depends only on the frequency prior π and n. Here excess error is measured relative to the optimal algorithm and not relative to the best model in some class. Formally, we denote by $\mathtt{errn}_S(\mathcal{A}, 1)$ the number of examples that appear once in the dataset S and are mislabeled by the classifier that $\mathcal{A}$ outputs on S. A special case of our theorem states:

$$\overline{\mathtt{err}}(\pi, \mathcal{F}, \mathcal{A}) \geq \mathtt{opt}(\pi, \mathcal{F}) + \tau_1 \cdot \mathbf{E}\left[\mathtt{errn}_S(\mathcal{A}, 1)\right]. \tag{1}$$

Here $\overline{\mathtt{err}}(\pi, \mathcal{F}, \mathcal{A})$ refers to the expected generalization error of $\mathcal{A}$ and $\mathtt{opt}(\pi, \mathcal{F})$ is the minimum achievable error by any algorithm (expectations are with respect to the process that generates the learning problem and also sampling of the dataset). The important quantity here is

$$\tau_1 := \frac{\mathbf{E}_{\alpha \sim \bar{\pi}^N}\left[\alpha^2 \cdot (1-\alpha)^{n-1}\right]}{\mathbf{E}_{\alpha \sim \bar{\pi}^N}\left[\alpha \cdot (1-\alpha)^{n-1}\right]},$$

where $\bar{\pi}^N$ is the actual marginal distribution over frequencies that results from our process and is, basically, a slightly smoothed version of π. We note that the optimal algorithm in this case does not depend on π and thus our modeling does not require the learning algorithm to know π to achieve near-optimal generalization error.

The quantity τ_1 is easy to compute given π. As a quick numerical example, for the prototypical long-tailed Zipf distribution (where the frequency of the i-th most frequent item is proportional to $1/i$) over the universe of size $N = 100,000$ and $n = 10,000$ samples, one gets the expected loss of at least $\approx 0.23/n$ per *every* example the learner does not fit. For comparison, the worst-case loss in this setting is determined by the least frequent element and is close to 0. Given that the expected fraction of samples that appear once is $\approx 35\%$, an algorithm that does not fit well will be suboptimal by $\approx 8\%$ (with the optimal top-1 error for 10 balanced classes being $\approx 31\%$ in this case). More generally, we show that τ_1 can be lower bounded by the total weight of the part of the prior π which has frequency on the order of $1/n$ and also that the absence of frequencies on this order will imply negligible τ_1 (see Sec. 2.3 for more details).

Continuous data distributions: Naturally, our simple setting in which individual points have significant probability cannot be applied to continuous and high-dimensional ML problems where each individual point has an exponentially small (in the dimension) probability. In this more general setting the prediction on the example itself has negligible effect on the generalization error. To show how the effects we demonstrated in the simple discrete setting can extend to continuous distributions, we consider mixture models of subpopulations. In our model, the frequencies of subpopulations (or mixture coefficients) are selected randomly according to the prior π as before. The labeling function is also chosen as before and is assumed to be constant over every subpopulation.

The discussion of fitting makes sense only if one assumes that the prediction on the data point in the dataset will affect the predictions on related points. Thus we assume that (with high probability) the learning algorithm's prediction on a single point from a subpopulation will be correlated with the prediction on a random example from the same subpopulation. We refer to this condition as coupling (Defn. 3.1) and show that eq. (1) still holds up to the adjustment for the strength of the coupling.

Intuitively, it is clear that this form of "coupling" is likely to apply to "local" learning rules such as the nearest neighbors algorithm. Indeed, our assumption can be seen as a more abstract version of geometric smoothness conditions on the marginal distribution of the label used in analysis of such methods (*e.g.* [CD14]). We also show that it applies to linear predictors/SVMs in high dimension provided that distinct subpopulations are sufficiently uncorrelated (see Sec. 3.1). Deep neural networks are known to have some of the properties of both nearest neighbor rules and linear classifiers in the last-hidden-layer representation (*e.g.* [CSG18]). Thus they are likely to exhibit this type of coupling as well.

From fitting to memorization and privacy: Our results so far have expressed suboptimality in terms of fitting the data. To relate these results to memorization we give a simple definition of what memorizing a label of a point in the dataset means (we are not aware of a prior formal definition of this notion). Formally, for a dataset $S = (x_i, y_i)_{i \in [n]}$ and $i \in [n]$ define

$$\mathtt{mem}(\mathcal{A}, S, i) := \left| \mathop{\mathbf{Pr}}_{h \sim \mathcal{A}(S)}[h(x_i) = y_i] - \mathop{\mathbf{Pr}}_{h \sim \mathcal{A}(S^{\setminus i})}[h(x_i) = y_i] \right|,$$

where $S^{\setminus i}$ denotes the dataset that is S with (x_i, y_i) removed. This definition is closely related to the classical leave-one-out notion of stability but focuses on the change in the label and not the incurred loss. An immediate corollary of this definition is that an algorithm that cannot memorize labels will be unable to fit the singleton data points whenever the algorithm cannot predict their labels based on the rest of the dataset. Two natural situations in which the algorithm will not be able to predict these labels are learning a complex labeling function (*e.g.* having large VC dimension) and computational hardness of finding a simple model of the data. A direct corollary of our results is that in these situations an algorithm that does not memorize labels will not be able to reach close-to-optimal generalization error. In particular, in these conditions differentially private algorithms will not achieve the same accuracy as non-private algorithms.

1.2 Known empirical evidence

The best results (that we are aware of) on modern benchmarks that are achieved without interpolation are those for differentially private (DP) training algorithms [Aba+16; PAEGT16; PAEGT17; MRTZ18]. While not interpolating is not the goal, the properties of DP imply that a DP algorithm with the privacy parameter $\epsilon = O(1)$ cannot memorize individual labels . Moreover, they result in remarkably low gap between the training and test error that is formally explained by the generalization properties of DP [DFHPRR14]. However, the test error results achieved in these works are well below the state-of-the-art using similar models and training algorithms. For example, Papernot et al. [PAEGT17] report accuracy of 98% and 82.7% on MNIST and SVHN as opposed to 99.2% and 92.8%, respectively when training the same models without privacy.

The motivation and inspiration for this work comes in part from attempts to understand why do DP algorithms fall short of their non-private counterparts and which examples are they more likely to misclassify. A thorough and recent exploration related to this question can be found in the work of Carlini et al. [CEP18]. They consider different ways to measure how "prototypical" each of the data points is according to several natural metrics and across MNIST, CIFAR-10, Fashion-MNIST and ImageNet datasets and compare between these metrics. One of those metrics is the highest level of privacy that a DP training algorithm can achieve while still correctly classifying an example that is correctly classified by a non-private model. As argued in that work and is clear from their comprehensive visualization, the examples on which a DP model errs are either outliers or atypical ones. To illustrate this point, we include the examples for MNIST digit "3" and CIFAR-10 "plane" class from their work as Fig. 2. In addition, the metric based on DP is well correlated with other metrics of being prototypical such as relative confidence of the (non-private) model and human annotation. Their concepts of most and least prototypical map naturally to the frequency of subpopulation in our model. Thus their work supports the view that the reason why learning with DP cannot achieve the same accuracy as non-private learning is that it cannot memorize the tail of the mixture distribution. This view also

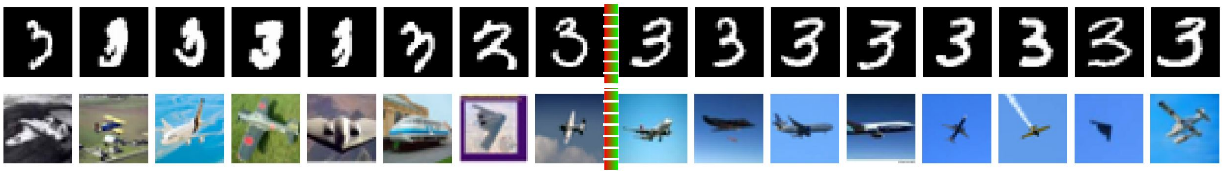


Figure 2: Hardest examples for a differentially private to predict accurately (among those accurately predicted by a non-private model) on the left vs the easiest ones on the right. Top row is for digit “3” from the MNIST dataset and the bottom row is for the class “plane” from the CIFAR-10 dataset. The figure is extracted from [CEP18] with the authors’ permission. Details of the training process can be found in the original work.

explains the recent empirical results showing that the decrease in accuracy is larger for less well represented subpopulations [BS19b].

Our theory also makes a number of predictions that merit empirical investigation. For example, the model predicts that for typical image and text datasets and learning algorithms, there is a significant fraction of examples whose memorization is necessary for predicting accurately on examples from the same subpopulation in the test set. More formally, there exist examples in the training set such that for each of them (1) the label is memorized by the learning algorithm in the sense defined above; (2) there exists a dependent example in the test set in the following sense: the accuracy of the model on the dependent test example drops significantly when the corresponding example from the training set is removed (with no significant effect on the accuracy on the other test examples). This prediction has been already confirmed on MNIST, CIFAR-10/100, SVHN and ImageNet datasets revealing numerous visually similar pairs of relatively atypical examples [FZ19].

1.3 Related work

One line of research motivated by the empirical phenomena we discuss here studies implicit regularization in the overparameterized regime (namely, when the parameter space is large enough that the learning algorithm can perfectly fit the dataset). For example, the classical margin theory [Vap82; CV95; SFBL98] for SVMs and boosting suggests that, while the ambient dimension is large, the learning algorithm implicitly maximizes the margin. The generalization gap can then be upper bounded in terms of the margin. Examples of this approach in the context of DNNs can be found in [NTS15; NBMS17; BFT17; NTSS17; LMZ18] (and references therein). These notions imply that it is beneficial to overparameterize and suffice for explaining why the training algorithm will select the best model among those that do fit the training set. However implicit regularization does not explain why, despite the regularization, the training error is near zero even when the generalization error is large.

Another line of research studies generalization properties of learning algorithm that fit the training data perfectly, often referred to as *interpolating* [BHM18; BMM18]. For example, a classical work of Cover and Hart [CH67] gives bounds on the generalization error of the 1-nearest neighbor algorithm. Recent wave of interest in such methods has lead to new analyses of existing interpolating methods as well as new algorithmic techniques [WOBM17; BRT18; BHM18; LR18; BMM18; RZ19; BLLT19; BHX19; HMRT19; MVS19]. These works bypass the classical approach to generalization outlined above and demonstrate that interpolating methods can generalize while tolerating some amount of noise. In particular, they show that interpolation can be “harmless” in the sense that interpolating methods can in some cases achieve asymptotically optimal generalization error. At the same time, for the problems studied in these works there also exist non-interpolating algorithms with the same (or better) generalization guarantees. Thus they do not explain why interpolation is common in the first place. We also remark that while interpolating the training set (with high generalization error) requires memorization, memorization also occurs without interpolation. For example, experiments of Zhang et al. [ZBHRV17] show that 9% training error is achieved by a standard deep learning algorithm on completely randomly labeled 1000-class Imagenet dataset (with generalization error being 99.9%).

It is known that in the convex setting SGD converges faster when all the loss functions have a joint minimizer [SST10; NWS14] and therefore it has been suggested that interpolation is the result of computational benefits of optimization via SGD [MBB18]. However this hypothesis is not well supported by empirical evidence since interpolation does not appear to significantly affect the speed with which the neural networks are trained [ZBHRV17]. In addition, methods like nearest neighbors, boosting, and bagging are not trained via SGD but tend to interpolate the data as well.

Algorithmic stability [BE02; SSSS09; HRS16; FV19] is essentially the only general approach that is known to imply generalization bounds beyond those achievable via uniform convergence [SSSS09; Fel16]. However it runs into exactly the same conceptual issue as capacity-based bounds: average stability needs to be increased by at least $1/n$ to fit an arbitrary label. In fact, an interpolating learning algorithm does not satisfy any non-trivial uniform stability (but may still be on-average stable).

2 Memorization in Unstructured Classification

Preliminaries: For a natural number n, we use $[n]$ to denote the set $\{1, \ldots, n\}$. For a condition O we use $\mathbf{1}(O)$ to denote the $\{0,1\}$-indicator function of the condition. A dataset is specified by an ordered n-tuple of examples $S = (x_1, y_1), \ldots, (x_n, y_n)$ but we will also treat it as the multi-set of examples it includes. Let X_S denote the set of all points that appear in S.

For a probability distribution D over X, $x \sim D$ denotes choosing x by sampling it randomly from D. For any condition $O \subseteq X$ and function F over X, we denote by $\mathbf{D}_{x \sim D}[F(x) \mid x \in O]$ the probability distribution of $F(x)$, when $x \sim D$ and is conditioned on $x \in O$. For two probability distributions D_1, D_2 over the same domain we use $\mathtt{TV}(D_1, D_2)$ to denote the total variation distance between them.

The goal of the learning algorithm is to predict the labels given a dataset $S = (x_1, y_1), \ldots, (x_n, y_n)$ consisting of i.i.d. samples from some unknown distribution P over $X \times Y$. For any function $h \colon X \to Y$ and distribution P over $X \times Y$, we denote $\mathtt{err}_P(h) := \mathbf{E}_{(x,y)\sim P}[h(x) \neq y]$. As usual, for a randomized learning algorithm $\mathcal{A}$ we denote its expected generalization error on a dataset S by

$$\mathtt{err}_P(\mathcal{A}, S) := \mathop{\mathbf{E}}_{h \sim \mathcal{A}(S)} \left[\mathtt{err}_P(h)\right],$$

where $h \sim \mathcal{A}(S)$ refers to h being the output of a (possibly) randomized algorithm. We also denote by $\mathtt{err}_P(\mathcal{A}) := \mathbf{E}_{S \sim P^n}\left[\mathtt{err}_P(\mathcal{A}, S)\right]$ the expectation of the generalization error of $\mathcal{A}$ when examples are drawn randomly from P.

2.1 Problem setup

To capture the main phenomenon we are interested in, we start by considering a simple and general prediction problem in which the domain does not have any underlying structure (such as the notion of distance). The domains X and Y are discrete, $|X| = N$ and $|Y| = m$ (for concreteness one can think of $X = [N]$ and $Y = [m]$).

The prior information about the labels is encoded using a distribution $\mathcal{F}$ over functions from X to Y. The key assumption is that nothing is known a priori about the frequency of any individual point aside from a prior distribution over the individual frequencies. One natural approach to capturing this assumption is to assume that the frequencies of the elements in X are known up to a permutation. That is, a distribution over X is defined by picking a random permutation of elements of the prior $\pi = (\pi_1, \dots, \pi_N)$. Exact knowledge of the entire frequency prior is also a rather strong assumption in most learning problems. We therefore use a related but different way to model the frequencies (which we have not encountered in prior work). In our model the frequency of each point in X is chosen randomly and independently from the list of possible frequencies π and then normalized to sum up to 1.

More formally, let $\mathcal{D}_\pi^X$ denote the distribution over probability mass functions on X defined as follows. For every $x \in X$, sample p_x randomly, independently and uniformly from the elements of π. Define the corresponding probability mass function on X as $D(x) = \frac{p_x}{\sum_{x \in X} p_x}$. This definition can be naturally generalized to sampling from a general distribution π over frequencies (instead of just the uniform over a list of frequencies). We also denote by $\bar{\pi}^N$ the resulting marginal distribution over the frequency of any single element in x. That is,

$$\bar{\pi}^N(\alpha) := \mathop{\mathbf{Pr}}_{D \sim \mathcal{D}_\pi^X}[D(x) = \alpha].$$

Note that, while π is used to define the process, the actual distribution over individual frequencies the process results in is $\bar{\pi}^N$ and our bounds will be stated in terms of properties of $\bar{\pi}^N$. At the same time, this distinction is not particularly significant for applications of our result since, as we will show later, $\bar{\pi}^N$ is essentially a slightly smoothed version of π.

The key property of this way to generate the frequency distribution is that it allows us to easily express the expected frequency of a sample conditioned on observing it in the dataset. Specifically, in Appendix A we prove the following lemma:

Lemma 2.1. *For any frequency prior π, $x \in X$ and a sequence of points $V = (x_1, \dots, x_n) \in X^n$ that includes x exactly ℓ times, we have*

$$\mathop{\mathbf{E}}_{D \sim \mathcal{D}_\pi^X, U \sim D^n}[D(x) \mid U = V] = \frac{\mathbf{E}_{\alpha \sim \bar{\pi}^N}\left[\alpha^{\ell+1} \cdot (1-\alpha)^{n-\ell}\right]}{\mathbf{E}_{\alpha \sim \bar{\pi}^N}\left[\alpha^{\ell} \cdot (1-\alpha)^{n-\ell}\right]}.$$

An instance of our learning problem is generated by picking a marginal distribution D randomly from $\mathcal{D}_\pi^X$ and picking the true labeling function randomly according to $\mathcal{F}$. We refer to the distribution of the labeled examples $(x, f(x))$ for $x \sim D$ by (D, f). We abbreviate $\mathcal{D}_\pi^X$ as $\mathcal{D}$ whenever the prior and X are clear from the context.

We are interested in evaluating the generalization error of a classification algorithm on instances of our learning problem. Our results apply (via a simple adaption) to the more common setup in statistical learning theory where F is a set of functions and worst case error with respect to a choice of $f \in F$ is considered. However for simplicity of notation and consistency with the random choice of D, we focus on the expectation of the generalization error on a randomly chosen learning problem:

$$\overline{\mathtt{err}}(\pi, \mathcal{F}, \mathcal{A}) := \mathop{\mathbf{E}}_{D \sim \mathcal{D}, f \sim \mathcal{F}}\left[\mathtt{err}_{D,f}(\mathcal{A})\right].$$

2.2 The cost of not fitting

Ability of an algorithm $\mathcal{A}$ to memorize the labels of points in the dataset is closely related to how well it can fit the dataset, or equivalently, to the lowest empirical error $\mathcal{A}$ can achieve. We will now demonstrate that for our simple problem there exists a precise relationship between how well an algorithm fits the labels of the points it observed and the excess generalization error of the algorithm. This relationship will be determined by the prior $\bar{\pi}^N$ and n. Importantly, this relationship will hold even when optimal achievable generalization error is high, a regime not covered by the usual analysis in the "realizable" setting.

In our results the effect of not fitting an example depends on the number of times it occurs in the dataset and therefore we count examples that $\mathcal{A}$ does not fit separately for each possible multiplicity. More formally,

Definition 2.2. *For a dataset $S \in (X \times Y)^n$ and $\ell \in [n]$, let $X_{S=\ell}$ denote the set of points x that appear exactly ℓ times in S. For a function $h \colon X \to Y$ let*

$$\mathtt{errn}_S(h, \ell) := |\{x \in X_{S=\ell} \mid h(x) \neq y\}|$$

and let

$$\mathtt{errn}_S(\mathcal{A}, \ell) := \mathop{\mathbf{E}}_{h \sim \mathcal{A}(S)}[\mathtt{errn}_S(h, \ell)].$$

It is not hard to see (and we show this below) that in this noiseless setting the optimal expected generalization error is achieved by memorizing the dataset. Namely, by the algorithm that outputs the function that on the points in the dataset predicts the observed label and on points outside the dataset predicts the most likely label according to the posterior distribution on $\mathcal{F}$. We will now quantify the excess error of any algorithm that does not fit the labels of all the observed data points. Our result holds for every single dataset (and not just in expectation). To make this formal, we define $\mathcal{G}$ to be the probability distribution over triplets (D, f, S) where $D \sim \mathcal{D}_\pi^X$, $f \sim \mathcal{F}$ and $S \sim (D, f)^n$. For any dataset $Z \in (X \times Y)^n$, let $\mathcal{G}(|Z)$ denote the marginal distribution over distribution-function pairs conditioned on $S = Z$. That is:

$$\mathcal{G}(|Z) := \mathop{\mathbf{D}}_{(D,f,S) \sim \mathcal{G}}[(D, f) \mid S = Z].$$

We then define the expected error of $\mathcal{A}$ conditioned on dataset being equal to Z as

$$\overline{\mathtt{err}}(\pi, \mathcal{F}, \mathcal{A} \mid Z) := \mathop{\mathbf{E}}_{(D,f) \sim \mathcal{G}(|Z)}\left[\mathtt{err}_{D,f}(\mathcal{A}, Z)\right].$$

We will also define $\mathtt{opt}(\pi, \mathcal{F} \mid Z)$ to be the minimum of $\overline{\mathtt{err}}(\pi, \mathcal{F}, \mathcal{A}' \mid Z)$ over all algorithms $\mathcal{A}'$.

Theorem 2.3. *Let π be a frequency prior with a corresponding marginal frequency distribution $\bar{\pi}^N$, and $\mathcal{F}$ be a distribution over Y^X. Then for every learning algorithm $\mathcal{A}$ and every dataset $Z \in (X \times Y)^n$:*

$$\overline{\mathtt{err}}(\pi, \mathcal{F}, \mathcal{A} \mid Z) \geq \mathtt{opt}(\pi, \mathcal{F} \mid Z) + \sum_{\ell \in [n]} \tau_\ell \cdot \mathtt{errn}_Z(\mathcal{A}, \ell),$$

where

$$\tau_\ell := \frac{\mathbf{E}_{\alpha \sim \bar{\pi}^N}\left[\alpha^{\ell+1} \cdot (1-\alpha)^{n-\ell}\right]}{\mathbf{E}_{\alpha \sim \bar{\pi}^N}\left[\alpha^{\ell} \cdot (1-\alpha)^{n-\ell}\right]}.$$

In particular,

$$\overline{\mathtt{err}}(\pi, \mathcal{F}, \mathcal{A}) \geq \mathtt{opt}(\pi, \mathcal{F}) + \mathop{\mathbf{E}}_{D \sim \mathcal{D}_\pi^X, f \sim \mathcal{F}, S \sim (D,f)^n}\left[\sum_{\ell \in [n]} \tau_\ell \cdot \mathtt{errn}_S(\mathcal{A}, \ell)\right].$$

Proof. We denote the marginal distribution of $\mathcal{G}(|Z)$ over D by $\mathcal{D}(|Z)$ and the marginal distribution over f by $\mathcal{F}(|Z)$. We begin by noting that for every $f'\colon X \to Y$ consistent with the examples in Z, the distribution of D conditioned on $f = f'$ is still $\mathcal{D}(|Z)$, since D is chosen independently of any labeling. Therefore we can conclude that $\mathcal{G}(|Z)$ is equal to the product distribution $\mathcal{D}(|Z) \times \mathcal{F}(|Z)$.

Let $X_{Z>0} := X \setminus X_{Z=0}$ denote the set of points in X that appear in one of the examples in Z. To prove the claim we will prove that

$$\overline{\mathtt{err}}(\pi, \mathcal{F}, \mathcal{A} \mid Z) = \sum_{\ell\in[n]} \tau_\ell \cdot \mathtt{errn}_Z(\mathcal{A}, \ell) + \sum_{x\in X_{Z=0}} \mathop{\mathbf{E}}_{h\sim\mathcal{A}(Z), f\sim\mathcal{F}(|Z)} [h(x) \neq f(x)] \cdot p(x, Z), \tag{2}$$

where $p(x, Z) := \mathbf{E}_{D\sim\mathcal{D}(|Z)}[D(x)]$. This will imply the claim since the bottom expression is minimized when for all $\ell \in [n]$, $\mathtt{errn}_Z(\mathcal{A}, \ell) = 0$ and for all $x \in X_{Z=0}$,

$$\mathop{\mathbf{E}}_{h\sim\mathcal{A}(Z), f\sim\mathcal{F}(|Z)} [h(x) \neq f(x)] = \min_{y\in Y} \mathop{\mathbf{E}}_{f\sim\mathcal{F}(|Z)} [f(x) \neq y].$$

Moreover, this minimum is achieved by the algorithm $\mathcal{A}^*$ that fits the examples in Z and predicts the label y that minimizes $\mathbf{E}_{f\sim\mathcal{F}(|Z)}[f(x) \neq y]$ on all the points in $X_{Z=0}$. Namely,

$$\begin{aligned}\sum_{x\in X_{Z=0}} \mathop{\mathbf{E}}_{h\sim\mathcal{A}(Z), f\sim\mathcal{F}(|Z)} [h(x) \neq f(x)] \cdot p(x, Z) &\geq \sum_{x\in X_{Z=0}} \min_{y\in Y} \mathop{\mathbf{E}}_{f\sim\mathcal{F}(|Z)} [f(x) \neq y] \cdot p(x, Z) \\ &= \overline{\mathtt{err}}(\pi, \mathcal{F}, \mathcal{A}^* \mid Z) = \mathtt{opt}(\pi, \mathcal{F} \mid Z).\end{aligned}$$

Plugging this into eq. (2) gives the first claim.

We now prove eq. (2).

$$\begin{aligned}\overline{\mathtt{err}}(\pi, \mathcal{F}, \mathcal{A} \mid Z) &= \mathop{\mathbf{E}}_{(D,f)\sim\mathcal{G}(|Z), h\sim\mathcal{A}(Z)} [\mathtt{err}_{D,f}(h)] \\ &= \mathop{\mathbf{E}}_{(D,f)\sim\mathcal{G}(|Z), h\sim\mathcal{A}(Z)} \left[\sum_{x\in X} \mathbf{1}\left(h(x) \neq f(x)\right) \cdot D(x)\right] \\ &= \sum_{x\in X_{Z>0}} \mathop{\mathbf{E}}_{(D,f)\sim\mathcal{G}(|Z), h\sim\mathcal{A}(Z)} \left[\mathbf{1}\left(h(x) \neq f(x)\right) \cdot D(x)\right] \qquad (3) \\ &+ \sum_{x\in X_{Z=0}} \mathop{\mathbf{E}}_{(D,f)\sim\mathcal{G}(|Z), h\sim\mathcal{A}(Z)} \left[\mathbf{1}\left(h(x) \neq f(x)\right) \cdot D(x)\right]. \qquad (4)\end{aligned}$$

Using the fact that $\mathcal{G}(|Z) = \mathcal{D}(|Z) \times \mathcal{F}(|Z)$, for every $x \in X_{Z=0}$ we get

$$\begin{aligned}\mathop{\mathbf{E}}_{(D,f)\sim\mathcal{G}(|Z), h\sim\mathcal{A}(Z)} \left[\mathbf{1}\left(h(x) \neq f(x)\right) \cdot D(x)\right] &= \mathop{\mathbf{Pr}}_{h\sim\mathcal{A}(Z), f\sim\mathcal{F}(|Z)} [h(x) \neq f(x)] \cdot \mathop{\mathbf{E}}_{D\sim\mathcal{D}(|Z)} [D(x)] \\ &= \mathop{\mathbf{Pr}}_{h\sim\mathcal{A}(Z), f\sim\mathcal{F}(|Z)} [h(x) \neq f(x)] \cdot p(x, Z).\end{aligned}$$

Hence we obtain that the term in line (4) is exactly equal to the second term on the right hand side of eq. (2).

For the term in line (3), we pick an arbitrary $x \in X_{Z=\ell}$ for some $\ell \in [n]$. We can decompose

$$\mathop{\mathbf{E}}_{(D,f)\sim\mathcal{G}(|Z), h\sim\mathcal{A}(Z)} \left[\mathbf{1}\left(h(x) \neq f(x)\right) \cdot D(x)\right] = \mathop{\mathbf{Pr}}_{h\sim\mathcal{A}(Z)} [h(x) \neq f(x)] \cdot \mathop{\mathbf{E}}_{D\sim\mathcal{D}(|Z)} [D(x)]$$

since additional conditioning on $h(x) \neq f(x)$ does not affect the distribution of $D(x)$ (as mentioned, $\mathcal{G}(|Z)$ is a product distribution). Let V denote the sequence of points in the dataset Z. The labels of these points do not affect the conditioning of D and therefore by Lemma 2.1,

$$\mathop{\mathbf{E}}_{D\sim\mathcal{D}(|Z)}[D(x)] = \mathop{\mathbf{E}}_{D\sim\mathcal{D},U\sim D^n}[D(x) \mid U = V] = \frac{\mathbf{E}_{\alpha\sim\bar{\pi}^N}\left[\alpha^{\ell+1}\cdot(1-\alpha)^{n-\ell}\right]}{\mathbf{E}_{\alpha\sim\bar{\pi}^N}\left[\alpha^{\ell}\cdot(1-\alpha)^{n-\ell}\right]} = \tau_\ell.$$

By combining these two equalities we obtain that, as claimed in eq.(2), line (3) is equal to

$$\begin{aligned}(3) &= \sum_{x\in X_{Z>0}} \mathop{\mathbf{E}}_{(D,f)\sim\mathcal{G}(|Z),h\sim\mathcal{A}(Z)}\left[\mathbf{1}\left(h(x)\neq f(x)\right)\cdot D(x)\right] \\ &= \sum_{\ell\in[n]}\sum_{x\in X_{Z=\ell}} \tau_\ell\cdot \mathop{\mathbf{Pr}}_{h\sim\mathcal{A}(Z)}[h(x)\neq f(x)] \\ &= \sum_{\ell\in[n]} \tau_\ell\cdot \mathtt{errn}_Z(\mathcal{A},\ell).\end{aligned}$$

To obtain the second part of the theorem we denote by $\mathcal{S}$ the marginal distribution of $\mathcal{G}$ over S. Observe that

$$\mathtt{opt}(\pi,\mathcal{F}) = \mathop{\mathbf{E}}_{Z\sim\mathcal{S}}[\mathtt{opt}(\pi,\mathcal{F}\mid Z)]$$

since the optimal algorithm is given Z as an input. The second claim now follows by taking the expectation over the marginal distribution over S:

$$\begin{aligned}\overline{\mathtt{err}}(\pi,\mathcal{F},\mathcal{A}) &= \mathop{\mathbf{E}}_{Z\sim\mathcal{S}}[\overline{\mathtt{err}}(\pi,\mathcal{F},\mathcal{A}\mid Z)] \\ &\geq \mathop{\mathbf{E}}_{Z\sim\mathcal{S}}\left[\mathtt{opt}(\pi,\mathcal{F}\mid Z) + \sum_{\ell\in[n]}\tau_\ell\cdot\mathtt{errn}_Z(\mathcal{A},\ell)\right] \\ &= \mathtt{opt}(\pi,\mathcal{F}) + \sum_{\ell\in[n]}\tau_\ell\cdot\mathop{\mathbf{E}}_{Z\sim\mathcal{S}}\left[\mathtt{errn}_Z(\mathcal{A},\ell)\right].\end{aligned}$$

□

2.3 From tails to bounds

Given a frequency prior π, Theorem 2.3 gives a general and easy way to compute the effect of not fitting an example in the dataset. We now spell out some simple and easier to interpret corollaries of this general result and show that the effect can be very significant. The primary case of interest is $\ell = 1$, namely examples that appear only once in S, which we refer to as *singleton* examples. In order to fit those, an algorithm needs memorize their labels (see Section 4.1 for a more detailed discussion). We first note that the expected number of singleton examples is determined by the weight of the entire tail of $\bar{\pi}^N$. Specifically, the expected fraction of the distribution D contributed by frequencies in the range $[\beta_1,\beta_2]$ is defined as:

$$\begin{aligned}\mathtt{weight}(\bar{\pi}^N,[\alpha,\beta]) &:= \mathop{\mathbf{E}}_{D\sim\mathcal{D}}\left[\sum_{x\in X} D(x)\cdot\mathbf{1}\left(D(x)\in[\beta_1,\beta_2]\right)\right] \\ &= N\cdot\mathop{\mathbf{E}}_{\alpha\sim\bar{\pi}^N}\left[\alpha\cdot\mathbf{1}\left(\alpha\in[\beta_1,\beta_2]\right)\right].\end{aligned}$$

At the same time the expected number of singleton points is:

$$\begin{aligned}
\texttt{single}(\bar{\pi}^N) &:= \mathop{\mathbf{E}}_{D\sim\mathcal{D}, V\sim D^n}\left[|X_{V=1}|\right] = \mathop{\mathbf{E}}_{D\sim\mathcal{D}}\left[\sum_{x\in X} \mathop{\mathbf{Pr}}_{V\sim D^n}[x \in X_{V=1}]\right] \\
&= \mathop{\mathbf{E}}_{D\sim\mathcal{D}}\left[\sum_{x\in X} n\cdot D(x)(1-D(x))^{n-1}\right] \\
&= \sum_{x\in X} n \mathop{\mathbf{E}}_{D\sim\mathcal{D}}\left[D(x)(1-D(x))^{n-1}\right] \\
&= nN\cdot \mathop{\mathbf{E}}_{\alpha\sim\bar{\pi}^N}\left[\alpha(1-\alpha)^{n-1}\right].
\end{aligned}$$

For every $\alpha \le 1/n$ we have that $(1-\alpha)^{n-1} \ge 1/3$ (for sufficiently large n). Therefore:

$$\texttt{single}(\bar{\pi}^N) \ge nN\cdot \mathop{\mathbf{E}}_{\alpha\sim\bar{\pi}^N}\left[\alpha(1-\alpha)^{n-1}\cdot \mathbf{1}\left(\alpha\in\left[0,\frac{1}{n}\right]\right)\right] \ge \frac{n}{3}\texttt{weight}\left(\bar{\pi}^N, \left[0,\frac{1}{n}\right]\right). \tag{5}$$

We will now show that the expected cost of not fitting any of the singleton examples is lower bounded by the weight contributed by frequencies on the order of $1/n$. Our bounds will be stated in terms of the properties of $\bar{\pi}^N$ (as opposed to π itself) and therefore, before proceeding, we briefly explain the relationship between these two.

Relationship between π and $\bar{\pi}^N$: Before the normalization step, for every $x \in X$, p_x is distributed exactly according to π (that is uniform over $(\pi_1,\dots,\pi_N)$. Therefore, it is sufficient to understand the distribution of the normalization factor conditioned on $p_x = \pi_i$ for some i. Under this condition the normalization factor s_i is distributed as the sum of $n-1$ independent samples from π plus π_i. The mean of each sample is exactly $1/N$ and thus standard concentration results can be used to obtain that s_i is concentrated around $\frac{N-1}{N} + \pi_i$. Tightness of this concentration depends on the properties of π, most importantly, the largest value $\pi_{\max} := \max_{j\in[N]} \pi_j$ and $\mathbf{Var}[\pi] := \frac{1}{N}\sum_{j\in[N]}(\pi_j - \frac{1}{N})^2 \le \pi_{\max}$. For $\pi_{\max} = o(1)$, $\bar{\pi}^N$ can be effectively seen as convolving each π_i multiplicatively by a factor whose inverse is a Gaussian-like distribution of mean $1 - 1/N + \pi_i$ and variance $\mathbf{Var}(\pi)$. More formally, using Bernstein's (or Bennett's) concentration inequality (*e.g.* [Sri02]) we can easily relate the total weight in a certain range of frequencies under $\bar{\pi}^N$ to the weight in a similar range under π.

Lemma 2.4. *Let $\pi = (\pi_1,\dots,\pi_N)$ be a frequency prior and $\bar{\pi}^N$ be the corresponding marginal distribution over frequencies. For any $0 < \beta_1 < \beta_2 < 1$ Then for and any $\gamma > 0$,*

$$\texttt{weight}(\bar{\pi}^N, [\beta_1,\beta_2]) \ge \frac{(1-\delta)}{1-\frac{1}{N}+\beta_2+\gamma}\cdot\texttt{weight}\left(\pi, \left[\frac{\beta_1}{1-\frac{1}{N}+\beta_1-\gamma}, \frac{\beta_2}{1-\frac{1}{N}+\beta_2+\gamma}\right]\right),$$

where $\pi_{\max} := \max_{j\in[N]}\pi_j$, $\mathbf{Var}[\pi] := \sum_{j\in[N]}(\pi_j - \frac{1}{N})^2$ and $\delta := 2\cdot e^{\frac{-\gamma^2}{2(N-1)\mathbf{Var}(\pi)+2\gamma\pi_{\max}/3}}$.

Note that

$$\mathbf{Var}[\pi] \le \frac{1}{N}\sum_{j\in[N]}\pi_j^2 \le \frac{\pi_{\max}}{N}\cdot\sum_{j\in[N]}\pi_j = \frac{\pi_{\max}}{N}.$$

By taking $\gamma = 1/4$, we can ensure that the boundaries of the frequency interval change by a factor of at most (roughly) $4/3$. For such γ we will obtain $\delta \le 2e^{-1/(40\pi_{\max})}$ and in particular $\pi_{\max} \le 1/200$ will suffice for making the correction $(1-\delta)$ at least $99/100$ (which is insignificant for our purposes).

Bounds for $\ell = 1$: We now show a simple lower bound on τ_1 in terms of $\texttt{weight}(\bar{\pi}^N, [1/2n, 1/n])$ (similar results hold for other choices of the interval $[c_1/n, c_2/n]$). We also do not optimize the constants in the bounds as our goal is to demonstrate the qualitative behavior.

Lemma 2.5. *For every frequency prior π and sufficiently large n, N,*

$$\tau_1 \geq \frac{1}{5n} \cdot \texttt{weight}\left(\bar{\pi}^N, \left[\frac{1}{3n}, \frac{2}{n}\right]\right).$$

If, in addition, $\pi_{\max} \leq 1/200$, then

$$\tau_1 \geq \frac{1}{7n} \cdot \texttt{weight}\left(\pi, \left[\frac{1}{2n}, \frac{1}{n}\right]\right).$$

Proof. We first observe that the denominator of τ_1 satisfies

$$\mathop{\mathbf{E}}_{\alpha \sim \bar{\pi}^N}\left[\alpha(1-\alpha)^{n-1}\right] \leq \mathop{\mathbf{E}}_{\alpha \sim \bar{\pi}^N}[\alpha] = \frac{1}{N}.$$

Now, by simple calculus, for every $\alpha \in \left[\frac{1}{3n}, \frac{2}{n}\right]$ and sufficiently large n,

$$\alpha^2(1-\alpha)^{n-1} \geq \frac{1}{5n} \cdot \alpha.$$

Therefore

$$\begin{aligned}
\tau_1 &= \frac{\mathbf{E}_{\alpha \sim \bar{\pi}^N}\left[\alpha^2(1-\alpha)^{n-1}\right]}{\mathbf{E}_{\alpha \sim \bar{\pi}^N}\left[\alpha(1-\alpha)^{n-1}\right]} \\
&\geq \frac{\frac{1}{5n} \cdot \mathbf{E}_{\alpha \sim \bar{\pi}^N}\left[\alpha \cdot \mathbf{1}\left(\alpha \in \left[\frac{1}{3n}, \frac{2}{n}\right]\right)\right]}{\frac{1}{N}} = \frac{1}{5n} \cdot \texttt{weight}\left(\bar{\pi}^N, \left[\frac{1}{3n}, \frac{2}{n}\right]\right).
\end{aligned}$$

To obtain the second part of the claim we apply Lemma 2.4 for $\gamma = 1/4$ (as discussed above). To verify, observe that for sufficiently large n and N, $\frac{\frac{1}{3n}}{1-\frac{1}{N}+\frac{1}{3n}-1/4} \leq \frac{1}{2n}$ and $\frac{\frac{2}{n}}{1-\frac{1}{N}+\frac{2}{n}+1/4} \geq \frac{1}{n}$, and $\frac{(1-\delta)}{1-\frac{1}{N}+\frac{2}{n}+\gamma} \geq \frac{3}{4}$. □

The value of $\tau_1 = \Omega(1/n)$ corresponds to paying on the order of $1/n$ in generalization error for every example that is not fit by the algorithm. Hence if the total weight of frequencies in the range of $1/n$ is at least some θ then the algorithm that does not fit them will be suboptimal by θ times the fraction of such examples in the dataset. By eq. (5), the fraction of such examples themselves is determined by the weight of the entire tail $\texttt{weight}(\bar{\pi}^N, [0, 1/n])$.

We can contrast this situation with the case where there are no frequencies that are on the order of $1/n$. Even when the data distribution has no elements with such frequency, the total weight of the frequencies in the tail and as a result the fraction of singleton points might be large. Still as we show in such case the cost of not fitting such examples will be negligible.

Lemma 2.6. *Let π be a frequency prior such that for some $\theta \leq \frac{1}{2n}$, $\texttt{weight}\left(\bar{\pi}^N, \left[\theta, \frac{t}{n}\right]\right) = 0$, where $t = \ln(1/(\theta\beta)) + 2$ for $\beta := \texttt{weight}\left(\bar{\pi}^N, [0, \theta]\right)$. Then $\tau_1 \leq 2\theta$.*

Proof. We first observe that the numerator of τ_1 is at most:

$$\begin{aligned}\mathop{\mathbf{E}}_{\alpha\sim\bar{\pi}^N}\left[\alpha^2(1-\alpha)^{n-1}\right] \leq \max_{\alpha\in[t/n,1]}\alpha^2(1-\alpha)^{n-1}\cdot\mathop{\mathbf{Pr}}_{\alpha\sim\bar{\pi}^N}\left[\alpha\geq\frac{t}{n}\right]\\ +\mathop{\mathbf{E}}_{\alpha\sim\bar{\pi}^N}\left[\alpha^2(1-\alpha)^{n-1}\cdot\mathbf{1}\left(\alpha\leq\theta\right)\right].\end{aligned}$$

By Markov's inequality, $\mathbf{E}_{\alpha\sim\bar{\pi}^N}[\alpha]=\frac{1}{N}$ implies

$$\mathop{\mathbf{Pr}}_{\alpha\sim\bar{\pi}^N}\left[\alpha\geq\frac{t}{n}\right]\leq\frac{n}{tN}.$$

In addition, by our definition of t,

$$\max_{\alpha\in[t/n,1]}\alpha^2(1-\alpha)^{n-1}\leq\frac{t}{n}\left(1-\frac{t}{n}\right)^{n-1}\leq\frac{t\beta\theta}{en}.$$

Therefore the first term in the numerator is upper bounded by $\frac{n}{tN}\frac{t\beta\theta}{en}\leq\frac{\beta\theta}{eN}$. At the same time the second term in the numerator satisfies:

$$\begin{aligned}\mathop{\mathbf{E}}_{\alpha\sim\bar{\pi}^N}\left[\alpha^2(1-\alpha)^{n-1}\cdot\mathbf{1}\left(\alpha\leq\theta\right)\right] &\geq\theta(1-\theta)^{n-1}\cdot\mathop{\mathbf{E}}_{\alpha\sim\bar{\pi}^N}\left[\alpha\cdot\mathbf{1}\left(\alpha\leq\theta\right)\right]\\ &\geq\theta\left(1-\frac{1}{2n}\right)^{n-1}\cdot\frac{\texttt{weight}\left(\bar{\pi}^N,[0,\theta]\right)}{N}\geq\frac{\theta\beta}{2N}.\end{aligned}$$

Therefore the second term is at least as large as the first term and we obtain that:

$$\begin{aligned}\mathop{\mathbf{E}}_{\alpha\sim\bar{\pi}^N}\left[\alpha^2(1-\alpha)^{n-1}\right] &\leq 2\cdot\mathop{\mathbf{E}}_{\alpha\sim\bar{\pi}^N}\left[\alpha^2(1-\alpha)^{n-1}\cdot\mathbf{1}\left(\alpha\leq\theta\right)\right]\\ &\leq 2\theta\cdot\mathop{\mathbf{E}}_{\alpha\sim\bar{\pi}^N}\left[\alpha(1-\alpha)^{n-1}\cdot\mathbf{1}\left(\alpha\leq\theta\right)\right]\\ &\leq 2\theta\cdot\mathop{\mathbf{E}}_{\alpha\sim\bar{\pi}^N}\left[\alpha(1-\alpha)^{n-1}\right].\end{aligned}$$

Thus $\tau_1\leq 2\theta$ as claimed. □

For $\theta=1/(2n^2)$, under the conditions of Lemma 2.6 we will obtain that the suboptimality of the algorithm that does not fit any of the singleton examples is at most $1/n$.

2.4 Comparison with standard approaches to generalization

We now briefly demonstrate that standard approaches for analysis of generalization error cannot be used to derive the conclusions of this section and do not capture our simple problem whenever $N\geq n$. For concreteness, we will use $m=2$ with the uniform prior over all labelings. Without any structure in the labels, a natural class of algorithms for the problem are algorithms that pick a subset of points whose labels are memorized and predict randomly on the other points in the domain.

First of all, it is clear that any approach that does not make any assumption on the marginal distribution D cannot adequately capture the generalization error of such algorithms. A distribution-independent generalization bound needs to apply to the uniform distribution over X. For this distribution the expected generalization error for a randomly chosen labeling function f will be at least $(1-n/N)/2$. In particular, no non-trivial bound on the generalization error will be possible for $N \gg n$. For sufficiently large N, the differences in the generalization error of different algorithms will be insignificant and therefore such notion will not be useful for guiding the choice of the algorithm.

Notions that are based on the algorithm knowing the input distribution D are not applicable to our setting. Indeed the main difficulty is that the algorithm does not know the exact frequencies of the singleton elements. An algorithm that knows D would not need to fit the points whose frequency is less than say $1/n^2$. Thus the algorithm would be able to achieve excess error of at most $1/n$ without fitting the dataset which is inconsistent with the conclusions in our model. As an extreme example, consider the case when the prior contains $n/2$ points of frequency $1/n$ and $n^2/2$ points of frequency $1/n^2$. In this case, the algorithm that knows D can fit only 50% of the points in the dataset and achieve excess generalization error of around $1/(2n)$. In contrast, our analysis shows that an algorithm that only knows the prior and fits only 50% of the dataset will be suboptimal by $> 13\%$.

Fairly tight data-dependent bounds on the generalization error can be obtained via the notion of empirical Rademacher complexity [Kol01; BM02]. Empirical Rademacher complexity for a dataset S and the class of all Boolean functions on X that memorize k points is $\geq \min\{k, |X_S|\}/n$. Similar bound can also be obtained via weak notions of stability such as average leave-one-out stability [BE02; RMP05; MNPR06; SSSS10]

$$\texttt{LOOstab}(P, \mathcal{A}) := \frac{1}{n} \sum_{i \in [n]} \mathop{\mathbf{E}}_{S \sim P^n} \left[\left| \mathop{\mathbf{Pr}}_{h \sim \mathcal{A}(S)} [h(x_i) = y_i] - \mathop{\mathbf{Pr}}_{h \sim \mathcal{A}(S^{\setminus i})} [h(x_i) = y_i] \right| \right], \tag{6}$$

where $S^{\setminus i}$ refers to S with i-th example removed. If we were to use either of these notions to pick k (the number of points to memorize), we would end up not fitting any of the singleton points. The simple reason for this is that, just like a learning algorithm cannot distinguish between “outlier” and “borderline” points given S in this setting, neither will any bound. Therefore any true upper bound on the generalization error that is not aware of the prior on the frequencies needs to be correct when all the points that occur once are “outliers”. Fitting any of the outliers does not improve the generalization error at all and therefore such upper bounds on the generalization error cannot be used to correctly guide the choice of k.

3 Prediction in Mixture Models

Our problem setting in Section 2 considers discrete domains without any structure on X. The results also focus on elements of the domain whose frequency is on the order of $1/n$. Naturally, practical prediction problems are high-dimensional with each individual point having an exponentially small (in the dimension) probability. Therefore direct application of our analysis from Section 2 for the unstructured case makes little sense. Indeed, any learning algorithm $\mathcal{A}$ can be modified to a learning algorithm $\mathcal{A}'$ that does not fit any of the points in the dataset and achieves basically the same generalization error as $\mathcal{A}$ simply by modifying $\mathcal{A}$’s predictions on the training data to different labels and vice versa (any algorithm can be made to fit the dataset without any effect on its generalization).

At the same time in high dimensional settings the points have additional structure that can be exploited by a learning algorithm. Most machine learning algorithms are very likely to produce the same prediction on points that are sufficiently “close” in some representation. The representation itself may be designed based on domain knowledge or data-derived (in a not too sensitive way). This is clearly true about k-NN, SVMs/linear predictors and has been empirically observed for neural networks once the trained representation in the last hidden layer is considered.

The second important aspect of natural image and text data is that it can be viewed as a mixture of numerous subpopulations. As we have discussed in the introduction, the relative frequency of these subpopulations has been observed to have a long-tailed distribution most obvious when considering the label distribution in extreme multiclass problems [ZAR14; BS17; WRH17; Kri+17; VHP17; CSSHB18; VH+18; BS19a] (see also Fig. 1). A natural way to think of and a common way to model subpopulations (or mixture components) is as consisting of points that are similar to each other yet sufficiently different from other points in the domain.

We capture the essence of these two properties using the following model that applies the ideas we developed in Section 2 to mixture models. To keep the main points clear we keep the model relatively simple by making relatively strong assumptions on the structure. (We discuss several ways in which the model's assumptions can be relaxed or generalized later).

We model the unlabeled data distribution as a mixture of a large number of fixed distribution $M_1, \dots, M_N$. For simplicity, we assume that these distributions have disjoint support, namely M_i is supported over X_i and $X_i \cap X_j = \emptyset$ for $i \neq j$ (without loss of generality $X = \cup_{i\in[N]} X_i$). For $x \in X$ we denote i_x to be the index of the sub-domain of x and by X_x (or M_x) the sub-domain (or subpopulation, respectively) itself.

The unknown distribution $M(x) \equiv \sum_{i\in[N]} \alpha_i M_i(x)$ for some vector of mixture coefficients $(\alpha_1, \dots, \alpha_N)$ that sums up to 1. We describe it as a distribution $D(x)$ over $[N]$ (that is $\alpha_i = D(i)$). As in our unstructured model, we assume that nothing is known a priori about the mixture coefficients aside from (possibly) a prior $\pi = (\pi_1, \dots, \pi_N)$ described by a list of frequencies. The mixture coefficients are generated, as before, by sampling D from $\mathcal{D}_\pi^{[N]}$. We denote by M_D the distribution over X defined as $M_D(x) \equiv \sum_{i\in[N]} D(i) M_i(x)$.

We assume that the entire subpopulation X_i is labeled by the same label and the label prior is captured via an arbitrary distribution $\mathcal{F}$ over functions from $[N]$ to Y. Note that such prior can be used to reflect a common situation where a subpopulation that is "close" to subpopulations i_1 and i_2 is likely to have the same label as either i_1 or i_2.The labeling function L for the entire domain X is sampled by first sampling $f \sim \mathcal{F}$ and defining $L_f(x) = f(i_x)$.

To model the properties of the learning algorithm we assume that for every point x in a dataset S the distribution over predictions $h(x)$ for a random predictor output by $\mathcal{A}(S)$ is close to (or at least not too different) from the distribution over predictions that $\mathcal{A}$ produces over the entire subpopulation of x. This follows the intuition that labeling x will have a measurable effect on the prediction over the entire subpopulation. This effect may depend on the number of other points from the same subpopulation and therefore our assumption will be parameterized by n parameters.

Definition 3.1. *Let X be a domain partitioned into sub-domains $\{X_i\}_{i\in[N]}$ with subpopulations $\{M_i\}_{i\in[N]}$ over the sub-domains. For a dataset S, let $X_{S=\ell}$ denote the union of subpopulations X_i such that points from X_i appear exactly ℓ times in S. For $\Lambda = (\lambda_1, \dots, \lambda_n)$, we say that an algorithm $\mathcal{A}$ is* Λ-subpopulation-coupled *if for every $S \in (X \times Y)^n$, $x \in X_{S=\ell}$,*

$$\mathtt{TV}\left(\underset{h\sim\mathcal{A}(S)}{\mathbf{D}}[h(x)], \underset{x'\sim M_x, h\sim\mathcal{A}(S)}{\mathbf{D}}[h(x')]\right) \leq 1 - \lambda_\ell.$$

Note that we do not restrict the algorithm to be coupled in this sense over subpopulations that are not represented in the data. This distinction is important since predictors output by most natural algorithms vary over regions from which no examples were observed. As a result the setting here cannot be derived by simply collapsing points in the sub-domain into a single point and applying the results from the unstructured case. However, the analysis and the results in Sec. 2 still apply essentially verbatim to this more general setup. All we need is to extend the definition of $\mathtt{errn}_S(\mathcal{A}, \ell)$ to look at the multiplicity of sub-domains and not points themselves and count mistakes just once per sub-domain. For a function $h\colon X \to Y$ let

$$\mathtt{errn}_S(h,\ell) = \frac{1}{\ell} \sum_{i\in[n]} \mathbf{1}\left(x_i \in X_{S=\ell} \text{ and } h(x_i) \neq y_i\right).$$

As before, $\mathtt{errn}_S(\mathcal{A},\ell) = \mathbf{E}_{h\sim\mathcal{A}(S)}[\mathtt{errn}_S(h,\ell)]$. With this definition we get the following generalization of Theorem 2 (we only state the version for the total expectation of the error but the per-dataset version holds as well):

Theorem 3.2. *Let $\{M_i\}_{i\in[N]}$ be subpopulations over sub-domains $\{X_i\}_{i\in[N]}$ and let π and $\mathcal{F}$ be some frequency and label priors. Then for every Λ-subpopulation-coupled learning algorithm $\mathcal{A}$:*

$$\overline{\mathtt{err}}(\pi,\mathcal{F},\mathcal{A}) \geq \mathtt{opt}(\pi,\mathcal{F}) + \mathop{\mathbf{E}}_{D\sim\mathcal{D}_\pi^{[N]},f\sim\mathcal{F},S\sim(M_D,L_f)^n}\left[\sum_{\ell\in[n]} \lambda_\ell \tau_\ell \cdot \mathtt{errn}_S(\mathcal{A},\ell)\right],$$

where τ_ℓ is defined in Thm. 2.3.

We now briefly discuss how the modeling assumptions can be relaxed. We first note that it suffices for subpopulation coupling to hold with high probability over the choice of dataset S from the marginal distribution over the datasets $\mathcal{S}$. Namely, if the property in Definition 3.1 holds with probability $1-\delta$ over the choice of $S \sim \mathcal{S}$ (where, $\mathcal{S}$ is the marginal distribution over the datasets) then the conclusion of the theorem holds up to an additional δ. This follows immediately from the fact that Theorem 3.2 holds for every dataset separately.

The assumption that the components of the mixture are supported on disjoint subdomains is potentially quite restrictive as it does not allow for ambiguous data points (for which Bayes optimal error is > 0). Subpopulations are also often modeled as Gaussians (or other distributions with unbounded support). If the probability of the overlap between the subpopulations is sufficiently small, then one can reduce this case to the disjoint one by modifying the components M_i to have disjoint supports while changing the marginal distribution over S by at most δ in the TV distance (and then appealing to the same argument as above). Dealing with a more general case allowing general overlap is significantly messier but the basic insight still applies: observing a single point sampled from some subpopulation increases the expectation of the frequency of the subpopulation under the posterior distribution. That increase can make this expectation significant making it necessary to memorize the label of the point.

3.1 Examples

We will now provide some intuition on why one would expect the Λ-subpopulation-coupling to hold for some natural classes of algorithms. Our goal here is not to propose or justify specific models of data but rather to relate properties of known learning systems (and corresponding properties of data) to subpopulation coupling. Importantly, we aim to demonstrate that the coupling emerges from the interaction between the algorithm and the geometric properties of the data distribution and not from any explicit knowledge of subpopulations.

Local algorithms: A simple example of a class of algorithms that will exhibit subpopulation coupling is k-NN-like algorithms and other algorithms that are in some sense locally smooth. If subpopulations are sufficiently "clustered" so that including the example (x,y) in the predictor will affect the prediction in the neighborhood of x and the total weight of affected neighborhood is some fraction λ_1 of the subpopulation, then we will obtain subpopulation coupling with λ_1. In the more concrete (and extreme case), when for every point $x \in X$, the most distant point in X_x is closer than the closest point from the other subpopulations we will get that any example from a subpopulation will cause a 1-NN classifier to predict in the same way over the entire subpopulation. In particular, it would make it Λ-subpopulation-coupled for $\Lambda = (1, \ldots, 1)$.

Linear classifiers: A more interesting case to understand is that of linear classifiers and by extension SVMs and (in a limited sense) neural networks. We will examine a high-dimensional setting, where $d \gg n$. We will assume that points within each subpopulation are likely to have relatively large inner product whereas for every subpopulation most points will, with high probability have, a substantially large component that is orthogonal to the span of n random samples from other populations. These conditions are impossible to satisfy when $d \leq n$ but are easy to satisfy when d is sufficiently large. Formally, we assume that points in most datasets sampled from the data distribution satisfy the following condition:

Definition 3.3. *Let $X \subset \mathbb{R}^d$ be a domain partitioned into subdomains $\{X_i\}_{i\in[N]}$. We say that a sequence of points $V = (x_1, \ldots, x_n)$ is (τ, θ)-independent if it holds that*

- *for all i, j such that $x_i, x_j \in X_t$ for some t, $\langle x_i, x_j\rangle \geq \tau\|x_i\|_2\|x_j\|_2$ and*
- *for all i such that $x_i \in X_t$, and any $v \in \mathtt{span}(V \setminus X_t)$, $|\langle x_i, v\rangle| \leq \theta\|x\|_2\|v\|_2$.*

We consider the performance of linear classifiers that approximately maximize the margin. Here, by "approximately" we will simply assume that they output classifiers that achieve at least $1/2$ of the optimal margin achievable when separating the same points in the given dataset. Note that algorithms with this property are easy to implement efficiently via SGD on the cross-entropy loss [SHNGS18] and also via simple regularization of the Perceptron algorithm [SSS05]. We will also assume that the linear classifiers output by the algorithm lie in the span of the points in the dataset[1] Formally, we define approximately margin-maximizing algorithms in this multi-class setting (for convenience, restricted to the homogeneous case) as follows:

Definition 3.4. *An algorithm $\mathcal{A}$ is an* approximately margin maximizing m-class linear classifier *if given a dataset $S = ((x_1, y_1), \ldots, (x_n, y_n)) \in (X \times [m])^n$ it outputs m linear classifiers $w_1, \ldots, w_m$ satisfying:*

- *for every $k \in [m]$, w_k lies in the span of $x_1, \ldots, x_n$;*
- *for every x, the prediction of $\mathcal{A}$ on x depends only on the predictions of the classifiers* $\mathsf{sign}(\langle x, w_k\rangle)$ *and;*
- *for every $k \in [m]$, let $V_- := \{x \in X_S \mid \langle x, w_k\rangle < 0\}$ and $V_+ := \{x \in X_S \mid \langle x, w_k\rangle \geq 0\}$. If V_- can be linearly separated from V_+ by a homogeneous linear separator with margin γ_k then for all $x \in X_S$, $|\langle x, w_k\rangle| \geq \frac{\gamma_k}{2}\|x\|_2$.*

We now show that linear classifiers over distributions that produce datasets independent in the sense of Definition 3.3 will have high subpopulation coupling. In order to guarantee strong coupling, we will assume that the set V of points in a random dataset together with the set of points V' that consists of additional samples from every mixture present in V (namely, $V' \sim \prod_{j\in[N]_{S=1}} M_j$) satisfy the independence condition with high probability. Formally, we establish the following result (the proof can be found in Appendix B).

[1] A linear classifier can always be projected to the span of the points without affecting the margins. This assumption allows us to avoid having to separately deal with spurious correlations between unseen parts of subpopulations and the produced classifiers.

Theorem 3.5. *Let $X \subset \mathbb{R}^d$ be a domain partitioned into sub-domains $\{X_i\}_{i\in[N]}$ with subpopulations $\{M_i\}_{i\in[N]}$ over the sub-domains. Let $\mathcal{A}$ be any approximately margin maximizing m-class linear classifier and π be a frequency prior. Assume that for $D \sim \mathcal{D}_\pi^{[N]}$ and $V \sim M_D^n$, $V' \sim \prod_{j\in[N]_{S=1}} M_j$, with probability at least $1-\delta^2$, $V \cup V'$ is $(\tau, \tau^2/(8\sqrt{n}))$-independent for some $\tau \in (0, 1/2]$. Then for any labeling prior $\mathcal{F}$, $\mathcal{A}$ is Λ-subpopulation-coupled with probability $1-\delta$ and $\lambda_1 \geq 1-\delta$.*

As a simple example of subpopulations that will produce sets of points that are $(\tau, \tau^2/(8\sqrt{n}))$-independent with high probability we pick each M_i to be a spherically-symmetric distribution supported on a ball of radius 1 around some center z_i of norm 1. We also pick the centers randomly and independently from the uniform distribution on the unit sphere. It is not hard to see that, by the standard concentration properties of spherically-symmetric distributions, a set V of t samples from an arbitrary mixture of such distributions will be (τ, θ)-independent with high probability for $\tau \geq 1/2 - o(1)$ and $\theta = \tilde{O}(\sqrt{t/d})$. Thus for $t < 2n$, $d = \tilde{O}(n^2)$ suffices to ensure that $\theta \leq \tau^2/(8\sqrt{n})$.

4 Memorization, Privacy and Stability

So far we have discussed memorization by learning algorithms informally. Below we will provide a simple definition of label memorization. We will show that bounds on the memorization ability of an algorithm can be easily translated into bounds on how well the algorithm can fit the dataset whenever there is enough (statistical or computational) uncertainty in the labels. This result immediately implies bounds on the generalization error of such algorithms in our problem setting. We will then show that (even relatively weak forms of) differential privacy imply that the algorithm cannot memorize well.

To keep the notation cleaner we will discuss these results in the context of our simpler model from Sec.2 but they can be easily adapted to our mixture model setting. For simplicity of notation, we will also focus on memorization of singleton elements.

4.1 Memorization

To measure the ability of an algorithm $\mathcal{A}$ to memorize labels we will look at how much the labeled example (x, y) affects the prediction of the model on x. This notion will be defined per specific dataset and example but in our applications we will use the expectation of this value when the dataset is drawn randomly.

Definition 4.1. *For a dataset $S = (x_i, y_i)_{i\in[n]}$ and $i \in [n]$ define*

$$\mathtt{mem}(\mathcal{A}, S, i) := \left| \mathop{\mathbf{Pr}}_{h\sim\mathcal{A}(S)}[h(x_i) = y_i] - \mathop{\mathbf{Pr}}_{h\sim\mathcal{A}(S^{\setminus i})}[h(x_i) = y_i] \right|,$$

where $S^{\setminus i}$ denotes the dataset that is S with (x_i, y_i) removed. We say that $\mathcal{A}$ is γ-memorization bounded for singletons if for all $S \in (X, Y)^n$ and all i such that $x_i \in X_{S=1}$ we have $\mathtt{mem}(\mathcal{A}, S, i) \leq \gamma$.

In this definition we measure the effect simply as the total variation distance between the distributions of the indicator of the label being y, but other notions of distance could be appropriate in other applications. For this notion of distance our definition of memorization is closely related to the leave-one-out stability of the algorithm (see eq. (6)). Indeed, it is easy to see from this definition that LOO stability upper bounds the expected memorization:

$$\frac{1}{n} \mathop{\mathbf{E}}_{S\sim P^n}\left[\sum_{i\in[n]} \mathtt{mem}(\mathcal{A}, S, i)\right] \leq \mathtt{LOOstab}(P, \mathcal{A}).$$

A simple corollary of this definition is that if $\mathcal{A}$ cannot predict the label y_i of x_i without observing it then it needs to memorize it to fit it. More formally,

Lemma 4.2. *For every distribution D and labeling prior $\mathcal{F}$,*

$$\mathop{\mathbf{E}}_{f\sim\mathcal{F},S\sim(D,f)^n}[\mathtt{errn}_S(\mathcal{A},1)] \geq \mathop{\mathbf{E}}_{f\sim\mathcal{F},S\sim(D,f)^n}\left[\sum_{i\in[n],\ x_i\in X_{S=1}} \mathop{\mathbf{Pr}}_{h\sim\mathcal{A}(S^{\setminus i})}[h(x_i)\neq y_i] - \mathtt{mem}(\mathcal{A},S,i)\right].$$

There can be several reasons why an algorithm $\mathcal{A}$ cannot predict the label on x_i without observing it. The simplest one is that if there is statistical uncertainty in the label. To measure the uncertainty in a distribution ρ over labels we will simply use the maximum probability of any specific label:

$$\|\rho\|_\infty := \max_{y\in Y}\rho(y).$$

Significant statistical uncertainly conditioned on knowing all the other labeled examples exists only when the labeling prior has high entropy (such as being uniform over a class of functions of VC dimension larger than n). In practice, there might exist a relatively simple model that explains the data well yet the learning algorithm cannot find (or even approximate) this model due to computational limitations. This can be modeled by considering the best accuracy in predicting the label of x_i given $S^{\setminus i}$ for the restricted class of algorithms to which $\mathcal{A}$ belongs. For example, the uniform prior can be achieved for all polynomial-time algorithms by using a pseudo-random labeling function [GGM86]. More generally, Lemma 4.2 implies that any upper bound on the expected accuracy of a learning algorithm on an unseen singleton example implies the need to memorize the label in order to fit it. Thus the results in the remainder of this section extend directly to computational notions of uncertainty in place of $\|\rho\|_\infty$. We now spell out the corollaries for the simple statistical notion of uncertainty.

Lemma 4.3. *Let ρ be an arbitrary distribution over Y. For a dataset $S=(x_i,y_i)_{i\in[n]}$, $i\in[n]$ and $y\in Y$, let $S^{i\leftarrow y}$ denote the dataset S with (x_i,y) in place of example (x_i,y_i). Then we have:*

$$\mathop{\mathbf{Pr}}_{y\sim\rho,h\sim\mathcal{A}(S^{i\leftarrow y})}[h(x)=y] \leq \|\rho\|_\infty + \mathop{\mathbf{E}}_{y\sim\rho}[\mathtt{mem}(\mathcal{A},S^{i\leftarrow y},i)].$$

In particular, for every distribution D and labeling prior $\mathcal{F}$,

$$\mathop{\mathbf{E}}_{f\sim\mathcal{F},S\sim(D,f)^n}[\mathtt{errn}_S(\mathcal{A},1)] \geq \mathop{\mathbf{E}}_{f\sim\mathcal{F},S\sim(D,f)^n}\left[\sum_{i\in[n],\ x_i\in X_{S=1}} 1-\|\mathcal{F}(x_i|S^{\setminus i})\|_\infty - \mathtt{mem}(\mathcal{A},S,i)\right],$$

where $\mathcal{F}(x_i|S^{\setminus i})$ denotes the conditional distribution over the label of x_i after observing all the other examples:

$$\mathcal{F}(x_i|S^{\setminus i}) = \mathop{\mathbf{D}}_{f\sim\mathcal{F},S\sim(D,f)^n}[f(x_i)\mid \forall j\neq i, f(x_j)=y_j].$$

Proof. Let ρ' denote the marginal distribution of $h(x)$ for $h\sim\mathcal{A}(S^{\setminus i})$. By Definition 4.1, for every y,

$$\mathop{\mathbf{Pr}}_{h\sim\mathcal{A}(S^{i\leftarrow y})}[h(x)=y] \leq \mathop{\mathbf{Pr}}_{h\sim\mathcal{A}(S^{\setminus i})}[h(x)=y] + \mathtt{mem}(\mathcal{A},S^{i\leftarrow y},i) = \rho'(y) + \mathtt{mem}(\mathcal{A},S^{i\leftarrow y},i).$$

Thus,

$$\mathop{\mathbf{E}}_{y\sim\rho,h\sim\mathcal{A}(S^{i\leftarrow y})}[h(x)=y] \leq \|\rho\|_\infty + \mathop{\mathbf{E}}_{y\sim\rho}[\mathtt{mem}(\mathcal{A},S^{i\leftarrow y},i)].$$

The rest of the claim follows from the definition of $\mathtt{errn}_S(\mathcal{A}, 1)$ and observing that an expectation is taken on $f \sim \mathcal{F}$ that ensures that for every point the error will be averaged over all labelings of the point according to conditional distribution of the corresponding label. □

Using these definitions and Lemma 4.3, we immediately obtain the following example corollary on the excess error of any algorithm that is γ-memorization bounded for singletons.

Corollary 4.4. *In the setting of Thm. 2.3, let $\mathcal{A}$ be any algorithm γ-memorization bounded for singletons. Then*

$$\overline{\mathtt{err}}(\pi, \mathcal{F}, \mathcal{A}) \geq \mathtt{opt}(\pi, \mathcal{F}) + \tau_1 \cdot \mathop{\mathbf{E}}_{D \sim D_\pi^X, f \sim \mathcal{F}, S \sim (D,f)^n} \left[\sum_{i \in [n],\ x_i \in X_{S=1}} 1 - \|\mathcal{F}(x_i | S^{\setminus i})\|_\infty - \gamma \right].$$

The bound in this corollary depends on the expectation of the uncertainty in the label $\|\mathcal{F}(x_i|S^{\setminus i})\|_\infty$. While, in general, this quantity might be hard to estimate it might be relatively easy to get a sufficiently strong upper bound. For example, if for $f \sim \mathcal{F}$ the labeling is k-wise independent for k that upper-bounds the typical number of distinct points (or subpopulations in the general case) then with high probability we will have that $\|\mathcal{F}(x_i|S^{\setminus i})\|_\infty \leq \max_{x \in X} \|\rho_x\|_\infty$, where ρ_x is the marginal distribution of $f(x)$ for $f \sim \mathcal{F}$.

4.2 Privacy

Memorization of the training data can be undesirable in a variety of settings. For example, in the context of user data privacy, memorization is known to lead to ability to mount black-box membership inference attacks (that discover the presence of a specific data point in the dataset) [SSSS17; LBG17; Lon+18; TLGYW18] as well as ability to extract planted secrets from language models [CLKES19]. The most common approaches toward defending such attacks are based on the notion of differential privacy [DMNS06] that are formally known to limit the probability of membership inference by requiring that the output distribution of the learning algorithm is not too sensitive to individual data points. Despite significant recent progress in training deep learning networks with differential privacy, they still lag substantially behind the state-of-the-art results trained without differential privacy [SS15; Aba+16; PAEGT16; WLKCJN17; PAEGT17; MRTZ18]. While some of this lag is likely to be closed by improved techniques, our results imply that the some of this gap is inherent due to the data being long-tailed. More formally, we will show that the requirements differential privacy imply a lower bound on the value of $\mathtt{errn}$ (for simplicity just for $\ell = 1$). We will prove that this limitation applies even to algorithms that satisfy a very weak form of privacy: label privacy for predictions. It protects only the privacy of the label as in [CH11] and also with respect to algorithms that only output a prediction on an (arbitrary) fixed point [DF18]. Formally, we define:

Definition 4.5. *Let $\mathcal{A}$ be an algorithm that given a dataset $S \in (X \times Y)^n$ outputs a random predictor $h \colon X \to Y$. We say that $\mathcal{A}$ is* (ϵ, δ)-differentially label-private prediction *algorithm if for every $x \in X$ and two datasets S, S' that only differ in a label of a single element we have for any subset of labels Y',*

$$\mathop{\mathbf{Pr}}_{h \sim \mathcal{A}(S)}[h(x) \in Y'] \leq e^\epsilon \cdot \mathop{\mathbf{Pr}}_{h \sim \mathcal{A}(S')}[h(x) \in Y'] + \delta.$$

It is easy to see that any algorithm that satisfies this notion of privacy is $(e^\epsilon - 1 + \delta)$-memorization bounded for singletons. A slightly more careful analysis in this case gives the following analogues of Lemma 4.3 and Corollary 4.4.

Theorem 4.6. *Let $\mathcal{A}$ be an (ϵ, δ)-differentially label-private prediction algorithm and let ρ be an arbitrary distribution over Y. For a dataset $S = (x_i, y_i)_{i \in [n]}$, $i \in [n]$ and $y \in Y$, we have:*

$$\mathop{\mathbf{E}}_{y \sim \rho, h \sim \mathcal{A}(S^{i \leftarrow y})} [h(x) = y] \leq e^{\epsilon} \cdot \|\rho\|_{\infty} + \delta.$$

In particular, in the setting of Thm. 2.3, for every distribution D and labeling prior $\mathcal{F}$,

$$\mathop{\mathbf{E}}_{f \sim \mathcal{F}, S \sim (D,f)^n} [\mathtt{errn}_S(\mathcal{A}, 1)] \geq \mathop{\mathbf{E}}_{f \sim \mathcal{F}, S \sim (D,f)^n} \left[\sum_{i \in [n],\ x_i \in X_{S=1}} 1 - e^{\epsilon} \cdot \|\mathcal{F}(x_i | S^{\setminus i})\|_{\infty} - \delta \right].$$

and, consequently,

$$\overline{\mathtt{err}}(\pi, \mathcal{F}, \mathcal{A}) \geq \mathtt{opt}(\pi, \mathcal{F}) + \tau_1 \cdot \mathop{\mathbf{E}}_{D \sim D_{\pi}^{X}, f \sim \mathcal{F}, S \sim (D,f)^n} \left[\sum_{i \in [n],\ x_i \in X_{S=1}} 1 - e^{\epsilon} \cdot \|\mathcal{F}(x_i | S^{\setminus i})\|_{\infty} - \delta \right].$$

Proof. Let ρ' denote the marginal distribution of $h(x)$ for $h \sim \mathcal{A}(S)$. By the definition of (ϵ, δ)-differential label privacy for predictions, for every y,

$$\mathop{\mathbf{Pr}}_{h \sim \mathcal{A}(S^{i \leftarrow y})} [h(x_i) = y] \leq e^{\epsilon} \cdot \mathop{\mathbf{Pr}}_{h \sim \mathcal{A}(S)} [h(x) = y] + \delta = e^{\epsilon} \rho'(y) + \delta$$

Thus,

$$\mathop{\mathbf{E}}_{y \sim \rho, h \sim \mathcal{A}(S^{i \leftarrow y})} [h(x_i) = y] \leq \mathop{\mathbf{E}}_{y \sim \rho} \left[e^{\epsilon} \rho'(y) + \delta \right] \leq e^{\epsilon} \|\rho\|_{\infty} + \delta.$$

The rest of the claim follows as before. □

This theorem is easy to extend to any subpopulation from which only ℓ examples have been observed using the group privacy property of differential privacy. This property implies that if ℓ labels are changed then the resulting distributions are $(\ell\epsilon, \ell e^{\ell - 1}\delta)$-close (in the same sense) [DR14]. The total weight of subpopulations that have at most ℓ examples for a small value of ℓ is likely to be significant in most modern datasets. Thus this may formally explain at least some of the gap in the results currently achieved using differentially private training algorithms and those achievable without the privacy constraint.

Uniform stability: A related notion of stability is uniform prediction stability [BE02; DF18] that, in the context of prediction, requires that changing any point in the dataset does not change the label distribution on any point by more than δ in total variation distance. This notion is useful in ensuring generalization [BE02; FV19] and as a way to ensure robustness of predictions against data poisoning. In this context, δ-uniform stability implies $(0, \delta)$-differential privacy for predictions and therefore Theorem 4.6 also implies limitations of such algorithms.

5 Discussion

Our work provides a natural and simple learning model in which memorization of labels and, in some cases interpolation, are necessary for achieving nearly optimal generalization when learning from a long-tailed data distribution. It suggests that the reason why many modern ML methods reach their best accuracy while (nearly) perfectly fitting the data is that these methods are (implicitly) tuned to handle the long tails of natural data distributions. Our model explicitly incorporates the prior distribution on the frequencies of subpopulations in the data and we argue that such modeling is necessary to avoid the disconnect between the classical view of generalization and the practice of ML. We hope that the insights derived from our approach will serve as the basis for future theoretical analyses of generalization that more faithfully reflect modern datasets and learning techniques. A recent example that such modeling has practical benefits can be found in [CWGAM19].

Our analysis does not consider some of the potentially significant costs of fitting/memorizing noisy examples. We first note that random label noise is easy to incorporate into the model. The optimal strategy in our setting is to predict the argmax of the posterior distribution over the label of each point. If it holds that observing a singleton example (x, y) makes the posterior probability of label y larger by at least some Δ than the posterior probability of any of the other labels (at x) then we will obtain the same result but with excess error for $\ell = 1$ scaled by Δ. In other words, despite the label noise, memorization might still be beneficial for these examples. At the same time, memorization of noisy examples *within* a frequent subpopulation is likely to be harmful for generalization and would not be explained by our model. Memorization of such examples by some algorithms can be explained by the fact that the learning algorithms we use are tuned for data distribution in which noise on typical examples is extremely rare. For such data the benefits of memorization outweigh the costs of memorizing some harmful noise.

Acknowledgements

Part of the inspiration and motivation for this work comes from empirical observations that differentially private algorithms have poor accuracy on atypical examples. I'm grateful to Nicholas Carlini, Ulfar Erlingsson and Nicolas Papernot for numerous illuminating discussions of experimental work on this topic [CEP18] and to Vitaly Shmatikov for sharing his insights on this phenomenon in the context of language models. I would like to thank my great colleagues Peter Bartlett, Misha Belkin, Olivier Bousquet, Edith Cohen, Roy Frostig, Daniel Hsu, Phil Long, Yishay Mansour, Mehryar Mohri, Tomer Koren, Sasha Rakhlin, Adam Smith, Kunal Talwar, Greg Valiant, and Chiyuan Zhang for insightful feedback and suggestions on this work. I thank the authors of [ZAR14] for the permission to include Figure 1 from their work.

References

[Aba+16] M. Abadi, A. Chu, I. Goodfellow, H. B. McMahan, I. Mironov, K. Talwar, and L. Zhang. "Deep learning with differential privacy". In: *Proceedings of the 2016 ACM SIGSAC Conference on Computer and Communications Security*. ACM. 2016, pp. 308–318.

[BE02] O. Bousquet and A. Elisseeff. "Stability and generalization". In: *JMLR* 2 (2002), pp. 499–526.

[BFT17] P. L. Bartlett, D. J. Foster, and M. J. Telgarsky. "Spectrally-normalized margin bounds for neural networks". In: *Advances in Neural Information Processing Systems*. 2017, pp. 6240–6249.

[BHM18] M. Belkin, D. J. Hsu, and P. Mitra. "Overfitting or perfect fitting? risk bounds for classification and regression rules that interpolate". In: *Advances in Neural Information Processing Systems*. 2018, pp. 2300–2311.

[BHX19] M. Belkin, D. Hsu, and J. Xu. "Two models of double descent for weak features". In: *arXiv preprint arXiv:1903.07571* (2019).

[BLLT19] P. L. Bartlett, P. M. Long, G. Lugosi, and A. Tsigler. “Benign Overfitting in Linear Regression”. In: *arXiv preprint arXiv:1906.11300* (2019).

[BM02] P. Bartlett and S. Mendelson. “Rademacher and Gaussian Complexities: Risk Bounds and Structural Results”. In: *Journal of Machine Learning Research* 3 (2002), pp. 463–482.

[BMM18] M. Belkin, S. Ma, and S. Mandal. “To Understand Deep Learning We Need to Understand Kernel Learning”. In: *ICML*. Vol. 80. Proceedings of Machine Learning Research. PMLR, 2018, pp. 541–549. URL: http://proceedings.mlr.press/v80/belkin18a.html.

[Bre01] L. Breiman. “Random forests”. In: *Machine learning* 45.1 (2001), pp. 5–32.

[BRT18] M. Belkin, A. Rakhlin, and A. B. Tsybakov. “Does data interpolation contradict statistical optimality?” In: *arXiv preprint arXiv:1806.09471* (2018).

[BS17] R. Babbar and B. Schölkopf. “Dismec: Distributed sparse machines for extreme multi-label classification”. In: *Proceedings of the tenth ACM international conference on web search and data mining*. ACM. 2017, pp. 721–729.

[BS19a] R. Babbar and B. Schölkopf. “Data scarcity, robustness and extreme multi-label classification”. In: *Machine Learning* (2019).

[BS19b] E. Bagdasaryan and V. Shmatikov. “Differential Privacy Has Disparate Impact on Model Accuracy”. In: *CoRR* abs/1905.12101 (2019). arXiv: 1905.12101. URL: http://arxiv.org/abs/1905.12101.

[CD14] K. Chaudhuri and S. Dasgupta. “Rates of Convergence for Nearest Neighbor Classification”. In: *NIPS*. 2014, pp. 3437–3445. URL: http://papers.nips.cc/paper/5439-rates-of-convergence-for-nearest-neighbor-classification.

[CEP18] N. Carlini, U. Erlingsson, and N. Papernot. “Prototypical Examples in Deep Learning: Metrics, Characteristics, and Utility”. In: (2018). URL: https://openreview.net/forum?id=r1xyx3R9tQ.

[CH11] K. Chaudhuri and D. Hsu. “Sample Complexity Bounds for Differentially Private Learning”. In: *COLT*. 2011, pp. 155–186.

[CH67] T. Cover and P. Hart. “Nearest neighbor pattern classification”. In: *IEEE transactions on information theory* 13.1 (1967), pp. 21–27.

[CLKES19] N. Carlini, C. Liu, J. Kos, Ú. Erlingsson, and D. Song. “The Secret Sharer: Evaluating and Testing Unintended Memorization in Neural Networks”. In: *Usenix Security (to appear)*. 2019.

[CSG18] G. Cohen, G. Sapiro, and R. Giryes. “DNN or k-NN: That is the Generalize vs. Memorize Question”. In: *arXiv preprint arXiv:1805.06822* (2018).

[CSSHB18] Y. Cui, Y. Song, C. Sun, A. Howard, and S. Belongie. “Large Scale Fine-Grained Categorization and Domain-Specific Transfer Learning”. In: *The IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*. 2018.

[CV95] C. Cortes and V. Vapnik. “Support-vector networks”. In: *Machine learning* 20.3 (1995), pp. 273–297.

[CWGAM19] K. Cao, C. Wei, A. Gaidon, N. Arechiga, and T. Ma. “Learning Imbalanced Datasets with Label-Distribution-Aware Margin Loss”. In: *arXiv preprint arXiv:1906.07413* (2019).

[DF18] C. Dwork and V. Feldman. “Privacy-preserving Prediction”. In: *Conference On Learning Theory*. 2018, pp. 1693–1702.

[DFHPRR14] C. Dwork, V. Feldman, M. Hardt, T. Pitassi, O. Reingold, and A. Roth. “Preserving Statistical Validity in Adaptive Data Analysis”. In: *CoRR* abs/1411.2664 (2014). Extended abstract in STOC 2015.

[DMNS06] C. Dwork, F. McSherry, K. Nissim, and A. Smith. “Calibrating noise to sensitivity in private data analysis”. In: *TCC*. 2006, pp. 265–284.

[DR14] C. Dwork and A. Roth. *The Algorithmic Foundations of Differential Privacy*. Vol. 9. 3-4. 2014, pp. 211–407. URL: `http://dx.doi.org/10.1561/0400000042`.

[Fel16] V. Feldman. “Generalization of ERM in Stochastic Convex Optimization: The Dimension Strikes Back”. In: *CoRR* abs/1608.04414 (2016). Extended abstract in NIPS 2016. URL: `http://arxiv.org/abs/1608.04414`.

[FS97] Y. Freund and R. Schapire. “A decision-theoretic generalization of on-line learning and an application to boosting”. In: *Journal of Computer and System Sciences* 55.1 (1997), pp. 119–139.

[FV19] V. Feldman and J. Vondrák. “High probability generalization bounds for uniformly stable algorithms with nearly optimal rate”. In: *CoRR* abs/1902.10710 (2019). arXiv: `1902.10710`. URL: `http://arxiv.org/abs/1902.10710`.

[FZ19] V. Feldman and C. Zhang. *Finding the memorized examples via fast influence estimation (working title)*. Unpublished manuscript. Short summary in `https://www.youtube.com/watch?v=YWy2Iwn-1S8`. 2019.

[GGM86] O. Goldreich, S. Goldwasser, and S. Micali. “How to construct random functions”. In: *Journal of the ACM* 33.4 (1986), pp. 792–807.

[HMRT19] T. Hastie, A. Montanari, S. Rosset, and R. J. Tibshirani. “Surprises in High-Dimensional Ridgeless Least Squares Interpolation”. In: *arXiv preprint arXiv:1903.08560* (2019).

[HRS16] M. Hardt, B. Recht, and Y. Singer. “Train faster, generalize better: Stability of stochastic gradient descent”. In: *ICML*. 2016, pp. 1225–1234. URL: `http://jmlr.org/proceedings/papers/v48/hardt16.html`.

[Kol01] V. Koltchinskii. “Rademacher penalties and structural risk minimization”. In: *IEEE Transactions on Information Theory* 47.5 (2001), pp. 1902–1914.

[Kri+17] R. Krishna, Y. Zhu, O. Groth, J. Johnson, K. Hata, J. Kravitz, S. Chen, Y. Kalantidis, L.-J. Li, D. A. Shamma, et al. “Visual genome: Connecting language and vision using crowdsourced dense image annotations”. In: *International Journal of Computer Vision* 123.1 (2017), pp. 32–73.

[LBG17] Y. Long, V. Bindschaedler, and C. A. Gunter. “Towards Measuring Membership Privacy”. In: *CoRR* abs/1712.09136 (2017). arXiv: `1712.09136`. URL: `http://arxiv.org/abs/1712.09136`.

[LMZ18] Y. Li, T. Ma, and H. Zhang. “Algorithmic Regularization in Over-parameterized Matrix Sensing and Neural Networks with Quadratic Activations”. In: *Conference On Learning Theory*. 2018, pp. 2–47.

[Lon+18] Y. Long, V. Bindschaedler, L. Wang, D. Bu, X. Wang, H. Tang, C. A. Gunter, and K. Chen. "Understanding Membership Inferences on Well-Generalized Learning Models". In: *CoRR* abs/1802.04889 (2018). arXiv: 1802.04889. URL: http://arxiv.org/abs/1802.04889.

[LR18] T. Liang and A. Rakhlin. "Just interpolate: Kernel" ridgeless" regression can generalize". In: *arXiv preprint arXiv:1808.00387* (2018).

[MBB18] S. Ma, R. Bassily, and M. Belkin. "The Power of Interpolation: Understanding the Effectiveness of SGD in Modern Over-parametrized Learning". In: *ICML*. 2018, pp. 3331–3340. URL: http://proceedings.mlr.press/v80/ma18a.html.

[MNPR06] S. Mukherjee, P. Niyogi, T. Poggio, and R. Rifkin. "Learning theory: stability is sufficient for generalization and necessary and sufficient for consistency of empirical risk minimization". In: *Advances in Computational Mathematics* 25.1-3 (2006), pp. 161–193.

[MRTZ18] B. McMahan, D. Ramage, K. Talwar, and L. Zhang. "Learning Differentially Private Recurrent Language Models". In: *International Conference on Learning Representations (ICLR)*. 2018. URL: https://openreview.net/pdf?id=BJ0hF1Z0b.

[MVS19] V. Muthukumar, K. Vodrahalli, and A. Sahai. "Harmless interpolation of noisy data in regression". In: *arXiv preprint arXiv:1903.09139* (2019).

[NBMS17] B. Neyshabur, S. Bhojanapalli, D. McAllester, and N. Srebro. "Exploring generalization in deep learning". In: *Advances in Neural Information Processing Systems*. 2017, pp. 5947–5956.

[NTS15] B. Neyshabur, R. Tomioka, and N. Srebro. "In Search of the Real Inductive Bias: On the Role of Implicit Regularization in Deep Learning". In: *ICLR*. 2015. URL: http://arxiv.org/abs/1412.6614.

[NTSS17] B. Neyshabur, R. Tomioka, R. Salakhutdinov, and N. Srebro. "Geometry of optimization and implicit regularization in deep learning". In: *arXiv preprint arXiv:1705.03071* (2017).

[NWS14] D. Needell, R. Ward, and N. Srebro. "Stochastic Gradient Descent, Weighted Sampling, and the Randomized Kaczmarz algorithm". In: *NIPS*. 2014, pp. 1017–1025. URL: http://papers.nips.cc/paper/5355-stochastic-gradient-descent-weighted-sampling-and-the-randomized-kaczmarz-algorithm.pdf.

[OS15] A. Orlitsky and A. T. Suresh. "Competitive distribution estimation: Why is good-turing good". In: *NIPS*. 2015, pp. 2143–2151.

[PAEGT16] N. Papernot, M. Abadi, Ú. Erlingsson, I. J. Goodfellow, and K. Talwar. "Semi-supervised Knowledge Transfer for Deep Learning from Private Training Data". In: *CoRR* abs/1610.05755 (2016). arXiv: 1610.05755. URL: http://arxiv.org/abs/1610.05755.

[PAEGT17] N. Papernot, M. Abadi, Ú. Erlingsson, I. J. Goodfellow, and K. Talwar. "Semi-supervised Knowledge Transfer for Deep Learning from Private Training Data". In: *Proceedings of the 5th International Conference on Learning Representations (ICLR)*. 2017.

[RMP05] A. Rakhlin, S. Mukherjee, and T. Poggio. "Stability Results In Learning Theory". In: *Analysis and Applications* 03.04 (2005), pp. 397–417.

[RZ19] A. Rakhlin and X. Zhai. "Consistency of Interpolation with Laplace Kernels is a High-Dimensional Phenomenon". In: *COLT*. Vol. 99. PMLR, 2019, pp. 2595–2623. URL: http://proceedings.mlr.press/v99/rakhlin19a.html.

[Sch13] R. E. Schapire. “Explaining adaboost”. In: *Empirical inference*. Springer, 2013, pp. 37–52.

[SFBL98] R. Schapire, Y. Freund, P. Bartlett, and W. Lee. “Boosting the margin: a new explanation for the effectiveness of voting methods”. In: *Annals of Statistics* 26.5 (1998), pp. 1651–1686.

[SHNGS18] D. Soudry, E. Hoffer, M. S. Nacson, S. Gunasekar, and N. Srebro. “The implicit bias of gradient descent on separable data”. In: *The Journal of Machine Learning Research* 19.1 (2018), pp. 2822–2878.

[Sri02] K. Sridharan. *A gentle introduction to concentration inequalities*. Tech. rep. 2002.

[SS15] R. Shokri and V. Shmatikov. “Privacy-preserving deep learning”. In: *Proceedings of the 22nd ACM SIGSAC conference on computer and communications security*. ACM. 2015, pp. 1310–1321.

[SSS05] S. Shalev-Shwartz and Y. Singer. “A new perspective on an old perceptron algorithm”. In: *International Conference on Computational Learning Theory*. Springer. 2005, pp. 264–278.

[SSSS09] S. Shalev-Shwartz, O. Shamir, N. Srebro, and K. Sridharan. “Stochastic Convex Optimization”. In: *COLT*. 2009.

[SSSS10] S. Shalev-Shwartz, O. Shamir, N. Srebro, and K. Sridharan. “Learnability, Stability and Uniform Convergence”. In: *Journal of Machine Learning Research* 11 (2010), pp. 2635–2670. URL: `http://portal.acm.org/citation.cfm?id=1953019`.

[SSSS17] R. Shokri, M. Stronati, C. Song, and V. Shmatikov. “Membership Inference Attacks Against Machine Learning Models”. In: *2017 IEEE Symposium on Security and Privacy, SP 2017*. 2017, pp. 3–18.

[SST10] N. Srebro, K. Sridharan, and A. Tewari. “Smoothness, Low Noise and Fast Rates”. In: *NIPS*. 2010, pp. 2199–2207. URL: `http://papers.nips.cc/paper/3894-smoothness-low-noise-and-fast-rates.pdf`.

[TLGYW18] S. Truex, L. Liu, M. E. Gursoy, L. Yu, and W. Wei. “Towards demystifying membership inference attacks”. In: *arXiv preprint arXiv:1807.09173* (2018).

[Vap82] V. N. Vapnik. *Estimation of Dependences Based on Empirical Data*. New York: Springer-Verlag, 1982.

[VH+18] G. Van Horn, O. Mac Aodha, Y. Song, Y. Cui, C. Sun, A. Shepard, H. Adam, P. Perona, and S. Belongie. “The inaturalist species classification and detection dataset”. In: *Proceedings of the IEEE conference on computer vision and pattern recognition*. 2018, pp. 8769–8778.

[VHP17] G. Van Horn and P. Perona. “The devil is in the tails: Fine-grained classification in the wild”. In: *arXiv preprint arXiv:1709.01450* (2017).

[VV16] G. Valiant and P. Valiant. “Instance optimal learning of discrete distributions”. In: *STOC*. ACM. 2016, pp. 142–155.

[WLKCJN17] X. Wu, F. Li, A. Kumar, K. Chaudhuri, S. Jha, and J. F. Naughton. “Bolt-on Differential Privacy for Scalable Stochastic Gradient Descent-based Analytics”. In: *SIGMOD*. 2017, pp. 1307–1322.

[WOBM17] A. J. Wyner, M. Olson, J. Bleich, and D. Mease. “Explaining the success of adaboost and random forests as interpolating classifiers”. In: *The Journal of Machine Learning Research* 18.1 (2017), pp. 1558–1590.

[WRH17] Y.-X. Wang, D. Ramanan, and M. Hebert. “Learning to model the tail”. In: *Advances in Neural Information Processing Systems*. 2017, pp. 7029–7039.

[XHEOT10] J. Xiao, J. Hays, K. A. Ehinger, A. Oliva, and A. Torralba. “Sun database: Large-scale scene recognition from abbey to zoo”. In: *2010 IEEE Computer Society Conference on Computer Vision and Pattern Recognition*. IEEE. 2010, pp. 3485–3492.

[ZAR14] X. Zhu, D. Anguelov, and D. Ramanan. “Capturing long-tail distributions of object subcategories”. In: *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*. 2014, pp. 915–922.

[ZBHRV17] C. Zhang, S. Bengio, M. Hardt, B. Recht, and O. Vinyals. “Understanding deep learning requires rethinking generalization”. In: *ICLR*. 2017. URL: `https://openreview.net/forum?id=Sy8gdB9xx`.

A Proof Lemma 2.1

The key property of our problem definition is that it allows to decompose the probability of a dataset (under the entire generative process) into a probability of seeing one of the points in the dataset and the probability of seeing the rest of the dataset under a similar generative process. Specifically, we prove the following lemma.

Lemma A.1. *For $x \in X$, a sequence of points $V = (x_1, \ldots, x_n) \in X^n$ that includes x exactly ℓ times, let $V \setminus x$ be equal to V with all the elements equal to x omitted. Then for any frequency prior π and α in the support of $\bar{\pi}^N$, we have*

$$\mathop{\mathbf{Pr}}_{D \sim \mathcal{D}_\pi^X, U \sim D^n}[U = V \mid D(x) = \alpha] = \alpha^\ell \cdot (1-\alpha)^{n-\ell} \cdot \mathop{\mathbf{Pr}}_{D' \sim \mathcal{D}_\pi^{X \setminus \{x\}}, U' \sim D^{n-\ell}}[U' = V \setminus x].$$

In particular:

$$\mathop{\mathbf{Pr}}_{D \sim \mathcal{D}_\pi^X, U \sim D^n}[U = V] = \mathop{\mathbf{E}}_{\alpha \sim \bar{\pi}^N}\left[\alpha^\ell \cdot (1-\alpha)^{n-\ell}\right] \cdot \mathop{\mathbf{Pr}}_{D' \sim \mathcal{D}_\pi^{X \setminus \{x\}}, U' \sim D^{n-\ell}}[U' = V \setminus x].$$

Proof. We consider the distribution of $D \sim \mathcal{D}_\pi^X$ conditioned on $D(x) = \alpha$ (which, by our assumption, is an event with positive probability). We denote this distribution by $\mathcal{D}_\pi^X(|D(x) = \alpha)$. From the definition of $\mathcal{D}_\pi^X$ we get that a random sample D from $\mathcal{D}_\pi^X(|D(x) = \alpha)$ can generated by setting $D(x) = \alpha$, then for all $z \in X \setminus \{x\}$, sampling p_z from π and normalizing the results to sum to $1 - \alpha$. That is, defining

$$D(z) = (1-\alpha)\frac{p_z}{\sum_{z \in X \setminus \{x\}} p_z}.$$

From here we obtain that an equivalent way to generate a random sample from $\mathcal{D}_\pi^X(|D(x) = \alpha)$ is to sample D' from $\mathcal{D}_\pi^{X \setminus \{x\}}$ and then multiply the resulting p.m.f. by $1 - \alpha$ (with $D(x) = \alpha$ as before). Naturally, for any D,

$$\mathop{\mathbf{Pr}}_{U \sim D^n}[U = V] = \prod_{i \in [n]} D(x_i).$$

Now we denote by I_{-x} the subset of indices of elements of V that are different from x: $I_x = \{i \in [n] \mid x_i \neq x\}$. We can now conclude:

$$\begin{aligned}
\mathop{\mathbf{Pr}}_{D \sim \mathcal{D}_\pi^X, U \sim D^n}[U = V \mid D(x) = \alpha] &= \mathop{\mathbf{Pr}}_{D \sim \mathcal{D}_\pi^X(|D(x)=\alpha), U \sim D^n}[U = V] \\
&= \mathop{\mathbf{E}}_{D \sim \mathcal{D}_\pi^X(|D(x)=\alpha)}\left[\prod_{i \in [n]} D(x_i)\right] \\
&= \mathop{\mathbf{E}}_{D \sim \mathcal{D}_\pi^X(|D(x)=\alpha)}\left[\alpha^\ell \prod_{i \in I_{-x}} D(x_i)\right] \\
&= \alpha^\ell \cdot (1-\alpha)^{n-\ell} \cdot \mathop{\mathbf{E}}_{D \sim \mathcal{D}_\pi^X(|D(x)=\alpha)}\left[\prod_{i \in I_{-x}} \frac{D(x_i)}{1-\alpha}\right] \\
&= \alpha^\ell \cdot (1-\alpha)^{n-\ell} \cdot \mathop{\mathbf{E}}_{D' \sim \mathcal{D}_\pi^{X \setminus \{x\}}}\left[\prod_{i \in I_{-x}} D'(x_i)\right] \\
&= \alpha^\ell \cdot (1-\alpha)^{n-\ell} \cdot \mathop{\mathbf{Pr}}_{D' \sim \mathcal{D}_\pi^{X \setminus \{x\}}, U' \sim D^{n-\ell}}[U' = V \setminus x].
\end{aligned}$$

The second part of the claim follows directly from the fact that, by definition of $\bar{\pi}^N$,

$$\mathop{\mathbf{Pr}}_{D \sim \mathcal{D}_\pi^X, U \sim D^n}[D(x) = \alpha] = \bar{\pi}^N(\alpha).$$

□

We can now prove Lemma 2.1 which we restate here for convenience.

Lemma A.2 (Lemma 2.1 restated)**.** *For any frequency prior π, $x \in X$ and a sequence of points $V = (x_1, \ldots, x_n) \in X^n$ that includes x exactly ℓ times, we have*

$$\mathop{\mathbf{E}}_{D \sim \mathcal{D}_\pi^X, U \sim D^n}[D(x) \mid U = V] = \frac{\mathbf{E}_{\alpha \sim \bar{\pi}^N}\left[\alpha^{\ell+1} \cdot (1-\alpha)^{n-\ell}\right]}{\mathbf{E}_{\alpha \sim \bar{\pi}^N}\left[\alpha^\ell \cdot (1-\alpha)^{n-\ell}\right]}.$$

Proof. We first observe that by the Bayes rule and Lemma A.1:

$$\begin{aligned}
\mathop{\mathbf{Pr}}_{D \sim \mathcal{D}_\pi^N, U \sim D^n}[D(x) = \alpha \mid U = V] &= \frac{\mathbf{Pr}_{D \sim \mathcal{D}_\pi^N, U \sim D^n}[U = V \mid D(x) = \alpha] \cdot \mathbf{Pr}_{D \sim \mathcal{D}_\pi^N, U \sim D^n}[D(x) = \alpha]}{\mathbf{Pr}_{D \sim \mathcal{D}_\pi^N, U \sim D^n}[U = V]} \\
&= \frac{\alpha^\ell \cdot (1-\alpha)^{n-\ell} \cdot \mathbf{Pr}_{D' \sim \mathcal{D}_\pi^{X \setminus \{x\}}, U' \sim D^{n-\ell}}[U' = V \setminus x] \cdot \bar{\pi}^N(\alpha)}{\mathbf{E}_{\beta \sim \bar{\pi}^N}\left[\beta^\ell \cdot (1-\beta)^{n-\ell}\right] \cdot \mathbf{Pr}_{D' \sim \mathcal{D}_\pi^{X \setminus \{x\}}, U' \sim D^{n-\ell}}[U' = V \setminus x]} \\
&= \frac{\alpha^\ell \cdot (1-\alpha)^{n-\ell} \cdot \bar{\pi}^N(\alpha)}{\mathbf{E}_{\beta \sim \bar{\pi}^N}\left[\beta^\ell \cdot (1-\beta)^{n-\ell}\right]}.
\end{aligned}$$

This leads to the claim:

$$\begin{aligned}\mathop{\mathbf{E}}_{D\sim\mathcal{D}_\pi^N, U\sim D^n}[D(x)\mid U=V] &= \sum_{\alpha\in\mathsf{supp}(\bar\pi^N)} \alpha\cdot \mathop{\mathbf{Pr}}_{D\sim\mathcal{D}_\pi^N, U\sim D^n}[D(x)=\alpha\mid U=V] \\ &= \sum_{\alpha\in\mathsf{supp}(\bar\pi^N)} \alpha\cdot \frac{\alpha^\ell\cdot(1-\alpha)^{n-\ell}\cdot\bar\pi^N(\alpha)}{\mathbf{E}_{\beta\sim\bar\pi^N}\left[\beta^\ell\cdot(1-\beta)^{n-\ell}\right]} \\ &= \frac{\mathbf{E}_{\alpha\sim\bar\pi^N}\left[\alpha^{\ell+1}\cdot(1-\alpha)^{n-\ell}\right]}{\mathbf{E}_{\alpha\sim\bar\pi^N}\left[\alpha^\ell\cdot(1-\alpha)^{n-\ell}\right]}.\end{aligned}$$

□

B Proof of Theorem 3.5

Theorem B.1 (Thm. 3.5 restated)**.** *Let $X\subset\mathbb{R}^d$ be a domain partitioned into sub-domains $\{X_i\}_{i\in[N]}$ with subpopulations $\{M_i\}_{i\in[N]}$ over the sub-domains. Let $\mathcal{A}$ be any approximately margin maximizing m-class linear classifier and π be a frequency prior. Assume that for $D\sim\mathcal{D}_\pi^{[N]}$ and $V\sim M_D^n$, $V'\sim\prod_{j\in[N]_{S=1}}M_j$, with probability at least $1-\delta^2$, $V\cup V'$ is $(\tau,\tau^2/(8\sqrt{n}))$-independent for some $\tau\in(0,1/2]$. Then for any labeling prior $\mathcal{F}$, $\mathcal{A}$ is Λ-subpopulation-coupled with probability $1-\delta$ and $\lambda_1\geq 1-\delta$.*

Proof. For the given priors π and $\mathcal{F}$, let $S=((x_1,y_1),\ldots,(x_n,y_n))$ be a dataset sampled from $(M_D,L_f)^n$ for $D\sim\mathcal{D}_\pi^{[N]}$ and $f\sim\mathcal{F}$. Let $V=(x_1,\ldots,x_n)$. Let $T:=[N]_{S=1}$ and let $V'=(x'_j)_{j\in K}$ be sampled from $\prod_{j\in T}M_j$, that is, V' consists of additional independent samples from every subpopulation with a single sample.

We will show that for any $V\cup V'$ that is $(\tau,\theta:=\tau^2/(8\sqrt{n}))$-independent, the output $w_1,\ldots,w_m$ of any approximately margin maximizing m-class linear classifier $\mathcal{A}$ gives predictions on V' that are consistent with those on V (which are defined by S): if $x_i\in X_t$ for $t\in T$ then for every $k\in[m]$,

$$\mathsf{sign}(\langle w_k,x'_t\rangle)=\mathsf{sign}(\langle w_k,x_i\rangle).$$

By Defn. 3.4, this implies that the prediction of the classifier on x'_t is identical to that on x_i. By our assumption, $V\cup V'$ is *not* $(\tau,\tau/(4\sqrt{n}))$-independent with probability at most δ^2. By Markov's inequality, probability over the choice of V such that, the probability over the choice of V' that $V\cup V'$ is not (τ,θ)-independent is more than δ, is at most δ. By our definition of V', the marginal distribution of x'_t is exactly M_t. This implies that, with probability at least $1-\delta$ over the choice of the dataset S, for every $x\in X_{S=1}$, and $x'\sim M_x$ we have

$$\mathtt{TV}\left(\mathop{\mathbf{D}}_{h\sim\mathcal{A}(S)}[h(x)],\mathop{\mathbf{D}}_{x'\sim M_x,h\sim\mathcal{A}(S)}[h(x')]\right)\leq\delta$$

as required by Defn. 3.1 (for $\ell=1$).

To prove the stated consistency property for $V\cup V'$ that is (τ,θ)-independent, we will first show that every subset of points in V can be separated from its complement with margin γ of $\Omega(1/\sqrt{n})$. We will then use the properties of approximately margin maximizing classifiers and, again, independence to obtain consistency.

For any vector v, we denote $\bar v:=v/\|v\|_2$. To show that the margin is large, we define the weights explicitly by using one representative point from every subpopulation in V. Without loss of generality, we can assume that these representatives are $x_1, \dots, x_r$ for some $r \leq n$. Let $z_1, \dots, z_r \in \{\pm 1\}$ be an arbitrary partition of these representatives into positively and negatively labeled ones. We define $w := \sum_{j \in [r]} z_j \bar{x}_j$ and consider the linear separator given by $\bar{w}$.

To evaluate the margin we first observe that $\|w\|_2 \leq \sqrt{2r}$. This follows via induction on r:

$$\begin{aligned}\left\|\sum_{j\in[r]} z_j\bar{x}_j\right\|_2^2 &= \left\|\sum_{j\in[r-1]} z_j\bar{x}_j\right\|_2^2 + \|\bar{x}_j\|_2^2 + 2z_r\left\langle \sum_{j\in[r-1]} z_j\bar{x}_j, \bar{x}_r\right\rangle \\ &\leq 2(r-1) + 1 + 2\frac{\tau^2}{8\sqrt{n}}\left\|\sum_{j\in[r-1]} z_j\bar{x}_j\right\|_2 \\ &\leq \frac{4(r-1)}{3} + 1 + \frac{1}{16\sqrt{n}} \cdot \sqrt{2(r-1)} \leq 2r.\end{aligned}$$

Now for $i \in [n]$, assume that $x_i \in X_t$ and (without loss of generality) that x_r is the representative of subdomain X_t. Then

$$\begin{aligned}z_r\langle \bar{x}_i, \bar{w}\rangle &= \frac{1}{\|w\|_2}\left(\langle \bar{x}_i, \bar{x}_r\rangle + z_r\left\langle \bar{x}_i, \sum_{j\in[r-1]} z_j\bar{x}_j\right\rangle\right) \\ &\geq \frac{1}{\|w\|_2}\left(\tau - \frac{\tau^2}{8\sqrt{n}}\left\|\sum_{j\in[r-1]} z_j\bar{x}_j\right\|_2\right) \\ &\geq \frac{\tau}{\|w\|_2}\left(1 - \frac{\tau\sqrt{2(r-1)}}{8\sqrt{n}}\right) \geq \frac{\tau}{2\sqrt{n}}.\end{aligned}$$

Thus we obtain that x_i is labeled in the same way as its representative x_r and with margin of at least $\frac{\tau}{2\sqrt{n}}$. This holds for all $i \in [n]$ and therefore $\bar{w}$ shows that the desired separation can be achieved with margin of at least $\frac{\tau}{2\sqrt{n}}$.

Let $w_1, \dots, w_k$ be the linear separators returned by $\mathcal{A}$. Let w be one of them. By our assumptions on $\mathcal{A}$, w separates V with margin of at least $\gamma := \frac{\tau}{4\sqrt{n}}$ and further it lies in the span on V. Namely, there exist $\alpha_1, \dots, \alpha_n$ such that $w = \sum_{i\in[n]} \alpha_i \bar{x}_i$.

We now pick an arbitrary singleton point from V. Without loss of generality we assume that it is x_n, $\langle x_n, w\rangle \geq \gamma\|x_n\|_2$ and let $x \in V'$ be the point from the same subdomain X_t. Let $v := \sum_{i\in[n-1]} \alpha_i\bar{x}_i$ be the part of w that excludes x_n. By our assumption, x_n is a singleton and therefore the points in $(x_1, \dots, x_{n-1})$ are from other subdomains. By the independence of V, this implies that $|\langle \bar{x}_n, v\rangle| \leq \theta\|v\|_2$ and $|\langle \bar{x}, v\rangle| \leq \theta\|v\|_2$.

Now we need to show that the margin condition implies that α_n is sufficiently large. Specifically,

$$\gamma \leq \langle \bar{x}_n, w\rangle = \alpha_n + \langle \bar{x}_n, v\rangle \leq \alpha_n + \theta\|v\|_2,$$

and thus

$$\alpha_n \geq \gamma - \theta\|v\|_2 \geq \gamma - \theta(1 + \alpha_n),$$

where we used the fact that, by the triangle inequality, $\|v\|_2 \leq \|w\|_2 + \|\alpha_n\bar{x}_n\|_2 \leq 1 + \alpha_n$. This implies that

$\alpha_n \geq \frac{\gamma-\theta}{1+\theta}$. We can now bound $\langle \bar{x}, w \rangle$

$$\langle \bar{x}, w \rangle = \langle \alpha_n \bar{x}, \bar{x}_n \rangle + \langle \bar{x}, v \rangle \geq \alpha_n \tau - \theta \|v\|_2 \geq \alpha_n \tau - \theta(1+\alpha_n) = \alpha_n(\tau - \theta) - \theta$$
$$\geq \frac{(\gamma-\theta)(\tau-\theta)}{1+\theta} - \theta \geq \frac{\left(\frac{\tau}{4\sqrt{n}} - \frac{\tau^2}{8\sqrt{n}}\right)\left(\tau - \frac{\tau^2}{8\sqrt{n}}\right)}{1+\frac{\tau^2}{8\sqrt{n}}} - \frac{\tau^2}{8\sqrt{n}} > 0.$$

where the last inequality assumes that $n \geq 4$. Thus we obtain that for every $w \in \{w_1, \ldots, w_m\}$, every point in $V' \cap X_{S=1}$ will be classified by w in the same way as the point from the same subpopulation in S. $\square$