A Priori Estimates of the Generalization Error for Two-layer Neural Networks

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Abstract

New estimates for the generalization error are established for the two-layer neural network model. These new estimates are a priori in nature in the sense that the bounds depend only on some norms of the underlying functions to be fitted, not the parameters in the model. In contrast, most existing results for neural networks are a posteriori in nature in the sense that the bounds depend on some norms of the model parameters. The error rates are comparable to that of the Monte Carlo method for integration problems. Moreover, these bounds are equally effective in the over-parametrized regime when the network size is much larger than the size of the dataset.

1 Introduction

One of the most important theoretical challenges in machine learning comes from the fact that classical learning theory cannot explain the effectiveness of over-parametrized models in which the number of parameters is much larger than the size of the training set. This is especially the case for neural network models, which have achieved remarkable performance for a wide variety of problems [2, 16, 26]. Understanding the mechanism behind these successes requires developing new analytical tools that can work effectively in the over-parametrized regime [30].

Our work is partly motivated by the situation in classical approximation theory and finite element analysis [8]. There are two kinds of error bounds in finite element analysis depending on whether the target solution (the ground truth) or the numerical solution enters into the bounds. Let \( f^* \) and \( \hat{f}_n \) be the true solution and the “numerical solution”, respectively. In “a priori” error estimates, only norms of the true solution enter into the bounds, namely

\[
\| \hat{f}_n - f^* \|_1 \leq C \| f^* \|_2.
\]

In “a posteriori” error estimates, the norms of the numerical solution enter into the bounds:

\[
\| \hat{f}_n - f^* \|_1 \leq C \| \hat{f}_n \|_3.
\]

Here \( \| \cdot \|_1, \| \cdot \|_2, \| \cdot \|_3 \) denote various norms.

In this language, most recent theoretical efforts [24, 4, 10, 21, 22, 23] on estimating the generalization error of neural networks should be viewed as “a posteriori” analysis, since the bounds depend on various norms of the solutions. Unfortunately, as observed in [1] and [23], the numerical values of these norms are usually quite large for real situations, yielding vacuous bounds.

In this paper we pursue a different line of attack by providing “a priori” analysis. For this purpose, a suitably regularized two-layer network is considered. It is proved that the generalization error of the regularized solutions is asymptotically sharp with constants depending only on the properties of...
In practice, we only have at our disposal the empirical risk. The ultimate goal is to minimize the generalization error (expected risk).

Following [6, 14], we consider target functions that are bounded and have finite spectral norm:

\[ \min_{\gamma(f) < \infty} \mathbb{E}_{\pi} \mathcal{R}(f) \]

We also define \( \gamma(f) \) to be the Fourier transform of \( f \) by

\[ \gamma(f) = \inf_{\tilde{F} \in L^2(\mathbb{R}^d), \tilde{F}[f] = f} \int_{\mathbb{R}^d} \|\omega\|_1 \tilde{F}(\omega) |d\omega. \]

We also define \( \hat{\gamma}(f) = \max\{\gamma(f), 1\} \).

**Assumption 1.** Following [6, 14], we consider target functions that are bounded and have finite spectral norm:

\[ \mathcal{F}_s := L^2(\Omega) \cap \{ f: \Omega \rightarrow \mathbb{R} \mid \gamma(f) < \infty, \|f\|_\infty \leq 1 \}, \]

We assume that \( f^* \in \mathcal{F}_s \).

As a consequence of the assumption that \( \|f^*\|_\infty \leq 1 \), we can truncate the network by \( T f(x) = \min\{|f(x)|, 1\} \text{sign}(f) \). By an abuse of notation, in the following we still use \( f(x) \) to denote \( T f(x) \).

The ultimate goal is to minimize the generalization error (expected risk)

\[ L(\theta) = \mathbb{E}_{x,y} [\ell(f(x; \theta), y)]. \]

In practice, we only have at our disposal the empirical risk

\[ \hat{L}_n(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i; \theta), y_i). \]

The generalization gap is defined as the difference between expected and empirical risk. Here the loss function is \( \ell(y_1, y_2) = (y_1 - y_2)^2 \), unless it is specified otherwise.

**1.2 Our Results**

We propose a regularized estimator \( \hat{\theta}_n \) (defined in Section 3) and prove a priori estimates for its generalization error shown in Table 1. As a comparison, we also list the result of [14] which analyzed a similar problem. It is worth mentioning that they require the network width \( m \) to be the orders of \( \text{poly}(n) \) whereas we allow arbitrary network width. See Theorem 8 and 9 for more details about the results.
2 Preliminary Results

In this section, we summarize some results on the approximation error and generalization bound for two-layer ReLU networks. These results are required by our subsequent a priori analysis.

2.1 Approximation Properties

Most of the content in this part is adapted from [3, 6, 14].

Proposition 1. For any \( f \in F_s \), one has the integral representation:

\[
 f(x) - f(0) - x \cdot \nabla f(0) = v \int_{[-1,1] \times [0,1] \times \mathbb{R}^d} h(x; z, t, \omega) dp(z, t, \omega),
\]

where

\[
 p(z, t, \omega) = |\hat{f}(\omega)||\omega||^2 \cos(||\omega||^2 z b(\omega)) |v \\
 s(z, t, \omega) = -\operatorname{sign} \left( \cos(||\omega||^2 z b(\omega)) \right) \\
 h(x; z, t, \omega) = s(z, t, \omega) (zx \cdot \omega/||\omega||_1 - t)_+.
\]

\( v \) is the normalization constant such that \( \int p(z, t, \omega) dzdt\omega = 1 \), which satisfies \( v \leq 2\gamma(f) \).

Proof. By an abuse of notation, let \( f \) be its own \( L^2 \) extension in \( \mathbb{R}^d \). Since \( f \in L^2(\mathbb{R}^d) \), \( f(x) - x \cdot \nabla f(0) - f(0) \) can be written as

\[
 \int_{\mathbb{R}^d} (e^{i\omega \cdot x} - i\omega \cdot x - 1) \hat{f}(\omega) d\omega. \tag{4}
\]

Note that the identity

\[
 -\int_0^c [(z-s)_+ e^{is} + (z-s)_- e^{-is}] ds = e^{iz} - iz - 1
\]

holds when \( |z| \leq c \). Choosing \( c = ||\omega||_1 \), \( z = \omega \cdot x \), we have

\[
 |z| \leq ||\omega||_1 ||x||_\infty \leq c.
\]

Let \( s = ||\omega||^2 t, 0 \leq t \leq 1 \), and \( \hat{\omega} = \omega/||\omega||_1 \), we have

\[
 -||\omega||^2 t \int_0^1 \left( (\hat{\omega} \cdot x - t)_+ e^{i||\omega||^2 t} + (-\hat{\omega} \cdot x - t)_+ e^{-i||\omega||^2 t} \right) dt = e^{i\omega \cdot x} - i\omega \cdot x - 1. \tag{5}
\]

Let \( \hat{f}(\omega) = e^{i\hat{b}(\omega)}|\hat{f}(\omega)| \), inserting (5) into (4) yields

\[
 f(x) - x \cdot \nabla f(0) - f(0) = \int_{\mathbb{R}^d} \int_0^1 g(t, \omega) dt\omega d\omega,
\]

where

\[
 g(t, \omega) = -||\omega||^2 ||\hat{f}(\omega)|| \left( (\hat{\omega} \cdot x - t)_+ \cos(||\omega||^2 t + b(\omega)) + (-\hat{\omega} \cdot x - t)_+ \cos(||\omega||^2 t - b(\omega)) \right).
\]
Consider a density on \( \{0,1\} \times [0,1] \times \mathbb{R}^d \) defined by
\[
p(z,t,\omega) = |\hat{f}(\omega)||\omega|^2 \cos (||\omega||_1 t - zb(\omega)) / v
\]
where the normalized constant \( v \) is given by
\[
v = \int_{\mathbb{R}^d} \int_0^1 |\hat{f}(\omega)||\omega|^2 \left( \cos (||\omega||_1 t + b(\omega)) + \cos (||\omega||_1 t - b(\omega)) \right) d\omega dt.
\]
Since \( f \) belongs to \( \mathcal{F}_s \), so we have
\[
v \leq 2\gamma(f) < +\infty,
\]
therefore the density \( p(z,t,\omega) \) is well-defined. To simplify the notations, we let
\[
s(z,t,\omega) = -\text{sign}(\cos(||\omega||_1 t - zb(\omega)))
\]
\[
h(x; z,t,\omega) = s(z,t,\omega)(z\hat{\omega} \cdot x - t)_+.
\]
Then we have
\[
f(x) - x \cdot \nabla f(0) - f(0) = v \int_{\{-1,1\} \times [0,B] \times \mathbb{R}^d} h(x; z,t,\omega) dp(z,t,\omega).
\]
Since \( x = (x)_+ - (-x)_+ \), we obtain
\[
f(x) = f(0) + (x \cdot \nabla f(0))_+ - (-x \cdot \nabla f(0))_+ + v \int_{\{-1,1\} \times [0,B] \times \mathbb{R}^d} h(x; z,t,\omega) dp(z,t,\omega).
\]

For simplicity, in the rest of this paper, we assume \( \nabla f(0) = 0, f(0) = 0 \). We take \( m \) samples \( T_m = \{(z_1,t_1,\omega_1), \ldots, (z_m,t_m,\omega_m)\} \) with \( (z_i,t_i,\omega_i) \) randomly drawn from \( p(z,t,\omega) \), and consider the empirical average \( \hat{f}_m(x) = \frac{1}{m} \sum_{k=1}^m h(x; z_k,t_k,\omega_k) \), which is exactly a two-layer ReLU network of width \( m \). The central limit theorem (CLT) tells us that the approximation error is roughly
\[
\mathbb{E}_{(z,t,\omega)} [h(x; z,t,\omega)] - \frac{1}{m} \sum_{k=1}^m h(x; z_k,t_k,\omega_k) \approx \sqrt{\frac{\text{Var}_{(z,t,\omega)}[h(x; z,t,\omega)]}{m}}.
\]
So as long as we can bound the variance at the right-hand side, we will have an estimate of the approximation error. The following result formalizes this intuition.

**Theorem 2.** For any distribution \( \pi \) with \( \text{supp}(\pi) \subset \Omega \) and any \( f \in \mathcal{F}_s \), there exists a two-layer network \( f(x; \hat{\theta}) \) of width \( m \) such that
\[
\mathbb{E}_{x \sim \pi} [f(x) - f(x; \hat{\theta})]^2 \leq \frac{16\gamma^2(f)}{m}.
\]
Furthermore \( \|\hat{\theta}\|_p \leq 4\gamma(f) \), i.e. the path norm of \( \hat{\theta} \) can be bounded by the spectral norm of the target function.

**Proof.** Let \( \hat{f}_m(x) = \frac{1}{m} \sum_{k=1}^m h(x; z_k,t_k,\omega_k) \) be the Monte-Carlo estimator, we have
\[
\mathbb{E}_T_m \mathbb{E}_x [f(x) - \hat{f}_m(x)]^2 = \mathbb{E}_x \mathbb{E}_{T_m} |f(x) - \hat{f}_m(x)|^2
\]
\[
= \frac{v^2}{m} \mathbb{E}_x (\mathbb{E}_{(z,t,\omega)}[h^2(x; z,t,\omega)] - f^2(x))
\]
\[
\leq \frac{v^2}{m} \mathbb{E}_x \mathbb{E}_{(z,t,\omega)}[h^2(x; z,t,\omega)]
\]
Furthermore, for any fixed \( x \), the variance can be upper bounded since
\[
\mathbb{E}_{z,t,\omega}[h^2(x; z, t, \omega)] \leq \mathbb{E}_{z,t,\omega}[(z\hat{\omega} \cdot x - t)^2] \\
\leq \mathbb{E}_{z,t,\omega}[(|\hat{\omega} \cdot x| + t)^2] \\
\leq 4.
\]
Hence we have
\[
\mathbb{E}_{z,m} \mathbb{E}_x[f(x) - \hat{f}_m(x)]^2 \leq \frac{4\nu^2}{m} \leq \frac{16\gamma^2(f)}{m}
\]
Therefore there must exist a set of \( T_m \), such that the corresponding empirical average satisfies
\[
\mathbb{E}_x[f - f_m]^2 \leq \frac{16\gamma^2(f)}{m}.
\]
Due to the special structure of the Monte-Carlo estimator, we have \(|a_k| = v/m, \|b_k\|_1 = 1, |c_k| \leq 1\). It follows Equation (7) that \( \|\hat{\theta}\|_p \leq 2\nu \leq 4\gamma(f). \)

### 2.2 Estimating the Generalization Gap

**Definition 3** (Rademacher complexity). Let \( \mathcal{H} \) be a hypothesis space, i.e. a set of functions. The Rademacher complexity of \( \mathcal{H} \) with respect to samples \( S = (z_1, z_2, \ldots, z_n) \) is defined as
\[
\hat{R}(\mathcal{H}) = \frac{1}{n} \mathbb{E}_{\xi} [\sup_{h \in \mathcal{H}} \sum_{i=1}^{n} h(z_i)\xi_i],
\]
where \( \{\xi_i\}_{i=1}^{n} \) are independent random variables with \( \mathbb{P}(\xi_i = +1) = \mathbb{P}(\xi_i = -1) = \frac{1}{2} \).

The generalization gap can be estimated via the Rademacher complexity by the following theorem (see [5, 25]).

**Theorem 3.** Fix a hypothesis space \( \mathcal{H} \). Assume that for any \( h \in \mathcal{H} \) and \( z \), \(|h(z)| \leq c\). Then for any \( \delta > 0 \), with probability at least \( 1 - \delta \) over the choice of \( S = (z_1, z_2, \ldots, z_n) \), we have
\[
\sup_{h \in \mathcal{H}} \left| \frac{1}{n} \sum_{i=1}^{n} h(z_i) - \mathbb{E}_z[h(z)] \right| \leq 2\mathbb{E}_S[\hat{R}(\mathcal{H})] + c\sqrt{\frac{2\log(2/\delta)}{n}}.
\]

Before to provide the upper bound for the Rademacher complexity of two-layer networks, we first need the following two lemmas.

**Lemma 1** (Lemma 26.11 of [25]). Let \( S = (x_1, \ldots, x_n) \) be \( n \) vectors in \( \mathbb{R}^d \). Then the Rademacher complexity of \( \mathcal{H}_1 = \{ x \mapsto u \cdot x \mid \|u\|_1 \leq 1 \} \) has the following upper bound,
\[
\hat{R}(\mathcal{H}_1) \leq \max_i \|x_i\|_\infty \sqrt{\frac{2\log(2d)}{n}}.
\]

The above lemma characterizes the Rademacher complexity of a linear predictor with \( \ell_1 \) norm bounded by 1. To handle the influence of nonlinear activation function, we need the following contraction lemma.

**Lemma 2** (Lemma 26.9 of [25]). Let \( \phi_i : \mathbb{R} \rightarrow \mathbb{R} \) be a \( \rho \)-Lipschitz function, i.e. for all \( \alpha, \beta \in \mathbb{R} \) we have \(|\phi_i(\alpha) - \phi_i(\beta)| \leq \rho|\alpha - \beta|\). For any \( a \in \mathbb{R}^n \), let \( \phi(a) = (\phi_1(a_1), \ldots, \phi_n(a_n)) \), then we have
\[
\hat{R}(\phi \circ \mathcal{H}) \leq \rho\hat{R}(\mathcal{H})
\]

We are now ready to characterize the Rademacher complexity of two-layer networks. Specifically, The path norm is used to control the complexity.
Lemma 3. Let \( F_Q = \{ f_m(x; \theta) \mid \| \theta \|_p \leq Q \} \) be the set of two-layer networks with path norm bounded by \( Q \), then we have
\[
\hat{R}(F_Q) \leq 2Q \sqrt{\frac{2 \log(2d)}{n}}
\]

Proof. To simplify the proof, we let \( c_k = 0 \), otherwise we can define \( b_k = (b_k^T, c_k)^T \) and \( \mathbf{x} = (x^T, 1)^T \).
\[
n \hat{R}(F_Q) = \mathbb{E}_\xi \left[ \sup_{\| \theta \|_p \leq Q} \sum_{i=1}^{n} \xi_i \sum_{k=1}^{m} a_k \| b_k \|_1 \sigma(b_k^T \mathbf{x}_i) \right]
\]
\[
\leq \mathbb{E}_\xi \left[ \sup_{\| \theta \|_p \leq Q, \| \mathbf{u}_k \|_1 = 1} \sum_{i=1}^{n} \xi_i \sum_{k=1}^{m} a_k \| b_k \|_1 \sigma(\mathbf{u}_k^T \mathbf{x}_i) \right]
\]
\[
= \mathbb{E}_\xi \left[ \sup_{\| \theta \|_p \leq Q, \| \mathbf{u}_k \|_1 = 1} \sum_{k=1}^{m} a_k \| b_k \|_1 \sum_{i=1}^{n} \xi_i \sigma(\mathbf{u}_k^T \mathbf{x}_i) \right]
\]
\[
\leq \mathbb{E}_\xi \left[ \sup_{\| \theta \|_p \leq Q} \sum_{k=1}^{m} a_k \| b_k \|_1 \sup_{\| \mathbf{u}_k \|_1} | \sum_{i=1}^{n} \xi_i \sigma(\mathbf{u}_k^T \mathbf{x}_i) | \right]
\]
\[
\leq Q \mathbb{E}_\xi \left[ \sup_{\| \mathbf{u}_k \|_1} | \sum_{i=1}^{n} \xi_i \sigma(\mathbf{u}_k^T \mathbf{x}_i) | \right]
\]

Due to the symmetry, we have that
\[
\mathbb{E}_\xi \left[ \sup_{\| \mathbf{u}_k \|_1 \leq 1} | \sum_{i=1}^{n} \xi_i \sigma(\mathbf{u}_k^T \mathbf{x}_i) | \right] \leq \mathbb{E}_\xi \left[ \sup_{\| \mathbf{u}_k \|_1 \leq 1} \sum_{i=1}^{n} \xi_i \sigma(\mathbf{u}_k^T \mathbf{x}_i) \right] + \mathbb{E}_\xi \left[ \sup_{\| \mathbf{u}_k \|_1 \leq 1} \sum_{i=1}^{n} -\xi_i \sigma(\mathbf{u}_k^T \mathbf{x}_i) \right]
\]
\[
= 2 \mathbb{E}_\xi \left[ \sup_{\| \mathbf{u}_k \|_1 \leq 1} \sum_{i=1}^{n} \xi_i \sigma(\mathbf{u}_k^T \mathbf{x}_i) \right]
\]

Since \( \sigma \) is Lipschitz continuous with Lipschitz constant 1, by applying Lemma 2 and Lemma 1, we obtain
\[
\hat{R}(F_Q) \leq 2Q \sqrt{\frac{2 \log(2d)}{n}}.
\]

Proposition 4. Assume the loss function \( \ell(\cdot, y) \) is \( \rho \)-Lipschitz continuous and bounded by \( B \), then with probability at least \( 1 - \delta \) we have,
\[
\sup_{\| \theta \|_p \leq Q} | L(\theta) - \hat{L}_n(\theta) | \leq 4\rho Q \sqrt{\frac{2 \log(2d)}{n}} + B \sqrt{\frac{2 \log(2/\delta)}{n}} \tag{8}
\]

Proof. Define \( \mathcal{H}_Q = \{ \ell \circ f \mid f \in F_Q \} \), then we have \( \hat{R}(\mathcal{H}_Q) \leq 2BQ \sqrt{\frac{2 \log(2d)}{n}} \), which follows from Lemma 2 and 3. Then directly applying Theorem 3 yields the result.

Theorem 5 (A posterior generalization bound). Assume the loss function \( \ell(\cdot, y) \) is \( \rho \)-Lipschitz continuous and bounded by \( B \). Then for any \( \delta > 0 \), with probability at least \( 1 - \delta \) over the choice of the training set \( S \), we have, for any two-layer network \( f(x; \theta) \),
\[
| L(\theta) - \hat{L}_n(\theta) \mid \leq 4\rho (\| \theta \|_p + 1) \sqrt{\frac{2 \log(2d)}{n}} + B \sqrt{\frac{2 \log(2c(1 + \| \theta \|_p)^2 / \delta)}{n}}, \tag{9}
\]
where \( c = \sum_{k=1}^{\infty} 1/k^2 \).

We can see that the generalization gap is roughly bounded by \( \| \theta \|_p \sqrt{n} \) up to some logarithmic terms.
Proof. Consider the decomposition $F = \bigcup_{l=1}^{\infty} F_l$, where $F_l = \{f_n(\mathbf{x}; \theta) \mid \|\theta\|_p \leq l\}$. Let $\delta_l = \frac{4}{c l^2}$ where $c = \sum_{l=1}^{\infty} \frac{1}{l^2}$. According to Theorem 4, if we fixed $l$ in advance, then with probability at least $1 - \delta_l$ over the choice of $S$,

$$
\sup_{\|\theta\|_p \leq 1} |L(\theta) - \hat{L}_n(\theta)| \leq 4\rho l \sqrt{\frac{2\log(2d)}{n}} + B \sqrt{\frac{2\log(2/\delta_l)}{n}}.
$$

So the probability that there exists at least one $l$ such that (2.2) fails is at most $\sum_{l=1}^{\infty} \delta_l = \delta$. In other words, with probability at least $1 - \delta$, the inequality (2.2) holds for all $l$.

Given an arbitrary set of parameters $\theta$, denote $l_0 = \min\{l \mid \|\theta\|_p \leq l\}$, then $l_0 \leq \|\theta\|_p + 1$. Equation (2.2) implies that

$$
|L(\theta) - \hat{L}_n(\theta)| \leq 4\rho l_0 \sqrt{\frac{2\log(2d)}{n}} + B \sqrt{\frac{2\log(2c(1 + \|\theta\|_p)^2/\delta)}{n}}.
$$

\[\square\]

3 A Priori Estimates

For simplicity we first consider the noiseless case, i.e. $\varepsilon_i = 0$. In the next section, we deal with the noise.

We see that the path norm of the special solution $\hat{\theta}$ which achieves the optimal approximation error is independent of the network size, and this norm can also be used to bound the generalization gap (Theorem 5). Therefore, if the path norm is suitably penalized during training, we should be able to control the generalization gap without harming the approximation accuracy. One possible implementation of this idea is through the structural empirical risk minimization [29, 25].

**Definition 4** (Path-norm regularized estimator). Define the regularized risk by

$$
J_\lambda(\theta) := \hat{L}_n(\theta) + \lambda \sqrt{\frac{2\log(2d)}{n}(1 + \|\theta\|_p)},
$$

where $\lambda$ is a positive constant. The **path-norm regularized estimator** is defined as

$$
\hat{\theta}_n = \arg\min J_\lambda(\theta).
$$

It is worth noting that the minimizer is not necessarily unique, and $\hat{\theta}_n$ should be understood as any of the minimizers. Without loss of generality, we also assume $2\log(2d) \geq 1$. In the following, we provide detailed analysis for the generalization error of the regularized estimator.

Since the path norm of the network associated with $\hat{\theta}$ is bounded, we have the following estimate of its regularized risk.

**Proposition 6.** Let $\hat{\theta}$ be the network constructed in Theorem 2. Then with probability at least $1 - \delta$, we have

$$
J_\lambda(\hat{\theta}) \leq L(\hat{\theta}) + \frac{1}{\sqrt{n}} \left(\hat{\gamma}(f^*) \left(4 + 5(\lambda + 4)\sqrt{2\log(2d)}\right) + \sqrt{2\log(2c/\delta)}\right).
$$

Proof. According to Definition 4 and the property that $\|\hat{\theta}\|_p \leq 4\gamma(f^*)$, the regularized cost of $\hat{\theta}$ satisfies

$$
J_\lambda(\hat{\theta}) = \hat{L}_n(\hat{\theta}) + \lambda \sqrt{\frac{2\log(2d)}{n}(\|\hat{\theta}\|_p + 1)} \\
\overset{(1)}{\leq} L(\hat{\theta}) + (4 + \lambda) \sqrt{\frac{2\log(2d)}{n}(|\hat{\theta}|_p + 1) + \sqrt{\frac{2\log(2c(1 + \|\hat{\theta}\|_p)^2/\delta)}{n}}} \\
\leq L(\hat{\theta}) + (4 + \lambda) \sqrt{\frac{2\log(2d)}{n}(4\gamma(f^*) + 1) + \sqrt{\frac{2\log(2c(1 + 4\gamma(f^*))^2/\delta)}{n}}},
$$

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where (1) follows from the generalization bound in Theorem 5 and the fact that \((f(x; \theta) - y_i)^2 \leq 4\). The last term can be simplified by using \(\sqrt{a + b} \leq \sqrt{a} + \sqrt{b}\) and \(\log(1 + a) = a\) for \(a \geq 0, b \geq 0\). So we have

\[
\sqrt{2\log(2c(1 + 4\gamma(f^*))^2/\delta)} \leq \sqrt{2\log(2c/\delta)} + \sqrt{4\log(1 + 4\gamma(f^*))} \\
\leq \sqrt{2\log(2c/\delta)} + 4\sqrt{\gamma(f^*)} \leq \sqrt{2\log(2c/\delta)} + 4\hat{\gamma}(f^*).
\]

By plugging it into Equation (13), and using \(\hat{\gamma}(f^*) \geq 1\), we obtain

\[
J_\lambda(\hat{\theta}) \leq L(\hat{\theta}) + \frac{1}{\sqrt{n}} \left(\hat{\gamma}(f^*) \left(4 + 5(\lambda + 4)\sqrt{2\log(2d)}\right) + \sqrt{2\log(2c/\delta)}\right).
\]

\[\square\]

**Proposition 7** (Properties of the regularized estimator). The path-norm regularized estimator \(\hat{\theta}_n\) satisfies:

\[
J_\lambda(\hat{\theta}_n) \leq J_\lambda(\hat{\theta}) \\
\frac{\|\hat{\theta}_n\|_p}{\sqrt{n}} \leq \lambda^{-1}L(\hat{\theta}) + n^{-1/2} \left(\hat{\gamma}(f^*)\left(5 + 24\lambda^{-1}\right) + \lambda^{-1}\sqrt{2\log(2c/\delta)}\right).
\]

**Proof.** The first claim follows from the definition of \(\hat{\theta}_n\). For the second claim, we have \(\lambda\sqrt{\frac{2\log(2d)}{n}}(\|\hat{\theta}_n\|_p + 1) \leq J_\lambda(\hat{\theta}_n) \leq J_\lambda(\hat{\theta})\), so \(\frac{\|\hat{\theta}_n\|_p}{\sqrt{n}} \leq \lambda^{-1}\sqrt{n}\frac{\frac{1}{2\log(2d)}}{J_\lambda(\hat{\theta})}\). By using Proposition 6 and \(2\log(2d) \geq 1\), we have

\[
\frac{\|\hat{\theta}_n\|_p}{\sqrt{n}} \leq \frac{\lambda^{-1}}{\sqrt{2\log(2d)}}L(\hat{\theta}) + \lambda^{-1}n^{-1/2} \left(\hat{\gamma}(f^*)\left(4\sqrt{\frac{2\log(2d)}{2\log(2d)}} + 5(\lambda + 4)\right) + \sqrt{2\log(2c/\delta)}\right)
\]

\[\leq \lambda^{-1}L(\hat{\theta}) + n^{-1/2} \left(\hat{\gamma}(f^*)\left(5 + 24\lambda^{-1}\right) + \lambda^{-1}\sqrt{2\log(2c/\delta)}\right).
\]

\[\square\]

**Remark 1.** The above proposition establishes the connection between the regularized solution and the special solution \(\hat{\theta}\) constructed in Theorem 2. In particular, the upper bound of the generalization gap of the regularized solution satisfies \(\frac{\|\hat{\theta}_n\|_p}{\sqrt{n}} \to \lambda^{-1}L(\hat{\theta})\) as \(n \to \infty\). This suggests that our regularization term is added appropriately, which forces the generalization gap to be roughly in the same order of approximation error.

**Theorem 8** (Main result, noiseless case). Under Assumption 1, there exists a pure constant \(C\) such that for any \(\delta > 0\) and \(\lambda \geq 4\), with probability at least \(1 - \delta\) over the choice of the training set \(S\), the generalization error of estimator (11) satisfies

\[
\mathbb{E}[f(x; \hat{\theta}_n) - f^*(x)]^2 \leq \frac{C\gamma^2(f^*)}{m} + \frac{C}{\sqrt{n}} \left(\sqrt{\log(2d)}\hat{\gamma}(f^*)\lambda + \frac{\hat{\gamma}(f^*)}{\sqrt{m\lambda}} \sqrt{\log(n/\delta)}\right) + \frac{\sqrt{C(\hat{\gamma}(f^*) + \log^{1/2}(1/\delta))}}{n}.
\]

**Remark 2.** It should be noted that both terms at the right hand side of the above result has a Monte Carlo nature (for numerical integration). From this viewpoint, the result is quite sharp.

**Proof.** We first have that

\[
L(\hat{\theta}_n) \overset{(1)}{\leq} \hat{L}_n(\hat{\theta}_n) + 4(\|\hat{\theta}_n\|_p + 1)\sqrt{\frac{2\log(2d)}{n}} + \sqrt{\frac{\log(2c(1 + \|\hat{\theta}_n\|_p)^2/\delta)}{n}} \\
\overset{(2)}{\leq} J_\lambda(\hat{\theta}_n) + \sqrt{\frac{\log(2c(1 + \|\hat{\theta}_n\|_p)^2/\delta)}{n}}
\]

\[8\]
Where (1) follows from the a posteriori generalization bound in Theorem 5, and (2) is due to $\lambda \geq 4$.

Furthermore,

$$\sqrt{\log(2c(1 + \|\hat{\theta}_n\|_p)^2/\delta)} \leq \sqrt{\log(2nc/\delta)} + \sqrt{2 \log(1 + n^{-1/2}\|\hat{\theta}_n\|_p)}$$

By Proposition 7 and the condition $\lambda \geq 4$, we have that

$$\|\hat{\theta}_n\|_p \leq \frac{\lambda - 1}{L(\hat{\theta}_n)} + 20 \frac{\sqrt{60(\hat{\gamma}(f^*) + \log(1/\delta))}}{n}.$$  

Thus we obtain that

$$\sqrt{\log(2c(1 + \|\hat{\theta}_n\|_p)^2/\delta)} \leq \sqrt{\log(2nc/\delta)} + \sqrt{2 \log(1 + n^{-1/2}\|\hat{\theta}_n\|_p)}.$$  

On the other hand, for $\lambda \geq 4$ we have

$$J_{\lambda}(\hat{\theta}_n) \leq J_{\lambda}(\hat{\theta}) \leq L(\hat{\theta}) + \frac{1}{\sqrt{n}} \left(11\lambda \hat{\gamma}(f^*) \sqrt{2 \log(2d)} + \sqrt{2 \log(2c/\delta)}\right)$$

By combining Equation (15) and (16), we obtain

$$L(\hat{\theta}_n) \leq L(\hat{\theta}) + \frac{C}{\sqrt{n}} \left(\sqrt{\log(2d)} \hat{\gamma}(f^*) L(\hat{\theta}) + \sqrt{\log(n/\delta)}\right) + \sqrt{60(\hat{\gamma}(f^*) + \log^{1/2}(1/\delta))} + \sqrt{60(\hat{\gamma}(f^*) + \log^{1/2}(1/\delta))} \frac{1}{n}.$$  

By applying $L(\hat{\theta}) \leq 16\gamma^2(f^*)/m$, we complete the proof.

**Remark 3.** From the proof, we can see that the requirement of $\lambda \geq 4$ is due to constant 4 appears in the upper bound of the generalization gap.

### 4 Tackling the Noise

This section is devoted to analyze the impact of noise. We first make the following assumption on the noise.

**Assumption 2.** We assume the noise has zero mean, and its probability distribution has an exponentially decaying tail, i.e.,

$$\mathbb{E}[\varepsilon] = 0, \quad \mathbb{P}(|\varepsilon| > t) \leq c_0 e^{-\frac{t^2}{\tau_0}} \quad \forall t \geq \tau_0.$$  

Here $c_0, \tau_0$ and $\sigma$ are constants.

In the presence of noise, the expected risk can be decomposed into

$$L(\theta) = \mathbb{E}_x[f(x; \theta) - f^*(x)]^2 + \mathbb{E}^2.$$  

This suggests that, in spite of the noise, we still have $\text{argmin}_\theta L(\theta) = \text{argmin}_\theta \mathbb{E}_x[f(x; \theta) - f^*(x)]^2$, and the latter is what we really want to minimize. However due to the noise, $\ell(f(x_i), y_i)$ could be unbounded. We cannot directly use the bound (9) to control the generalization gap. To address this issue, we consider the truncated risk defined as follows.

$$L_B(\theta) = \mathbb{E}_{x, y}[(f(x, \theta) - y)^2 \wedge B]^2, \quad \hat{L}_B(\theta) = \frac{1}{n} \sum_{i=1}^n (f(x_i; \theta) - y_i)^2 \wedge B^2.$$  

Correspondingly, we define the regularized estimator for noisy case as follows,
Definition 5. Let \( B_n = 1 + \max\{\tau_0, \sigma^2 \log n\} \), and define the regularized risk by

\[
J_\lambda(\theta) := \tilde{L}_{B_n}(\theta) + \lambda B_n \sqrt{\frac{2 \log(2d)}{n}} (1 + \|\theta\|_p).
\]

The corresponding regularized estimator is given by \( \hat{\theta}_n = \text{argmin} J_\lambda(\theta) \).

Lemma 4. Under Assumption 2, we have \( \sup_{\theta} |L(\theta) - L_{B_n}(\theta)| \leq \frac{2c_0 \sigma^2}{\sqrt{n}} \).

Proof. Let \( Z = f_n(x; \theta) - f^*(x) - \varepsilon \), then for any \( B \geq 2 + \tau_0 \), we have

\[
|L(\theta) - L_B(\theta)| = E \left[ (Z^2 - B^2)1_{|Z| \geq B} \right] \\
= \int_0^\infty P(Z^2 - B^2 \geq t^2) dt^2 \leq \int_0^\infty P(|Z| \geq \sqrt{B^2 + t^2}) dt^2 \\
\leq c_0 \int_0^\infty e^{-\frac{t^2}{2\sigma^2}} dt = 2c_0 \sigma^2 e^{-B^2/2\sigma^2}
\]

Since \( B_n \geq \sigma^2 \log n \), we have \( 2c_0 \sigma^2 e^{-\frac{n^2}{2\sigma^2}} \leq 2c_0 \sigma^2 n^{-1/2} \). We thus complete the proof.

Therefore, \( L(\theta) = L(\theta) - L_{B_n}(\theta) + L_{B_n}(\theta) \leq \frac{2c_0 \sigma^2}{\sqrt{n}} + L_{B_n}(\theta) \). This suggests that as long as we can bound the truncated expected risk, then the original risk will be bounded accordingly. This leads to the following result.

Theorem 9 (Main result, noisy case). Under Assumptions 1 and 2, there exists a pure constant \( C \) such that for any \( \delta > 0 \) and \( \lambda \geq 4 \), with probability at least \( 1 - \delta \) over the choice of the training set \( S \), the generalization error for the estimator \( (11) \) satisfies

\[
E[f(x; \hat{\theta}_n) - f^*(x)]^2 \leq \frac{16\gamma^2(f^*)}{m} + \frac{CB_n^2}{\sqrt{n}} \left( \sqrt{\log(2d)\gamma(f^*)} \lambda + \sqrt{\frac{m^{-1} \gamma^2(f^*) + E[\varepsilon^2]}{\lambda}} + \sqrt{\log(n/\delta)} \right) \\
+ \frac{4c_0 \sigma^2}{\sqrt{n}} + \frac{C(c_0 \sigma^2 + \hat{\gamma}(f^*) + \log^{1/2}(1/\delta))}{n}.
\]

Compared to the result (14) for noiseless case, the noise introduces at most a logarithmic term, and the result is consistent, as \( B_n = 1 \) when \( \tau_0 = 0, \sigma = 0 \). In the following, we give the proof, which is almost the same as the noiseless case.

Proof. By analogy with the proof of Proposition 6, we can obtain that with probability at least \( 1 - \delta \) the following inequality holds,

\[
J_\lambda(\hat{\theta}) \leq L_{B_n}(\hat{\theta}) + \frac{B_n^2}{\sqrt{n}} \left( \hat{\gamma}(f^*) \left( 3 + 5(\lambda + 4)\sqrt{\log(2d)} \right) + \sqrt{\log(2c/\delta)} \right).
\]

Following the proof in Proposition 7, similarly we can obtain \( J_\lambda(\hat{\theta}_n) \leq J_\lambda(\hat{\theta}) \) as well as

\[
\|\hat{\theta}_n\|_p \leq \lambda^{-1} L_{B_n}(\hat{\theta}) + n^{-1/2} \left( \hat{\gamma}(f^*)(5 + 24\lambda^{-1}) + \lambda^{-1} \sqrt{2\log(2c/\delta)} \right).
\]

Following the proof of Theorem 8, by combining (13) and (23) we have

\[
L_{B_n}(\hat{\theta}_n) \leq L_{B_n}(\hat{\theta}) + \frac{CB_n^2}{\sqrt{n}} \left( \sqrt{\log(2d)\gamma(f^*)} \lambda + \sqrt{\frac{L_{B_n}(\hat{\theta})}{\lambda}} + \sqrt{\log(n/\delta)} \right) \\
+ \frac{C(\hat{\gamma}(f^*) + \log^{1/2}(1/\delta))}{n}.
\]

By plugging Lemma 4 and the decomposition (19), we can obtain the result.
5 Numerical Experiments

We evaluate the properties of the regularized estimator on both MNIST\(^1\) [17] and CIFAR-10\(^2\) [15] datasets. Each example in MNIST is a 28 \times 28 grayscale image, while each example in CIFAR-10 is a 32 \times 32 \times 3 color image. To be consistent with our setup (regression of a scalar function) in the theoretical analysis, we use mean squared error rather than cross entropy as the surrogate loss function to handle the binary classification problem. For MNIST, we map numbers \{0, 1, 2, 3, 4\} to label 0 and \{5, 6, 7, 8, 9\} to 1. For CIFAR-10, we select the examples with labels 0 and 1 to construct our new training and validation sets. Thus, our new MNIST has 60,000 training examples, and CIFAR-10 has 10,000 training examples.

Following the standard initialization strategy [12], the two-layer ReLU network is initialized using \(a_i \sim \mathcal{N}(0, \frac{2\kappa}{m})\), \(b_{i,j} \sim \mathcal{N}(0, 2\kappa/d)\), \(c_i = 0\). We use \(\kappa = 1\) and train the models using the Adam optimizer [13] for \(T = 10,000\) steps, unless it is specified otherwise. The initial learning rate is set to be 0.001, and it is then multiplied by a decay factor of 0.1 at \(0.7T\) and again at \(0.9T\). We set the trade-off parameter \(\lambda = 0.1\) for the regularized models. Although the theoretical results suggest \(\lambda \geq 4\), we find in practice usually a smaller \(\lambda\) can achieve better test performance.

5.1 The Non-vacuous Upper Bound of the Generalization Gap

Theorem 5 shows that the generalization gap can be bounded by \(\|\theta\|_p \sqrt{\frac{p}{n}}\) up to some logarithmic terms. To see how this works in practice, we trained both the regularized models with \(\lambda = 0.1\) and un-regularized models (\(\lambda = 0\)) for fixed network width \(m = 10,000\). To cover the over-parameterization regime, we also consider \(n = 100\) where \(m/n = 100 \gg 1\). The results are summarized in Table 2.

Table 2: Comparison of regularized (\(\lambda = 0.1\)) and un-regularized (\(\lambda = 0\)) models. The experiments are repeated for 5 times, and the mean values are reported.

| dataset  | \(\lambda\) | \(n\)  | training accuracy | test accuracy | \(\|\theta\|_p \sqrt{\frac{p}{n}}\) |
|----------|-------------|--------|-------------------|---------------|----------------------------------|
| CIFAR-10 | 0           | \(10^4\) | 100\%             | 84.5\%        | 58                               |
|          |             | 100    | 100\%             | 70.5\%        | 507                              |
|          | 0.1         | \(10^4\) | 87.4\%            | 86.9\%        | 0.14                             |
|          |             | 100    | 91.0\%            | 72.0\%        | 0.43                             |
| MNIST    | 0           | \(6 \times 10^4\) | 100\%       | 98.8\%        | 58                               |
|          |             | 100    | 100\%             | 78.7\%        | 162                              |
|          | 0.1         | \(6 \times 10^4\) | 98.1\%       | 97.8%          | 0.27                             |
|          |             | 100    | 100\%             | 74.9%          | 0.41                             |

Figure 1: Comparison of the path norms between the regularized and un-regularized solutions for varying widths.

As we can see, the test accuracies of both the regularized and un-regularized solutions are generally comparable, but the upper bounds of generalization gap \(\|\theta\|_p \sqrt{\frac{p}{n}}\) are drastically different. Specifically, for

\(^1\)http://yann.lecun.com/exdb/mnist/
\(^2\)https://www.cs.toronto.edu/~kriz/cifar.html
the un-regularized models, the bounds are always vacuous, since they are several orders of magnitude larger than the naive upper bound 1. This is consistent with the observations in [1] and [23]. However, for regularized models, the bounds are non-vacuous, although they are not sharp. These numerical observations are consistent with our theoretical prediction in Proposition 7.

To further explore the impact of over-parameterization, we trained various models with different widths. For both datasets, all the training examples are used. In Figure 1, we display how the upper bound \( \|\theta\|_P \sqrt{n} \) of the learned solution varies with the network width. We find that this quantity for the regularized model is almost constant, whereas for the un-regularized model it increases with network width.

### 5.2 Dependence on the Initialization

Since the neural network model is non-convex, it is interesting to see how initialization affects the performance of the solutions, especially in the over-parametrized regime. To this end, we fix \( m = 10000, n = 100 \) and vary the variance of random initialization \( \kappa \). The results are reported in Figure 2. In general, we find that regularized models are much more stable than the un-regularized models. For large initialization, the regularized model always performs significantly better.

![Figure 2: Test accuracies of solutions obtained from different initializations. Each experiment is repeated for 5 times, and we report the mean and standard deviation.](image)

### 6 Concluding Remarks

The most unsatisfactory aspect of our result is that it is proved for the regularized model. In practice it is uncommon to add explicit regularizations. Instead, practitioners rely on the so-called “implicit regularization” [30, 20]. At the moment it is unclear where the “implicit regularization” comes from and how it actually works. But there are overwhelming evidence that by tuning extensively the details of the optimization procedure, including the algorithm, the initialization, the hyper-parameters, etc., one can find solutions with superior performance on the test data. The disadvantage is that excessive tuning and serious experience is required to find good solutions. Until we have a good understanding about the mysteries surrounding implicit regularization, the business of parameter tuning will remain an art. In contrast, the regularized model is rather robust and much more fool-proof. Borrowing the terminology from mathematical physics, one is tempted to say that the regularized model is “well-posed” whereas the un-regularized model is “ill-posed” [28].

There are two clear paths moving forward. One is to study other regularized models. In fact to avoid the slight loss of test accuracy shown for the MNIST dataset in Figure 1, one can consider regularizations that vanish for small values of the path norm. Our main results should hold for this kind of regularizations. The other is to study the so-called “implicit regularization”. Recently, assuming that the data is well-separated, [7, 18] proved that for two-layer networks, the number of iterations required for SGD to achieve certain accuracy for the classification problem is independent of the network size. Implicit regularization has also been studied in other problems, such as logistic...
regression [27] and matrix factorization [19, 11]. However, we still lack a general understanding of the mechanism behind implicit regularization.

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