Good linear classifiers are abundant in the interpolating regime

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Abstract

Within the machine learning community, the widely-used uniform convergence framework seeks to answer the question of how complex models such as modern neural networks can generalize well to new data. This approach bounds the test error of the worst-case model one could have fit to the data, which presents fundamental limitations. In this paper, we revisit the statistical mechanics approach to learning, which instead attempts to understand the behavior of the typical model. To quantify this typicality in the setting of over-parameterized linear classification, we develop a methodology to compute the full distribution of test errors among interpolating classifiers. We apply our method to compute this distribution for several real and synthetic datasets. We find that in many regimes of interest, an overwhelming proportion of interpolating classifiers have good test performance, even though—as we demonstrate—classifiers with very high test error do exist. This shows that the behavior of the worst-case model can deviate substantially from that of the usual model. Furthermore, we observe that for a given training set and testing distribution, there is a critical value $\epsilon^* > 0$ which is typical, in the sense that nearly all test errors eventually concentrate around it. Based on these empirical results, we study this phenomenon theoretically under simplifying assumptions on the data, and we derive simple asymptotic expressions for both the distribution of test errors as well as the critical value $\epsilon^*$. Both of these results qualitatively reproduce our empirical findings. Our results show that the usual style of analysis in statistical learning theory may not be fine-grained enough to capture the good generalization performance observed in practice, and that approaches based on the statistical mechanics of learning offer a promising alternative.

1 Introduction

The phenomenon of good generalization in highly over-parameterized models, especially neural networks, has largely eluded theoretical understanding. Recently, however, progress has been made towards understanding over-parameterization in several simpler settings. Important examples include the variety of results demonstrating “double descent” phenomena in linear regression [1, 2, 3, 4] (and, in particular, how it is essentially a consequence of a transition between two different phases of learning [5]), nearest neighbors models [6], and binary classification [7, 8]. These results are typically derived by defining a specific estimator (e.g., the least-norm estimator in linear regression), and carefully examining its test risk. This approach presents a challenge when extending these analyses to the setting of neural networks, where no such estimator

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can easily be defined. In these situations, almost all results rely, in one way or another, on the framework of uniform convergence; that is, results which bound a quantity of the form
\[
\varepsilon_{\text{unif}} := \sup_{f \in \mathcal{F}} \left| \mathcal{E}_n(f) - \mathcal{E}(f) \right|
\]
where \( \mathcal{F} \) is a given function class, \( \mathcal{E}_n \) is the training error on a dataset of \( n \) points, and \( \mathcal{E} \) is the population error. Recently, it has been drawn into question whether this approach is fine-grained enough to capture the good generalization properties observed in deep learning [9, 10]. One issue that arises when using the uniform convergence framework is that for any given training set \( \{(x_1, y_1), \ldots, (x_n, y_n)\} \), and a sufficiently complex function class \( \mathcal{F} \), the worst-case estimator \( f \in \mathcal{F} \) fitting the training data may indeed perform quite poorly—thus dooming quantities like (1)—even if we are extremely unlikely to encounter such models in practice. One line of work has attempted to tackle this problem by studying the implicit biases of the algorithms used to train modern machine learning models [11, 12, 13] (by using what may be called implicit regularization in non-exact approximation algorithms [14]). Still, such results are mostly limited to simplified settings, and a comprehensive understanding of the relationship between optimization and generalization remains elusive.

In this work, we revisit several old ideas originating out of the statistical physics literature, which offer an alternative to the uniform convergence framework. (Such a perspective, while less common in statistical learning theory today, has a long history [9, 15, 16, 17, 18].) Rather than studying the worst-case estimator \( f \in \mathcal{F} \), the statistical mechanics approach seeks to understand the behavior of the typical function \( f \). This typicality can be characterized in a number of ways. A natural measure, from the statistical physics perspective, would be the entropy (or log density of states), which captures the number of models at any given test error value. As we review in the next section, several of these prior works calculate the entropy, or entropy-like quantities, in various settings. However, in part because these calculations are technically challenging, these works typically operate under significant simplifying assumptions, which limits their usefulness in describing real-world learning problems.

In this work, rather than computing an entropy directly, we will develop a methodology to compute the full distribution of test errors among interpolating linear classifiers. While this distribution captures much of the same information as an entropy would, it is considerably more interpretable, and allows us to precisely study how common different test error values are. Of course, a naïve way to answer such a question might be to fit many interpolating models, using some standard training algorithm, and then construct an empirical distribution of test errors. Such an approach was the subject of, e.g., [19]. However, this approach conflates a number of factors. For example, it will naturally be biased by the choice of optimization algorithm used to fit these models. While the study of such biases is an interesting question in its own right, we are instead interested in more fundamental properties of the learning problem.

In Section 3, we state a formal definition of the distribution of test errors as the fraction of interpolating models which achieve a given test error \( \varepsilon \). We then specialize to the setting of linear classification, and leverage recent work [20] to develop an efficient method to compute this distribution accurately, even in very high dimensions. In Section 4, we then apply this method to several learning tasks with both real and synthetic data. Our empirical results lead to a number of interesting observations. First, we find that, in many regimes, the fraction of interpolating classifiers with test error at most \( \varepsilon \) is nearly 1, indicating that essentially all classifiers perfectly fitting the data have test error less than \( \varepsilon \). Second, we also construct interpolating classifiers with test error much worse than \( \varepsilon \), demonstrating that, for these problems, bad classifiers do exist, but they are exceedingly rare. This fact draws into question whether a worst-case analysis of test errors is sufficiently fine-grained to capture to complexity (or simplicity) of these tasks. Third, we observe an intriguing phenomenon: for given training set and test distribution, there is a critical value \( \varepsilon^* \) around which almost all test errors eventually (in certain limits) concentrate.
Using these empirical observations as guidance, in Section 5, we study the distribution of test errors for interpolating classifiers theoretically, given simplifying assumptions on the training and testing data. In this setting, we provide asymptotic expressions for the distribution of test errors, and we precisely characterize the asymptotic behavior of the critical value $\varepsilon^*$. Both of these results qualitatively replicate the behavior from our empirical investigation, and they provide insight into the structure of the data which make good classifiers abundant.

2 Notation and background

In this section, we begin with some notation that will be used throughout the paper, and then we provide relevant background on the statistical mechanics approach to learning.

We will consider the setting of binary classification, and denote a training dataset $S_n = \{(x_1, y_1), \ldots, (x_n, y_n)\}$, with samples $x_i \in \mathbb{R}^d$ and labels $y_i \in \{-1, 1\}$. We let $\mathcal{F}$ be a class of functions $f : \mathbb{R}^d \to \{-1, 1\}$, and we define the version space to be the following subset of $\mathcal{F}$:

$$\text{VS}(S_n) = \{f \in \mathcal{F} : f(x_1) = y_1, \ldots, f(x_n) = y_n\}. \quad (2)$$

That is, the version space is the set of “interpolating” functions, i.e., those which perfectly fit the dataset $S_n$. We also use $\mathbb{P}$ to denote a probability measure defined over $\mathcal{F}$. We use $S_{\text{test}} = \{(x_{n+1}, y_{n+1}), \ldots, (x_{n+m}, y_{n+m})\}$ to denote a set of $m$ testing points, and $\mathbb{P}_{X,Y}$ to denote a testing distribution over the data $(x, y)$. Using these, we define the empirical and population testing errors:

$$\mathcal{E}_m(f) = \frac{1}{m} \sum_{h=1}^{m} \mathbb{I}(-y_{n+h}f(x_{n+h}) > 0), \quad \text{and} \quad \mathcal{E}(f) = \mathbb{E}_{X,Y}[\mathbb{I}(-yf(x) > 0)]. \quad (3)$$

From the viewpoint of statistical mechanics, the functions $f \in \mathcal{F}$ are “microscopic” variables which, for the purposes of learning, are summarized entirely by the corresponding “macroscopic” variables $\mathcal{E}_m(f)$ and $\mathcal{E}(f)$. Rather than measuring a worst-case error, à la (1), the statistical mechanics approach seeks to understand the typical behavior of the macroscopic variables $\mathcal{E}(f)$ and $\mathcal{E}_m(f)$, for classifiers $f$ perfectly fitting the training set, i.e., among $f \in \text{VS}(S_n)$. A natural way to do this is to divide up the version space into sets $\Omega_\varepsilon = \{f \in \text{VS}(S_n) : \mathcal{E}(f) \leq \varepsilon\}$ of classifiers obtaining test error at most $\varepsilon$. If $\mathbb{P}(\Omega_\varepsilon)$ is large (relative to $\mathbb{P}(\text{VS}(S_n))$), then interpolating classifiers with error at most $\varepsilon$ are correspondingly abundant.

Many works from the nineties studied learning behavior from the perspective of statistical physics [15, 16, 17, 18], and it has more recently been noted that revisiting this line of work would help to understand generalization in more modern applications [9]. Most similar in style to PAC-style generalization bounds were the results of [17], which derived generalization error bounds for functions $f \in \text{VS}(S_n)$, in the case of a finite class $\mathcal{F}$. In this case, the functions $f$ can only take on finitely many test error values $\varepsilon_1, \ldots, \varepsilon_r$, with each value $\varepsilon_j$ corresponding to a “shell” $\Omega_j = \{f : \mathcal{E}(f) = \varepsilon_j\}$. The error of a given classifier $f \in \text{VS}(S_n)$ can then be decomposed in terms of these shells, providing rigorous error bounds depending on a trade-off between the values $1 - \varepsilon_j$ and the cardinalities $|\Omega_j|$. Unfortunately, in addition to the obvious shortcoming of requiring $\mathcal{F}$ to be finite, this approach can be difficult to apply in many practical situations, in particular because the values $\varepsilon_j$ and $|\Omega_j|$ cannot be calculated, except for a few very special cases.

To generalize the analysis beyond finite classes $\mathcal{F}$, it is natural to use the measure $\mathbb{P}$ defined over $\mathcal{F}$, in which case the notion of “size” is captured by the volumes $\mathbb{P}(\Omega_\varepsilon)$. Work in the nineties studied such quantities for the class $\mathcal{F}_\text{lin} = \{f(x) = \text{sign}(w^T x) : w \in \mathbb{R}^d\}$ of linear classifiers. For example, [18] showed that if $\mathbb{P}$ is the
uniform measure on the sphere, for large \( d \) and the number of training samples scaling as \( n = \alpha d \), then \( \mathbb{P}(\Omega_\varepsilon) \) is asymptotically proportional to
\[
\exp \left( d \left[ \frac{1}{2} \log \sin^2(\pi \varepsilon) + \alpha \log(1 - \varepsilon) \right] \right). \tag{4}
\]
For a given scaling \( \alpha \), and \( d \) sufficiently large, these volumes exhibit a typicalness, in that they concentrate at a test error value \( \varepsilon^*(\alpha) \), which goes to zero as \( \alpha \to \infty \). An important simplifying assumption on which these results rely, however, is that the labels \( y_i \) are generated via a teacher \( w_* \), such that \( y_i = \text{sign}(w_*^t x_i) \), for all \( i = 1, \ldots, n \). In the present work, we will relax this assumption—no longer requiring that the labels be generated via a teacher—and we will focus particularly on the over-parameterized setting with \( n < d \). This relaxation allows us to study the test errors of classifiers fit to arbitrary datasets, without assumptions on how the labels are generated. We will show that, in certain regimes, test errors still concentrate at a value \( \varepsilon^* \), and that this value can differ significantly from the uniform error \( \varepsilon_{\text{unif}} \).

There are several other important works which are related to what we present here, such as [21, 22, 23], which we do not review in detail, but refer the interested reader to. Similarly, the wonderful text [18] provides a rich introduction to the statistical mechanics of learning.

3 Efficiently calculating the distribution of test errors for interpolating classifiers

In this section, we formally define the test error distribution of interpolating classifiers, and, in the linear case, provide an efficient method to compute it.

**Definition 1.** Given a function class \( \mathcal{F} \), a measure \( \mathbb{P} \) over \( \mathcal{F} \), and a training set \( S_n \), let
\[
R_{n,m}(\varepsilon) := \frac{\mathbb{P}(\{\mathcal{E}_m(f) \leq \varepsilon\} \cap \text{VS}(S_n))}{\mathbb{P}(\text{VS}(S_n))} = \mathbb{P}(\mathcal{E}_m(f) \leq \varepsilon \mid \text{VS}(S_n)), \tag{5}
\]
and
\[
R_n(\varepsilon) := \frac{\mathbb{P}(\{\mathcal{E}(f) \leq \varepsilon\} \cap \text{VS}(S_n))}{\mathbb{P}(\text{VS}(S_n))} = \mathbb{P}(\mathcal{E}(f) \leq \varepsilon \mid \text{VS}(S_n)). \tag{6}
\]
That is, the quantities \( R_{n,m}(\varepsilon) \) and \( R_n(\varepsilon) \) are the cumulative distribution functions (CDFs) of the errors \( \mathcal{E}_m \) and \( \mathcal{E} \), conditioned on perfectly fitting the training data. Intuitively, these quantities measure the fraction of interpolating classifiers \( f \in \text{VS}(S_n) \) that have test error at most \( \varepsilon \).

An advantage of our definition of \( R_{n,m}(\varepsilon) \) is that it is defined only relative to fixed training and testing sets, \( S_n \) and \( S_{\text{test}} \). This means that, at least in principle, \( R_{n,m}(\varepsilon) \) can be computed exactly (without explicit knowledge of the training and testing distributions). To do this naively would require computing the ratio of two (in general very small) high-dimensional volumes, which would be infeasible. Below, we introduce a technique to estimate \( R_{n,m}(\varepsilon) \) and \( R_n(\varepsilon) \) accurately, using the function class \( \mathcal{F}_{\text{lin}} = \{ f(x) = \text{sign}(w^t x) : w \in \mathbb{R}^d \} \) of linear classifiers.

Notice that for \( \mathcal{F} = \mathcal{F}_{\text{lin}} \), a probability measure \( \mathbb{P} \) over \( \mathcal{F} \) is simply a distribution over \( \mathbb{R}^d \). For the version space \( \text{VS}(S_n) \) to be non-trivial in general, we will focus on the regime where \( d > n \). Throughout this paper, we will assume that \( \mathbb{P} \) is the uniform distribution on the sphere \( \mathbb{S}^{d-1} = \{ w \in \mathbb{R}^d : \|w\| = 1 \} \). For the sake of computation, it will be convenient to make use of the equivalence (up to scaling) of this distribution with the
Gaussian distribution $\mathcal{N}(0, I)$, which is a consequence of the spherical symmetry of the Gaussian (see the Appendix for details).

If we define $L_n(w) = \prod_{i=1}^n 1(y_i w^T x_i \geq 0)$, then we can represent $R_n(\varepsilon)$ as

$$R_n(\varepsilon) = P(\mathcal{E}(w) \leq \varepsilon \mid VS(S_n)) = P(\mathcal{E}(w) \leq \varepsilon \mid L_n(w) = 1). \quad (7)$$

That is, we are interested in estimating a probability under the posterior distribution $P(\cdot \mid L_n(w) = 1)$. We can compute estimates of these probabilities by leveraging recent work [20], which developed the LIN-ESS algorithm (an extension of Elliptical Slice Sampling [24]). LIN-ESS is a Markov Chain Monte Carlo algorithm which can be used to draw samples $\tilde{w}$ from the posterior $P(\cdot \mid L_n(w) = 1)$ under the prior distribution $P = \mathcal{N}(0, I)$. Using traditional Monte Carlo methods, this task would be computationally infeasible in high dimensions, since if we naively drew samples from $P$ and rejected those not lying in the domain $\{L_n(w) = 1\}$, then drawing a reasonable number of samples could take an exponential amount of time. LIN-ESS is able to exploit special properties of the linear constraints $y_i w^T x_i \geq 0$ to draw samples without rejection. In particular, in our setup, we can use this to generate samples $\tilde{w}_1, \ldots, \tilde{w}_M \sim P(\cdot \mid L_n(w) = 1)$ efficiently, even in high dimensions. As we explain below, this allows us to generate accurate estimators for $R_{n,m}(\varepsilon)$ and $R_n(\varepsilon)$.

Using samples generated from LIN-ESS, we can define estimators for $R_{n,m}(\varepsilon)$ and $R_n(\varepsilon)$ as follows: given samples $\tilde{w}_1, \ldots, \tilde{w}_M \sim P(\cdot \mid L_n(w) = 1)$, let

$$\overline{R}_{n,m}(\varepsilon) = \frac{1}{M} \sum_{j=1}^M 1(\mathcal{E}_m(\tilde{w}_j) \leq \varepsilon), \quad \text{and} \quad \overline{R}_n(\varepsilon) = \frac{1}{M} \sum_{j=1}^M 1(\mathcal{E}(\tilde{w}_j) \leq \varepsilon). \quad (8)$$

Importantly, these estimators do not require the direct computation of the either $P(VS(S_n))$ or $P(\{\mathcal{E}(f) \leq \varepsilon\} \cap VS(S_n))$, nor the ratio of these quantities, and thus they are much more numerically stable than naive estimation of the ratio.

### 4 Computation of test error distributions for real and synthetic datasets

In this section, we compute the estimated test error distributions $\overline{R}_{n,m}(\varepsilon)$ and $\overline{R}_n(\varepsilon)$ on both real benchmark data as well as illustrative synthetic data, and we use this to obtain results on the abundance of good linear classifiers in the under-determined/over-parameterized regime.

#### 4.1 Evaluation on image datasets

For our first set of evaluations, we compute $\overline{R}_{n,m}(\varepsilon)$ for high-dimensional image datasets used in modern machine learning. In particular, we focus on the MNIST and FASHION-MNIST datasets, which consist of images in $d = 784$ dimensional space. Thus, throughout this section, we only consider values of $n < 784$. Since we are specialized to the binary classification setting, we focus of the MNIST 0 vs 1 task, and on the shirt vs pants task for FASHION-MNIST, though in the Appendix, we include results for other combinations of classes (leading to similar conclusions). For both of these tasks, the data has been centered and scaled, so as to have mean 0 and variance 1.

In Figure 1, we plot the $\overline{R}_{n,m}(\varepsilon)$ for various values of $n$. For each of the plots in this section, estimators $\overline{R}_{n,m}(\varepsilon)$ are formed with $M = 10,000$ samples from $P(\cdot \mid L_n(w) = 1)$ using the LIN-ESS algorithm, and they are evaluated on $m = 5000$ testing points.
Observation 1: Good classifiers are abundant. Our first observation is that, for reasonable $n$, most interpolating classifiers have good test set performance. For example, for the MNIST dataset, we see that at $n = 350$, nearly 100% of the models that perfectly fit the training data achieve at least 95% ($\varepsilon = 0.05$) test accuracy. This indicates that, for this particular training set, bad classifiers (with error $> 5\%$) make up a set with very small measure. On the other hand, for the FASHION-MNIST task, only about 60% of classifiers perfectly fitting the training data get 95% test performance at $n = 350$ samples, but nearly 100% of such classifiers get 92% accuracy.

Observation 2: Existence of bad classifiers. A natural question that may arise out of these results is whether or not bad interpolating classifiers even exist for these tasks, at least for the parameter settings we consider. Here, we demonstrate a simple method for finding bad classifiers which, together with the previous results, shows that bad classifiers exist and constitute a tiny fraction of the version space. Given a dataset $S_n$, with $n < d$, we can append up to $n_b \leq (d - 1) - n$ “bad” samples, to form a new dataset $S'_n$ with $n' = n + n_b$ samples. Notice that any model $w \in \text{VS}(S'_n)$ must also belong to $\text{VS}(S_n)$, since $\text{VS}(S'_n) \subseteq \text{VS}(S_n)$. Here, we construct $n_b = (d - 1) - n$ “bad” points lying in the span of the set $\{-y_1x_1, \ldots, -y_nx_n\}$. In Figure 2, we plot the test error of interpolating classifiers constructed in this manner, fit using gradient descent with a logistic loss, for varying levels of $n$. We see that this method finds classifiers with test error at least worse than $1/2$, and in many regimes nearly 1.

We are therefore left with an insightful contrast: in Figure 1, we observe that, for example, at $n = 350$, the set of interpolating MNIST classifiers with test accuracy $\geq 95\%$ comprise a set of measure essentially 1, while in Figure 2, we have demonstrated that there exist interpolating classifiers for this task with test accuracy $1/2$.

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1Of course, one could fit a model from a more complicated function class and obtain even better test performance.

2We explain in more detail why this works in the Appendix.
nearly 0%. Thus we see that the performance of the worst-case classifier can give basically no insight into the performance of the typical classifier, indicating that a uniform convergence-type analysis is not appropriate in this setting. This is also information that cannot be gleaned by looking at a summary statistic, like the expected test error of interpolating classifiers, i.e., $E[\mathcal{E}_m(w) \mid VS(S_n)]$, alone—it is necessary to consider the full distribution.

4.2 Evaluation on synthetic datasets

For our next set of experiments, we compute $R_n(\epsilon)$ for synthetic data generated from the Gaussian mixture distribution

$$(x, y) \sim \frac{1}{2}(N_+, 1) + \frac{1}{2}(N_-, -1)$$

where $N_+ \sim \mathcal{N}(\mu, \Sigma)$, $N_- \sim \mathcal{N}(-\mu, \Sigma)$ and $\mu \in \mathbb{R}^d$, $\Sigma \in S_d^+$. The purpose of this synthetic model is twofold: first, it allows us to demonstrate the ubiquity of the phenomena observed on the MNIST and FASHION-MNIST tasks. Second, it allows us to investigate the effect of varying the dimension $d$, which we could not do on the datasets studied in the previous section, as this was fixed at $d = 784$. This reveals that test errors begin to concentrate around a value $\epsilon^*$ as the dimension $d$ increases.

For this model, we have that $y x \sim \mathcal{N}(\mu, \Sigma)$, so we can characterize the set $\{w : \mathcal{E}(w) \leq \epsilon\}$ with the condition

$$\mathcal{E}(w) = \Pr_{x,y}(yw^T x < 0) = \Phi\left(\frac{-w^T \mu}{\sqrt{w^T \Sigma w}}\right) \leq \epsilon \iff \frac{w^T \mu}{\sqrt{w^T \Sigma w}} \geq -\Phi^{-1}(\epsilon),$$

where $\Phi(\cdot)$ is the CDF of a $\mathcal{N}(0, 1)$ distribution. Given a training set $S_n$ and samples $\tilde{w}_1, \ldots, \tilde{w}_M \sim \mathcal{P}(\cdot \mid VS(S_n))$, this expression allows us to compute an estimate $\hat{R}_n(\epsilon) = \frac{1}{M} \sum_{j=1}^M 1(\mathcal{E}(\tilde{w}_j) \leq \epsilon)$ in a straightforward manner.

As with many Gaussian models, the signal-to-noise ratio (SNR), which we define as $\sqrt{\mu^T \Sigma^{-1} \mu}$ (or simply $\|\mu\|/\sigma$ when $\Sigma = \sigma^2 I$), controls much of the complexity of this task. In Figure 3, we plot $\hat{R}_n(\epsilon)$ for $d = 100, 500, 1000$, and with SNR = 1, 5. For these experiments, we take $\Sigma = I$ and, to keep the SNR constant as we vary the dimension, we set $\mu = (\text{SNR}/\sqrt{d}, \ldots, \text{SNR}/\sqrt{d})^T$.

**Observation 3:** Concentration at critical value $\epsilon^*$. Our main observation in this section is the existence of a critical value $\epsilon^*$ around which test errors eventually concentrate. Indeed, we see in Figure 3 that as $d$
grows, the distributions $R_n(\varepsilon)$ seem to approach the threshold function $\mathbb{1}(\varepsilon \geq \varepsilon^*)$ at a critical value $\varepsilon^*$, which depends on the aspect ratio $\alpha = n/d$. Therefore, in the large $d$ regime, almost all interpolating classifiers have test error exactly $\varepsilon^*$, and so this critical value almost completely characterizes the distribution of test errors for interpolating classifiers. We also observe that this value is largely determined by the value of the SNR.

The following lemma supports this observation by providing a lower bound on $\varepsilon^*$ in terms of the SNR.

**Lemma 1.** For the Gaussian model (9), and any value $\varepsilon^* \geq \inf\{\varepsilon : R_n(\varepsilon) > 0\}$, we have

$$\varepsilon^* \geq \Phi(-\sqrt{\mu^T \Sigma^{-1} \mu}).$$ \hspace{1cm} (11)

When $\Sigma = \sigma^2 I$, this lower bound reduces to the usual signal-to-noise ratio: $\Phi(-\frac{\mu}{\sigma})$.

In the next section, we give a more formal definition of the critical value $\varepsilon^*$, and we describe a simple setting in which $R_n(\varepsilon)$ provably converges to $\mathbb{1}(\varepsilon \geq \varepsilon^*)$, for a precisely quantified critical value $\varepsilon^*$.

## 5 Characterizing the distribution of test errors in a simplified setting

In this section, we present a simple model, and we prove that this model exhibits the main qualitative properties we observed in Section 4 on synthetic and real datasets.

A full mathematical characterization of $R_{n,m}(\varepsilon)$ and/or $R_n(\varepsilon)$ is a challenging task. To see why, even in the context of linear classification, let us define the random variables $\zeta_i = y_i w^T x_i$ for $(x_i, y_i) \in S_n$ and $\zeta_{n+h} = y_{n+h} w^T x_{n+h}$ for $(x_{n+h}, y_{n+h}) \in S_{test}$ (where we emphasize that the randomness is due to $w$).

Then, for example, the normalization term $\mathbb{P}(\mathbb{V}(S_n))$ can be expressed as

$$\mathbb{P}(\mathbb{V}(S_n)) = \int \prod_{i=1}^{n} \mathbb{1}(y_i w^T x_i \geq 0) d(w) \hspace{1cm} (12)$$

$$= \mathbb{P}(\zeta_1 \geq 0, \zeta_2 \geq 0, \ldots, \zeta_n \geq 0). \hspace{1cm} (13)$$

That is, $\mathbb{P}(\mathbb{V}(S_n))$ can be seen as an orthant probability under the distribution $\mathbb{P}$. When $\mathbb{P} = \mathcal{N}(0, I)$, we find that $\zeta = (\zeta_1, \zeta_2, \ldots, \zeta_n) \sim \mathcal{N}(0, ZZ^T)$, where $Z$ is the $n \times d$ matrix whose $i^{th}$ row is $(y_i x_i)^T$. Computing such a Gaussian orthant probability for a general covariance matrix is a classical problem, and explicit formulae for them are known only in dimensions $\leq 5$ and in a few other special cases [25, 26, 27].

Hence, to present a model we can analyze, here we consider an idealized setting where the training samples have a fixed positive correlation with each other, i.e., for fixed $0 \leq \rho \leq 1$, $y_i y_j x_i^T x_j = \rho > 0$ for each pair $i \neq j$ (where here we assume the data are normalized, without loss of generality). To allow for more heterogeneity in the data, we model both positive and negative correlations between the test and training data, namely, either $y_i y_{n+h} x_i^T x_{n+h} = \rho > 0$ or $y_i y_{n+h} x_i^T x_{n+h} = -\rho < 0$ for each pair $(x_{n+h}, y_{n+h}) \in S_{test}$ and $(x_j, y_j) \in S_n$.

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3By correlation between data points, we mean $y_i y_j x_i^T x_j$ for $i \neq j$. 

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Figure 4: Plot of expression for $R_n(\varepsilon)$ given in Theorem 2. Blue curves correspond to $\rho = 0.2$, $\delta = 0.75$; red curves correspond to $\rho = 0.6$, $\delta = 0.9$. 

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Theorem 2. Let $\delta = \sqrt{1 - \rho}Z_i + B_i \sqrt{\rho}Z$, where $Z, Z_1, Z_2, \ldots, Z_n$ are i.i.d. $\mathcal{N}(0, 1)$ and $B_i$ is either $-1$ or $+1$.

In order to derive asymptotically valid expressions for $R_n(\varepsilon)$ and $R_{n,m}(\varepsilon)$, one may be tempted to use off-the-shelf techniques for approximating high-dimensional integrals, e.g., Laplace’s method. However, there are a number of pitfalls with this approach. First, it is difficult to quantify the approximation errors and results that do exist are not precise enough for our purposes. Second, certain conditions for Laplace’s method or other standard integral expansions do not hold in our setting. Nevertheless, we can leverage special properties of the Gaussian distribution and quantile functions to prove several non-trivial results. Henceforth, for sequences $\{a_n\}$ and $\{b_n\}$, the notation $a_n \sim b_n$ means $a_n = b_n(1 + o(1))$ as $n \to \infty$.

Our first result considers the setting of a single testing point $(x_{n+1}, y_{n+1})$, and demonstrates 1) a fundamental trade-off between the number of positive and negative correlations and 2) the effect of a larger correlation $\rho$ on the probability of correctly classifying a new test point. Furthermore, it shows that, at least for this simple setting, we can expect the probability of correctly classifying a testing point to converge to 1 at a $O(1/n)$ rate.

**Theorem 1.** Suppose we have a single test point $(x_{n+1}, y_{n+1})$, which has positive correlation $\rho$ with $n - n_0$ of the training samples and negative correlation $-\rho$ with $n_0$ of the training samples, where $n_0 = o(n)$. Then, as $n \to \infty$,

$$
\mathbb{P}(y_{n+1} = \text{sign}(w^T x_{n+1}) \mid \text{VS}(S_n)) \sim 1 - \frac{n_0 + (1 - \rho)/\rho}{n}.
$$

(14)

Before stating our next result, we provide a formal definition of a critical value $\varepsilon^*$ which we will reference therein.

**Definition 2.** We say that $\varepsilon^*$ is a critical value if for each $c > 0$, $R_n(\varepsilon^* - c) = 0$ and $R_n(\varepsilon^* + c) \to 1$ as $n \to \infty$.

Our next result provides an expression for $R_n(\varepsilon)$ and as a consequence provides a connection between the critical value $\varepsilon^*$ and the expected fraction $\delta$ of positively correlated test points.

**Theorem 2.** Let $\delta > 1/2$ be the expected fraction of test points that have positive correlation $\rho$ with the training points, conditional on the training data. Define the random variable

$$
U \overset{d}{=} 1 - \delta + \frac{2\delta - 1}{2n}V, \quad \text{where } V \sim \chi^2 \left( \frac{2(1 - \rho)}{\rho} \right).
$$

(15)

Then, as $n \to \infty$,

$$
R_n(\varepsilon) \sim \mathbb{P}(U \leq \varepsilon).
$$

(16)

In particular,

$$
\varepsilon^* = 1 - \delta + \left( \frac{1 - \rho}{n\rho} \right)(2\delta - 1)
$$

(17)

is a critical value.

Recall that by definition, $R_n(\varepsilon)$ is the cumulative distribution function of $\mathcal{E}$, conditioned on perfectly fitting the training data. Under the stated assumptions, Theorem 2 characterizes, asymptotically, this CDF as that of a shifted and scaled chi-square random variable. This result immediately implies that, in the large $n$ limit, the critical value $\varepsilon^*$ is simply the fraction $1 - \delta$ of negative correlations, and that $R_n(\varepsilon) \to 1(\varepsilon \geq 1 - \delta)$. In Figure 4, we plot this CDF for two different values of $\rho$ and $\delta$. In this simple setting, these two parameters completely determine the distribution $R_n(\varepsilon)$; both control the alignment of the datapoints. If $\rho$ is close to

---

4For example, the maximum of the function in the exponent of the integrand occurs at infinity.

5That is, it should not be confused with “has the probability distribution of” which uses the same notation.
1, then the datapoints are nearly parallel, and we will have that the test errors sharply concentrate around the critical value $\varepsilon^*$, even for $n$ small. On the other hand, if $\delta$ is close to 1, then we can expect to have an abundance of interpolating classifiers with test error near zero. Of course, for real datasets, there will be a more subtle and complicated relationship between the correlations and the distribution $R_n(\varepsilon)$, which will likely be difficult to characterize precisely. Nonetheless, this result provides insight into the structure of the data which can lead to the results observed in Section 4.

6 Conclusions

In this paper, we built on previous literature on the statistical mechanics of learning to develop a framework to study the typical generalization error of a classifier, which we propose as an alternative to the more standard uniform convergence approach. We define the full distribution of test errors among interpolating classifiers; and, after specializing to the setting of linear classification, we introduce a method to compute this distribution accurately on real datasets. One of the most important findings of our investigation is that, given a particular training and testing setup, there exists a critical value $\varepsilon^*$ around which almost all interpolating classifiers’ test errors eventually concentrate. This will not come as a surprise to the statistical physicist: such values commonly appear in physical systems. However, as we have demonstrated, this critical value can differ significantly from the error $\varepsilon_{\text{unif}}$, which one would obtain via a uniform convergence analysis, especially in the interpolating/over-parameterized regime, and which may be more familiar to the machine learner.

Our results should motivate further research into alternatives to the uniform convergence framework, either through the lens of statistical physics or some other (likely related) perspective, and ultimately help resolve questions surrounding the good performance of over-parameterized machine learning models. As a first step, we state a few potential directions for future work building off of the results presented here.

A conjecture. First, a conjecture, which is empirically supported by our results on Gaussian data in Section 4.2:

*For the model class $\mathcal{F}_{\text{lin}}$, a dataset $S_n$, testing distribution $\Pr_{x,y}$ and scaling $0 < \alpha < 1$, there exists a critical value $\varepsilon^*(\alpha)$ such that $\lim_{n,d \to \infty, n/d \to \alpha} R_n(\varepsilon) = 1(\varepsilon \geq \varepsilon^*(\alpha))$.\* 

This can be seen as a generalization of Theorem 2, without restrictions on the correlation matrix $ZZ^T$. A result of this form can also be deduced from Equation (4), in the case when the labels are generated via a teacher network. However, the more interesting, and technically challenging, case is when no such teacher exists, and the value $\varepsilon^*$ is characterized only by properties of the dataset $S_n$ and distribution $\Pr_{x,y}$.

More general function classes. An important point regarding our setting is that it in fact naturally extends to function classes of the form $\mathcal{F}_\varphi = \{ f(x) = \text{sign}(w^T \varphi(x)) : w \in \mathbb{R}^k \}$, where $\varphi : \mathbb{R}^d \to \mathbb{R}^k$ is some fixed embedding. This would facilitate, for example, the study of random feature models or kernel classifiers. An interesting direction for future work would be to investigate the effect of the choice of embedding $\varphi$ and dimension $k$.

While a full (distribution-dependent but data-agnostic) theoretical analysis of general neural networks seems challenging, our empirical and theoretical results do strongly suggest that a semi-empirical theory can be developed to study quantities like $R_n(\varepsilon)$, hopefully yielding insight into the empirical successes of these (and other) models.

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A Appendix

Equivalence of $\mathcal{N}(0, I)$ and uniform distribution on $\mathbb{S}^{d-1}$

We use the following two simple facts: 1) binary linear classification is invariant to positive scaling of the parameter vector and 2) if $w \sim \mathcal{N}(0, I)$, then $w \overset{d}{=} u \times Q$, where $u$ is uniformly distributed on $\mathbb{S}^{d-1}$ and $Q$ is an independent chi-square random variable with $d$ degrees of freedom. Thus, any quantity defined by a set of linear thresholds at zero with $w$, i.e., $y_i w^\top x_i \geq 0$, has the same distribution if the linear thresholds at zero are replaced with $u$, i.e., $y_i u^\top x_i \geq 0$.

Constructing bad classifiers

In Section 4, we demonstrated that we can construct bad classifiers by appending “bad” data points to a given training set. To see a simple way to construct bad points, recall that in Section 5, we saw that the size of the version space was largely controlled by the correlations $y_i y_j x_i^\top x_j$. We can explicitly construct an additional point $(y', x')$ with the smallest average correlation with the training points by observing that

$$\frac{1}{n} \sum_{i=1}^{n} (y_i x_i, y' x') = \left( \frac{1}{n} \sum_{i=1}^{n} y_i x_i, y' x' \right) \geq - \left\| \frac{1}{n} \sum_{i=1}^{n} y_i x_i \right\| \| y' x' \|.$$

This lower bound can be attained by taking $y' x'$ proportional to $- \sum_{i=1}^{n} y_i x_i$, e.g., by taking $y' = 1$ and $x' = - \sum_{i=1}^{n} y_i x_i$. In Section 4, we construct $n_b$ bad data points in this fashion, by first constructing a new bad point $(x', y')$, and then appending this to the original dataset and repeating the process $n_b$ times.

Proofs of our main theoretical results

Proof of Lemma 1. Define the norm $\| x \|_{\Sigma}^2 = x^\top \Sigma x$. The value $\varepsilon^*$ satisfies

$$-\Phi^{-1}(\varepsilon^*) = \text{ess sup}_{w \in \mathbb{S}} \frac{w^\top \mu}{\sqrt{w^\top \Sigma w}} \leq \sup_{w \in \mathbb{S}} \frac{w^\top \mu}{\sqrt{w^\top \Sigma w}} = \sup_{w \in \mathbb{S}, \|w\|_{\Sigma} = 1} w^\top \mu \leq \sup_{\|w\|_{\Sigma} = 1} w^\top \mu = \|\mu\|_{\Sigma^{-1}} = \sqrt{\mu^\top \Sigma^{-1} \mu},$$

where we use the fact that $\| \cdot \|_{\Sigma^{-1}}$ is the dual norm to $\| \cdot \|_{\Sigma}$. Hence solving for $\varepsilon^*$, we get the lower bound

$$\varepsilon^* \geq \Phi(-\sqrt{\mu^\top \Sigma^{-1} \mu}).$$

When $\Sigma = \sigma^{-2} I$, this lower bound reduces to the usual signal-to-noise ratio $\Phi(-\|\mu\|_{\sigma})$. \qed

Proof of Theorem 1. The assumptions on the correlation structure imply that $\zeta_i \overset{d}{=} \sqrt{1 - \rho} Z_i - \sqrt{\rho} Z$ for $i = 1, 2, \ldots, n_0$ and $\zeta_i \overset{d}{=} \sqrt{1 - \rho} Z_i + \sqrt{\rho} Z$ for $i = n_0 + 1, n_0 + 2, \ldots, n + 1$. Let $a = \sqrt{\frac{\rho}{1 - \rho}}$. Note that

$$P(\zeta_1 \geq 0, \zeta_2 \geq 0, \ldots, \zeta_n \geq 0) = \mathbb{E}_{Z \sim N(0, 1)} \left[ (1 - \Phi(aZ))^n_0 (\Phi(aZ))^{n-n_0} \right] = \int_{-\infty}^{\infty} (1 - \Phi(az))^n_0 (\Phi(az))^{n-n_0} \phi(z) dz,$$

(18)
where $\phi(\cdot)$ is the density of a $N(0, 1)$ distribution. Make the change of variables $u = (n - n_0)(1 - \Phi(az))$. Then the integral (18) becomes

$$
\frac{(2\pi)^{\frac{1}{2}}(\frac{1}{a^2})^{-1}}{(n - n_0)a} \int_0^{n-n_0} \left( u/(n-n_0) \right)^{n_0} (1 - u/(n-n_0))^{n-n_0} \phi(\Phi^{-1}(1-u/(n-n_0))) \frac{1}{\sqrt{\pi}} \nu^{-1} du. \tag{19}
$$

Next, consider the so-called “density quantile function” $\phi(\Phi^{-1}(v))$. Using a standard asymptotic expression for Mills’ ratio [28], we have

$$
\frac{1 - \Phi(x)}{\phi(x)} = \frac{1}{x} \left( 1 + O\left( \frac{1}{x^2} \right) \right), \quad x \to \infty. \tag{20}
$$

Furthermore, the quantile function $\Phi^{-1}(v)$ has the following asymptotic expression [29]

$$
\Phi^{-1}(v) = \sqrt{2\log(1/(1-v))} \left( 1 + O\left( \frac{\log \log(1/(1-v))}{\log(1/(1-v))} \right) \right), \quad v \uparrow 1. \tag{21}
$$

Combining these two facts ((20) and (21)) yields

$$
\phi(\Phi^{-1}(v)) = (1-v)\sqrt{2\log(1/(1-v))} \left( 1 + O\left( \frac{\log \log(1/(1-v))}{\log(1/(1-v))} \right) \right), \quad v \uparrow 1.
$$

Using this asymptotic expression for $\phi(\Phi^{-1}(v))$, we find that

$$
\int_0^{n-n_0} \left( u/(n-n_0) \right)^{n_0} (1 - u/(n-n_0))^{n-n_0} \phi(\Phi^{-1}(1-u/(n-n_0))) \frac{1}{\sqrt{\pi}} \nu^{-1} du
$$

from (19) is asymptotically

$$
(n - n_0)^{1-n_0-1/a^2} \left( 2\log(n-n_0) \right)^{\frac{1}{4} \left( \frac{1}{a^2} - 1 \right)} \int_0^{n-n_0} \left( 1 + \frac{\log(1/u)}{\log(n-n_0)} \right)^{\frac{1}{2} \left( \frac{1}{a^2} - 1 \right)} u^{n_0+1/a^2-1} e^{-u} du. \tag{22}
$$

Finally, by the dominated convergence theorem, $\int_0^{n-n_0} \left( 1 + \frac{\log(1/u)}{\log(n-n_0)} \right)^{\frac{1}{2} \left( \frac{1}{a^2} - 1 \right)} u^{n_0+1/a^2-1} e^{-u} du$ is asymptotically

$$
\int_0^\infty u^{n_0+1/a^2-1} e^{-u} du = \Gamma(n_0 + 1/a^2).
$$

Therefore, (22) is asymptotically

$$
(n - n_0)^{1-n_0-1/a^2} \left( 2\log(n-n_0) \right)^{\frac{1}{4} \left( \frac{1}{a^2} - 1 \right)} \Gamma(n_0 + 1/a^2). \tag{23}
$$

Combining (19) and (23), we have

$$
P(\zeta_1 \geq 0, \zeta_2 \geq 0, \ldots, \zeta_n \geq 0) \sim \frac{\Gamma(n_0 + 1/a^2)}{a} \left( 4\pi \log(n-n_0) \right)^{\frac{1}{2} \left( \frac{1}{a^2} - 1 \right)} (n - n_0)^{-n_0-1/a^2}. \tag{24}
$$

Having given an asymptotic expression for the orthant probabilities, we turn our attention to the ratio $R_{n,1}(0) = P(y_{n+1} = f(x_{n+1}) \mid VS(S_n))$. Note that

$$
R_{n,1}(0) = 1 - \frac{P\left( \{y_{n+1} \neq f(x_{n+1})\} \cap VS(S_n) \right)}{P(VS(S_n))}.
$$

Next, we recognize that the set $\{y_{n+1} \neq f(x_{n+1})\} \cap VS(S_n)$ is another version space with $n + 1$ samples and the same correlation structure as before, but with $n_0 + 1$ of the $\zeta_i$ equal in distribution to $\sqrt{1 - \rho} Z_i + \sqrt{\rho} Z_i$.
instead of \( n_0 \). Therefore, using the above asymptotic formula (24) for \( \mathbb{P}(\zeta_1 \geq 0, \zeta_2 \geq 0, \ldots, \zeta_n \geq 0) \), we have that
\[
\mathbb{P}(\{(y_{n+1} \neq f(x_{n+1})) \cap \text{VS}(S_n)\}) = 1 - R_{n,1}(0)
\]
is asymptotically
\[
\frac{\Gamma((n+1) + 1/a^2)}{a} \frac{(4 \pi \log((n + 1) - (n_0 + 1)))^{1/2(a-1)}}{(n + 1) - (n_0 + 1)} - (n_0 + 1)^{-1/a^2} \frac{\Gamma(n_0 + 1/a^2)}{a} \frac{(4 \pi \log(n - n_0))^{1/2(a-1)}}{(n - n_0)} - n_0^{-1/a^2}
\]
thus completing the proof of (14).

**Proof of Theorem 2.** The following specifications satisfy the assumed correlation structure between the test and training samples. For the test samples, \( \zeta_{n+h} \stackrel{d}{=} \sqrt{1-\rho}Z_{n+h} + B_{n+h}\sqrt{\rho}Z \), where \( B_{n+h} \) are i.i.d. Rademacher(\( \delta \)) and for the training samples, \( \zeta_i \stackrel{d}{=} \sqrt{1-\rho}Z_i + \sqrt{\rho}Z \). This means that among the training samples, the \( \zeta_i \) have positive correlation \( \rho \). Also, if
\[
T = \sum_{(x_{n+h}, y_{n+h}) \in \text{last}, (x_i, y_i) \in S_n} \mathbb{I}(y_{n+h} x_{n+h}^T x_i > 0) = n \sum_{(x_{n+h}, y_{n+h}) \in \text{last}} \mathbb{I}(B_{n+h} = 1)
\]
is the observed number of test samples that have positive correlation with the training samples, then \( E_{\text{last}}[T | S_n] = nm\delta \).

To begin with the asymptotic derivations, note that by definition
\[
R_{n,m}(\varepsilon) = \frac{\mathbb{P}(\{E_m(f) \leq \varepsilon\} \cap \text{VS}(S_n))}{\mathbb{P}(\text{VS}(S_n))} \quad (25)
\]
Using the representation of \( \zeta_i \) in terms of \( Z \) and \( Z_i \), we have \( E_m(f) \stackrel{d}{=} \frac{1}{m} \sum_{i=1}^{m} \mathbb{I}(Z_i < -aB_i Z) \) and \( E(f) \stackrel{d}{=} \lim_m \frac{1}{m} \sum_{i=1}^{m} \mathbb{I}(Z_i < -aB_i Z) \), where \( a = \Theta \). Henceforth, we take these distributional equivalents as the definitions of \( E_m(f) \) and \( E(f) \). Now,
\[
\mathbb{P}(\{E_m(f) \leq \varepsilon\} \cap \text{VS}(S_n)) = \mathbb{E}_{Z \sim N(0,1)} [\mathbb{P}(E_m(f) \leq \varepsilon \mid Z) \Phi^n(aZ)]
\]
By the strong law of large numbers, given \( Z \), \( \frac{1}{m} \sum_{i=1}^{m} \mathbb{I}(Z_i < -aB_i Z) \) converges almost surely (with respect to the test data \( S_{\text{last}} \) and \( Z_1, Z_2, \ldots \)) to its mean \( \Phi(-aZ) + (1-\delta)\Phi(aZ) = 1-\delta + (2\delta - 1)(1-\Phi(aZ)) \). Thus, by the dominated convergence theorem, almost surely,
\[
\lim_m \mathbb{P}(E_m(f) \leq \varepsilon \mid Z) = \mathbb{1}(1-\delta + (2\delta - 1)(1-\Phi(aZ)) \leq \varepsilon).
\]
Therefore, it follows that, almost surely,
\[
\mathbb{P}(E(f) \leq \varepsilon \mid Z) = \mathbb{1}(1-\delta + (2\delta - 1)(1-\Phi(aZ)) \leq \varepsilon).
\]
The above indicator function is equal to 0 when \( \delta > 1/2 \) and \( \varepsilon \leq 1-\delta \), so we consider the case where \( \delta > 1/2 \) and \( \varepsilon > 1-\delta \). Let \( \tau = (\varepsilon - (1-\delta))/(2\delta - 1) \). Then,
\[
R_n(\varepsilon) = \frac{\mathbb{P}(\{E(f) \leq \varepsilon\} \cap \text{VS}(S_n))}{\mathbb{P}(\text{VS}(S_n))} \leq \mathbb{E}_{Z \sim N(0,1)} [\mathbb{1}(1-\Phi(aZ) \leq \tau) \Phi^n(aZ)]
\]
\[
= \int_0^{\tau} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u}{2}\right) du
\]
\[
= \frac{1}{\sqrt{2\pi}} \int_0^{\tau} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u}{2}\right) du
\]
\[
= \frac{1}{\sqrt{2\pi}} \int_0^{\tau} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u}{2}\right) du \quad (26)
\]
where for the final equality, we use (19) from Theorem 2 with \( n_0 = 0 \). Using the same techniques as Theorem 2 to derive asymptotic integral expressions therein (in fact, the integrands of the integrals are identical), (26) is asymptotically equivalent to
\[
\frac{\int_0^{\tau n} u^{1/\rho^2 - 1} e^{-u} du}{\int_0^{\infty} u^{1/\rho^2 - 1} e^{-u} du} = \mathbb{P}(V \leq 2n\tau) = \mathbb{P}(U \leq \varepsilon),
\]
which proves the first claim (16).

To prove the second claim (17) about the critical value, let \( c > 0 \) be arbitrary. Then,
\[
\mathbb{P}(U \leq \varepsilon^* + c) = \mathbb{P}(V \leq 2(1 - \rho)/\rho + 2nc/(2\delta - 1)) \rightarrow 1,
\]
preserved \( np \rightarrow \infty \). On the other hand, for \( np \) large enough, \( 2(1 - \rho)/\rho - 2nc/(2\delta - 1) < 0 \) and hence,
\[
\mathbb{P}(U \leq \varepsilon^* - c) = \mathbb{P}(V \leq 2(1 - \rho)/\rho - 2nc/(2\delta - 1)) = 0.
\]

Additional empirical results

In Figure 5, we plot the same quantities shown in Figure 1, using different choices of classes for the binary problem – specifically, 6 vs 9 for MNIST and sandal vs bag for FASHION-MNIST.