An analysis of training and generalization errors in shallow and deep networks

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Abstract

An open problem around deep networks is the apparent absence of over-fitting despite large over-parametrization which allows perfect fitting of the training data. In this paper, we analyze this phenomenon in the case of regression problems when each unit evaluates a trigonometric polynomial. It is well understood that a trigonometric monomial can be synthesized with a good degree of approximation by neural networks with fixed weights and thresholds. Approximation by trigonometric polynomials serves as a “role model” for every other approximation process, including that by neural and RBF networks. In this paper, we argue that the maximum loss functional is necessary to measure the generalization error. We give estimates on exactly how many parameters ensure both zero training error as well as a good generalization error. We prove that a solution of a regularization problem is guaranteed to yield a good training error as well as a good generalization error and estimate how much error to expect at which test data.

Keywords: Deep learning, generalization error, interpolatory approximation

1 Introduction

The main problem of machine learning is the following. Given data \((x, y)\) sampled from an unknown probability distribution \(\mu\), the goal is find a function \(P\) that minimizes the generalization error \(E_\mu((y - P)^2)\) among all functions in some function class that is thought to represent the prior information about the distribution. Since we do not know \(\mu\), classical machine learning paradigm expresses the generalization error as a sum of three components: the variance, the approximation error, and the sampling error. The variance is a lower bound on the generalization error, and the estimation typically focuses on the other two errors. The sum of these two is given by \(E((f - P)^2)\), where the expectation is with respect to the marginal distribution of \(x\) and the target function \(f\) is the conditional expectation of \(y\) given \(x\). If the marginal distribution of \(x\) is known, then the split between approximation and sampling errors is no longer necessary, and one can obtain estimates as well as constructions directly from characteristics of the training data (e.g., [7, 13, 17]). In the classical paradigm where this distribution is not known, the approximation error decreases as the number of parameters in \(P\) increases to \(\infty\). However, this makes the empirical risk minimization problem harder to solve; making it essential to choose the number of parameters in \(P\) to balance the two errors. In turn, this explains a commonly observed phenomenon that if one achieves a zero empirical risk on the training data by over-parametrized model \(P\), the test error is generally not good.

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There are several recent papers that demonstrate that this phenomenon is often not observed (e.g., [10, 21, 24, 27, 22]). One of the vexing problems around deep learning is to explain the generalization error; why do the deep learning models, despite being highly over-parameterized, still predict well? There are a few recent papers that address this issue in the case of classification problems, Belkin, Hsu, and Mitra [1] analyze the “excess error” in least square fits by piecewise linear interpolants over that obtained by the optimal Bayes’ classifier. In [22, 23], the question is analyzed from the perspective of the geometry of the error surface with respect to different loss functions near the local extrema. In particular, it is shown in [22] that substituting the ReLU activation function by a polynomial approximation exhibits the same behavior as the original network.

In this paper, we focus on regression problems. We wish to consider the overfitting puzzle for universal approximation in a more intrinsic and theoretical manner, independent of the training mechanism used. For example, it is obvious that a network (or any other model) that uses less number of parameters than the amount of training data cannot in general produce a zero training error in the absence of some strong prior knowledge about the target function that generated the training data, no matter what training algorithm is used. We wish to address the following issues about the phenomenon of zero/small training error and small test error for universal approximation:

1. What characteristics of the data govern a zero training error and a good generalization error?

2. How much over-parametrization will give a mathematical guarantee of the model to exhibit this behavior?

3. Propose a regularization scheme whose solution will guarantee a good (but not necessarily zero) training error while maintaining a good generalization error at the same time.

4. How much generalization error can be guaranteed by the solution of the (global) regularization scheme at each point in the test data (rather than a global error estimate), compared to the nearest neighbor in the training data?

We do not propose any algorithm to find a solution of the regularization problem. The objective is to study the nature of the problem itself intrinsically and with mathematical guarantees.

In recent years, convolutional neural networks (CNNs) have achieved a revolution in machine learning. A good survey can be found in [11]. From a practical point of view, the central features of CNNs are locality and weight sharing. From a strictly mathematical point of view, convolution is a very special operation that requires a group structure on the data. According to the book [8], the CNNs “are a specialized kind of neural network for processing data that has a known, grid-like topology. Examples include time-series data, which can be thought of as a 1D grid taking samples at regular time intervals, and image data, which can be thought of as a 2D grid of pixels.” For this kind of data, it is customary to treat it either as a data on the whole real line/plane with zero-padding, or otherwise use a symmetrical extension to treat it as a data on a circle/torus so that the standard group operations on these spaces can be used to define the operation of convolution.

In this paper, we will focus on function approximation on the torus. The most fundamental class for this purpose is the class of all trigonometric polynomials. Accordingly, we will study the problem of the lack of overfitting in the context of approximation by trigonometric polynomials. We will explain in Section 2.2 the theoretical relationship between trigonometric polynomials and neural/RBF networks in the periodic setting.

In the study of approximation error in deep learning, it is observed in [19] that the compositional structure of the target function can be utilized effectively via a property called good propagation of error to obtain substantially better error bounds allowing us to overcome the curse of dimensionality observed in shallow networks. This allows us to “lift” many results on approximation by shallow networks to those on deep networks. However, there are a few barriers that prevent a straightforward extension.
One is that we do not know the functions evaluated at each node in the intervening layers; just the input/output relations between the data and output of the ultimate layers. There are some recent efforts in the direction of designing deep networks in some special applications using domain knowledge (e.g., [9, 18]). It is conceivable that this problem does not appear in these contexts.

The other problem is even more fundamental, requiring a change in the traditional notion of generalization error. For example, suppose we wish to approximate a function \( f^* = f(f_1(x_1), f_2(x_2)) \) by a network of the form \( P^* = P(P_1(x_1), P_2(x_2)) \), where \( x_1, x_2 \in \mathbb{R}^d \). Without the compositional structure, \( f^* \) has to be treated as a function of \( 2d \) variables. The compositional structure allows us to treat the approximation problem as a set of three approximation problems: approximating functions \( f_1, f_2 \) as functions of \( d \) variables each, and a function \( f \) of 2 variables.

How do we define generalization error? Defining it in terms of the original distribution of \( ((x_1, x_2), y) \) is not sensitive to the compositional structure. On the other hand, the input \( (f_1, f_2) \) to the function \( f \) is not the same (even may not have the same distribution) as the input \( (P_1, P_2) \) to the approximation \( P \).

Therefore, we measure in this paper the errors in the uniform norm rather than searching for appropriate \( L^2 \) norms suitable for the compositionality structure of the target function. Thus, we define the generalization error as the maximal error between the target function and the model at all possible test points. One consequence is that the decomposition of the generalization error into three parts breaks down. Therefore, new ideas are required to achieve the approximation in terms of the training data alone. The approximation errors themselves are studied in [19, 14, 15], but the techniques suggested there require the data points \( x_j \) to be sufficiently dense in the domain (Euclidean space, sphere, cube, etc.). When the data is not dense, it is clearly not expected to get a good approximation on the whole domain. However, if the data does become dense on some subset of the domain, one can expect a good approximation at points close by to the training data. Thus, we will establish pointwise bounds for the generalization error obtained by a solution of the suggested regularization scheme.

In Section 2, we develop some notation and provide some background information that has motivated our current paper. In Section 3, we state our theorems for the case of shallow networks (where each neuron calculates a trigonometric monomial). In Section 4, we state and prove the analogues of the results in Section 3 in the case of deep networks. The proofs of the results in Sections 3 and 4 are given in Section 5.

2 Background

The purpose of this section is to explain the connection between trigonometric polynomials and neural networks (Section 2.2) as well as explain a classical theorem which provides a motivation for our theorems in this paper (Section 2.3). In order to do so, we need first to develop some notation. This is done in Section 2.1.

2.1 Notation

Let \( q \geq 1 \) be an integer, \( \mathbb{T}^q \) be the \( q \) dimensional torus \( (\mathbb{R}^q/(2\pi\mathbb{Z})^q) \). For \( x, y \in \mathbb{T}^q \),

\[
|x - y| = \max_{1 \leq i \leq q} |x_i - y_i|(\text{mod } 2\pi).
\]

For multi-integer \( k \), \( |k|_p \) is \( \ell^p \) norm of \( k \).

The space of all continuous functions \( f : \mathbb{T}^q \to \mathbb{R} \), equipped with the supremum norm will be denoted by \( C^* \) (or \( C^*(\mathbb{T}^q) \) if we wish to emphasize the input dimension to the functions). The norm on \( C^*(\mathbb{T}^q) \) will be denoted by \( \| \cdot \| \) or \( \| \cdot \|_q \) if it is important to identify the dimension. For \( n > 0 \), the space \( \mathbb{H}^n_q \) of trigonometric polynomials in \( q \) variables with (spherical) degree \( < n \) is defined by

\[
\mathbb{H}^n_q = \text{span}\{\exp(ik \cdot \circ) : |k|_2 < n\}.
\]
The dimension of \( \mathbb{H}_n^q \) is \( \sim n^q \). If \( f \in C^\infty(\mathbb{T}^q) \), then its Fourier coefficients are defined by
\[
\hat{f}(k) = \frac{1}{(2\pi)^q} \int_{\mathbb{T}^q} f(x) \exp(-ik \cdot x) dx, \quad k \in \mathbb{Z}^q,
\]
and its degree of approximation from \( \mathbb{H}_n^q \) is defined by
\[
E_n(f) = E_n(q; f) := \inf_{T \in \mathbb{H}_n^q} \| f - T \|.
\]

When our models are trigonometric polynomials in \( \mathbb{H}_n^q \), the quantity \( E_n(f) \) denotes the ideal generalization error for the target function \( f \).

For any finite subset \( \mathcal{C} \subset \mathbb{T}^q \), we define its minimal separation by
\[
\eta(\mathcal{C}) = \min_{x, y \in \mathcal{C}, x \neq y} |x - y|.
\]

We assume a training data of the form \( D = \{(x_j, y_j)\}_{j=1}^M \), where \( \mathcal{C} = \{x_j\}_{j=1}^M \subset \mathbb{T}^q \), and \( y_j = f(x_j) + \epsilon_j \) for some \( f \in C^\infty \). We denote
\[
\epsilon = \max_{1 \leq j \leq M} |\epsilon_j|.
\]

The quantity \( \epsilon \) plays the role of variance in our theory in this paper.

**The constant convention**

The symbols \( c, c_1, \ldots \) will denote generic positive constants, depending on such fixed parameters of the problem as \( q, h, G, \) and \( S \) (to be introduced later), etc. and other quantities explicitly indicated, but their value may differ at different occurrences, even within a single formula. The notation \( A \sim B \) means that \( c_1 A \leq B \leq c_2 A \).

### 2.2 Neural networks and trigonometric polynomials

Let \( \phi \in C^\infty(\mathbb{T}) \) and \( \phi(1) \neq 0 \). Then for \( k \in \mathbb{Z}^q \) and \( x \in \mathbb{T}^q \), it is not difficult to verify that
\[
\exp(i k \cdot x) = \frac{1}{2\pi \phi(1)} \int_{\mathbb{T}} \phi(t) \exp(i(k \cdot x - t)) dt = \frac{1}{2\pi \phi(1)} \int_{\mathbb{T}} \phi(k \cdot x - t) \exp(it) dt.
\]

Discretizing the integral expression above, it can be shown (cf. [12 Proposition 4.2.1]) that for any integer \( N \geq 1 \),
\[
\left\| \exp(i k \cdot (\cdot)) - \frac{1}{(2N + 1) \phi(1)} \sum_{j=0}^{2N} \exp \left( \frac{2\pi i j}{2N + 1} \right) \phi \left( k \cdot (\cdot) - \frac{2\pi j}{2N + 1} \right) \right\| \leq \frac{4}{|\phi(1)|} E_N(1; \phi).
\]

In particular, if \( T \) is a trigonometric polynomial of coordinatewise degree \( < n \),
\[
\left\| T - \frac{1}{(2N + 1) \phi(1)} \sum_{j=0}^{2N} \exp \left( \frac{2\pi i j}{2N + 1} \right) \sum_{|k| \leq n} \hat{T}(k) \phi \left( k \cdot (\cdot) - \frac{2\pi j}{2N + 1} \right) \right\| \leq \frac{4}{|\phi(1)|} E_N(1; \phi) \sum_{|k| \leq n} |\hat{T}(k)|.
\]

For example, if \( \phi(t) \) is a periodization of the smooth ReLU function \( te^t/(1 + e^t) \), then \( E_N(1; \phi) \) decreases to zero exponentially fast in terms of \( N \). Thus, a trigonometric polynomial can be approximated by a neural network with activation function \( \phi \) and the error bounds can be obtained by keeping track of the
degree of approximation of the target function by trigonometric polynomials, the magnitude of its Fourier coefficients and the bound in (2.5) (cf. [15] for some examples).

We note that the weights and thresholds of this neural network are independent of the target function. Therefore, an estimate on the degree of approximation by trigonometric polynomials yields at once an estimate on the degree of approximation by neural networks with an appropriate number of neurons. This idea is generalized to many other settings, and algorithms are known to find the approximation to the target function using the training data, without assuming any prior on the target function (see, e.g. [12] for an early construction). However, formulating the problem directly as a minimization of the supremum norm error between the function and the neural network model may not work. The theory implies certain relationships between the coefficients and the weights and thresholds.

Conversely, one can approximate $\phi$ by trigonometric polynomials. Therefore, if one can obtain or assume some bounds on the coefficients of a neural network with $\phi$ as the activation function, then these bounds can be translated to bounds on the degree of approximation by trigonometric polynomials. This part is hard to do on the torus with neural networks, but has been done in a far more general setting with kernel based approximation [13].

2.3 Interpolatory approximation

In the language of classical approximation theory, the problem of achieving a zero training error is the problem of interpolation. In the context of trigonometric polynomials, since an element of $H^1_n$ has $2n + 1$ free parameters, for any data of the form $\{(\theta_j, y_j)\}_{j=0}^{2n}, y_j \in \mathbb{R}, \theta_j \in \mathbb{T}$, and $\theta_j \neq \theta_k$ if $j \neq k$, there exists $T \in H^1_n$ such that $T(\theta_j) = y_j$ for $j = 0, \ldots, 2n$. Thus, it is easy to obtain a zero training error with a minimal number of free parameters. As we argued in the introduction, the test error in this context should be measured in terms of uniform approximation to the target function. A well known theorem attributed in [20] to Faber and Bernstein states that no sequence of interpolatory trigonometric polynomials (with minimal degree as above) can converge uniformly to every function in $C^*(\mathbb{T})$.

In 1943, Erdös [6] initiated (in the context of algebraic polynomials) a study of the question whether one can get a convergent sequence of interpolatory polynomials if one allows a polynomial of higher than minimal degree. A positive answer was given by Szabados in [25]. Although the answer is given in terms of algebraic polynomials, Szabados remarks that the same is clearly true for trigonometric polynomials as well. An explicit statement to this effect is the following [16, Theorem 3.1(a)].

**Theorem 2.1** Let $\theta_1, \ldots, \theta_N$ be distinct points in $[-\pi, \pi], \theta_{N+1} := \theta_1 + 2\pi, \alpha > 0$, and

$$\min_{1 \leq k \leq N} |\theta_{k+1} - \theta_k| =: \eta.$$  

Then for $f \in C^*(\mathbb{T})$, there exists a trigonometric polynomial $T$ of degree at most $(1 + 2/\alpha)(\pi/\eta)$ such that $f(\theta_j) = T(\theta_j), 1 \leq j \leq N$, and

$$\|f - T\| \leq (2 + \alpha)E_m(1; f)$$

where $m = (1 + 2/\alpha)(\pi/\eta)$.

3 Shallow networks

Our first theorem in this section shows the connection between the structural properties of the training data and the existence of a trigonometric polynomial $T^0_N(D)$ that can interpolate the noisy data (i.e., achieve a zero training error), as well as achieve a good generalization error in the sense defined in Section 1. The following theorem is a generalization of Theorem 2.1. Our proof is much simpler than that of Theorem 2.1 in either [16] or [25].
Theorem 3.1 Let $f \in C^*$. There exists $B > 0$ with the following property: for $N \geq B\eta(C)^{-1}$, there exists $T^\#_N(D) \in \mathbb{H}_N^q$ such that
\[
T^\#_N(D)(x_j) = y_j, \quad j = 1, \cdots, M, \quad \text{(Zero training error)} \tag{3.1}
\]
and
\[
\|f - T^\#_N(D)\| \leq c \left\{ \epsilon + E_{N/2}(f) \right\}. \quad \text{(Good generalization error).} \tag{3.2}
\]

Remark 3.1 A volume comparison argument shows that the number of data points $M$ satisfies $M \leq c\eta(C)q^{-q}$. Thus, Theorem 3.1 shows that for a right configuration of the training data, a good generalization error as well as zero training error can be achieved by choosing the number of parameters proportional to the number of data points. It is demonstrated in [2] that for RBF approximation, this phenomenon seems to hold in many applications with the number of parameters exactly equal to the number of data points.

Remark 3.2 In practice, the training data is high dimensional and sparse; i.e., $\eta(C)$ is large. The requirement that $N \geq B\eta(C)^{-1}$ is therefore satisfied with moderate degrees $N$.

Remark 3.3 A curious feature of Theorem 3.1 is that one obtains the bound (3.2) on the generalization on the entire torus $T^q$ without requiring that the training data $C$ be “dense” in $T^q$. Of course, Theorem 3.1 is not constructive. The proof of this theorem shows that the polynomial $T^\#_N$ actually utilizes also the Fourier coefficients of the target function in addition to the information contained in $D$.

Clearly, one cannot construct $T^\#_N(D)$ based only on the training data $C$, unless $C$ is sufficiently dense on $T^q$. If we anticipate a scenario where the training data sets become denser and denser on some compact subset $K \subset T^q$, then we cannot expect convergence of trigonometric polynomials that interpolate a noisy data, where the noise level does not decrease as well. The following discussion suggests a construction that keeps both training and generalization errors under control.

A straightforward approach is to consider the localized kernel $\Phi_N$ defined in (5.1), and solve the system of linear equations for $a_k$'s:
\[
\frac{1}{\Phi_N(0)} \sum_{k=1}^M a_k \Phi_N(x_j - x_k) = y_j, \quad j = 1, \cdots, M. \tag{3.3}
\]

The matrix involved is well-conditioned if $N \geq c\eta(C)^{-1}$. It is not difficult to show estimates analogous to those given in Theorem 3.2 below for approximation by the resulting polynomial, but they are not as good (cf. Remark 5.1). Also, an even simpler approach of just considering
\[
\frac{1}{\Phi_N(0)} \sum_{k=1}^M y_k \Phi_N(\circ - x_k)
\]
yields similar bounds on the generalization error as those obtained by solving (3.3).

Another approach, described in [3], is to minimize a high order Sobolev norm of the trigonometric polynomial subject to the interpolatory conditions. This approach has been used to great advantage for a numerical solution of some notoriously hard partial differential equations in 2 or 3 dimensions. However, the calculations are very ill-conditioned and require very carefully designed algorithms.

We describe a softer regularization scheme that does not require high order Sobolev norms, and yields both good training and generalization errors.

The space $W^* = W^*(T^q)$ consists of all continuously differentiable functions $f \in C^*$. We define
\[
\|f\|_{W^*} = \|f\|_{W^*(T^q)} = \sum_{j=1}^q \|D_j f\|.
\tag{3.4}
\]
For $n > 0$ and $T \in \mathbb{H}^n$, let

$$R_n(T) = \max_{1 \leq j \leq M} |y_j - T(x_j)| + \frac{1}{n} \|T\|_{\mathcal{W}}^n. \quad (3.5)$$

**Theorem 3.2** Let $f \in W^*$, $B$ be as in Theorem 3.1 and $N \geq Bn^{-1}$. Then

$$\min_{T \in \mathbb{H}_N^n} R_N(T) \leq c \left\{ \epsilon + \frac{1}{N} \|f\|_{\mathcal{W}}^* \right\}. \quad (Good \ training \ error) \quad (3.6)$$

Let $T^*(D) = \arg \min_{T \in \mathbb{H}_N^n} R_N(T)$, $x \in \mathbb{R}^n$, and $\delta = \min_{1 \leq j \leq M} |x - x_j|$. Then

$$|f(x) - T^*(D)(x)| \leq c(1 + N\delta) \left\{ \epsilon + \frac{1}{N} \|f\|_{\mathcal{W}}^* \right\}. \quad (Good \ generalization \ error). \quad (3.7)$$

**Remark 3.4** The estimate (3.7) shows that if $x$ is very close to the training data so that $N\delta < 1$, then the generalization error at $x$ is of the same order of magnitude as the loss in the training data measured by $R_N(T^*)$. As remarked earlier in Remark 3.2, we have greater liberty in choosing a large $N$ when the data is sparse. To take advantage of this fact, let $x$ be such that $N\delta \geq 1$. Then (3.7) can be reformulated in the form

$$|f(x) - T^*(D)(x)| \leq c\delta \left\{ N\epsilon + \|f\|_{\mathcal{W}}^* \right\}. \quad (3.8)$$

The term $\delta \|f\|_{\mathcal{W}}^*$ is clearly a customary bound from numerical analysis in view of the mean value theorem. If $\epsilon \leq \eta(C)\|f\|_{\mathcal{W}}^*$, it is possible to choose $N$ so that error bound is $c\delta \|f\|_{\mathcal{W}}^*$.

**Remark 3.5** It is well known (cf. [28, Chapter X, Theorem 7.28] for the univariate case) that for any $T \in \mathbb{H}_N^n$,

$$\|T\| \sim \max_{|k|_\infty \leq 3N^{-1}} \left| T \left( \frac{2\pi k}{3N} \right) \right|. \quad (3.9)$$

Therefore, the term $\|T\|_{\mathcal{W}}^*$ in regularization functional $R_n(T)$ can be calculated in terms of the Fourier coefficients of $T$ via matrix vector multiplications involving the discrete evaluations of $D_jT$ as in (3.9). The results are not affected except for the actual values of the constants involved.

**Remark 3.6** As explained in Section 2.2, any trigonometric polynomial can be re-cast approximately as a neural network. Therefore, the polynomial constructed in Theorem 3.2 can be converted to a neural network with a small extra error as given in (2.5). It is therefore tempting to set up the regularization functional (3.5) directly with neural networks with free coefficients, weights, and thresholds to be determined by a suitable optimization technique. However, the estimate (2.5) implies a strong connection between these parameters for the network approximating a trigonometric polynomial. Therefore, the solution to such a direct approach with neural networks is not guaranteed to give the right training and testing errors.

### 4 Deep networks

The following discussion about the terminology about the deep networks, including Figure 1, is based on the discussion in [19], and elaborates upon the same.

Let $G$ be a directed acyclic graph (DAG), with the set of nodes $V$. A $G$-function is defined as follows. The in-edges to each node of $G$ represents an input real variable. For each node $v$, we denote its in-degree by $d(v)$. The node $v$ itself represents the evaluation of a real valued function $f_v$ of the $d(v)$ inputs. The out-edges fan out the result of this evaluation. Each of the source node obtains an input from some
Euclidean space. Other nodes can also obtain such an input, but by introducing dummy nodes, it is convenient to assume that only the source nodes obtain an input from the Euclidean space. The set of all source nodes of $G$ will be denoted by $S$ (or $S(G)$ if necessary).

We note that if $q$ is the number of source nodes in $G$, a $G$–function is a function on $\mathbb{R}^q$. Viewed only as a function on $\mathbb{R}^q$, it is not clear whether two different DAG structures can give rise to the same function. Even if we assume a certain DAG, it is not clear that the choice of the constituent functions is uniquely determined for a given function on $\mathbb{R}^q$. For example, one can write
\[
\cos^4 x = ((\cos x)^2)^2 = (\cos^2 x)^2 = (1/4)(1 + \cos(2x))^2.
\]
The second expression above has the structure $h_{19}(h_{18}(h_{17}(x)))$, and the other two have the structures $g_1(g_2(x))$ or $f_1(f_2(x))$, both representing the same DAG but with different constituent functions. Thus, the question of whether a given multivariate function is in fact compositional cannot be answered.

For our mathematical analysis, we therefore find it convenient to think of a $G$–function as a set of functions $f = \{f_v : \mathbb{R}^{d(v)} \to \mathbb{R}\}_{v \in V}$, rather than a single function on $\mathbb{R}^q$. The individual functions $f_v$ will be called constituent functions.

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{An example of a $G$–function ($f^*$ given in (4.1)). The vertices of the DAG $G$ are denoted by red dots. The black dots represent the input to the various nodes as indicated by the in–edges of the red nodes, and the blue dot indicates the output value of the $G$–function, $f^*$ in this example.}
\end{figure}

For example, the DAG $G$ in Figure 1 represents the compositional function
\[
f^*(x_1, \cdots, x_9) = h_{19}(h_{17}(h_{13}(h_{10}(x_1, x_2, x_3, h_{16}(h_{12}(x_6, x_7, x_8, x_9)))))), h_{11}(x_4, x_5)),
\]
\[h_{14}(h_{10}, h_{11}), h_{16}), h_{18}(h_{15}(h_{11}, h_{12}), h_{16})).
\]
(4.1)
The $G$–function is $\{h_{10}, \cdots, h_{19} = f^*\}$.

We assume that there is only one sink node, $v^*$ (or $v^*(G)$) whose output is denoted by $f^*$. Technically, there are two functions involved here: one is the final output as a function of all the inputs to all source
variables, namely the outputs of \( h \) from the context. A similar convention is followed with respect to each of the constituent functions as well. For example, in the DAG of Figure 1, the function \( h_{14} \) can be thought of both as a function of two variables, namely the outputs of \( h_{10} \) and \( h_{11} \) as well as a function of five variables \( x_1, \ldots, x_5 \).

In this paper, we are interested only in the case where each of the inputs to each of the source node is in \( \mathbb{T} \) rather than \( \mathbb{R} \). Although this is no longer true for the non-source nodes, it is possible to accomplish this in the case when each of the constituent functions is continuous, as follows. Let \( f_v \) be one of the constituent functions. With a re-normalization, we may assume that the range of \( f_v \) is a subset of \([−1,1]\). Then the function \( f_v^*(x) = \arccos(f_v(x)) \), extended to \( \mathbb{T} \) as an even function, is a function whose range is a subset of \( \mathbb{T} \). Rather than complicating our notations, we will therefore assume in this paper that the domain of each constituent function is a torus, and the range is a subset of \( \mathbb{T} \). In particular, we may assume that every constituent function \( f_v \in C^* (\mathbb{T}^d(v)) \).

We adopt the convention that for any function class \( X(\mathbb{T}^d) \), the class \( G-X \) denotes the set of \( G \) functions \( f = \{f_v\}_{v \in V} \), where each constituent function \( f_v \in X(\mathbb{T}^d(v)) \). We define

\[
\|f\|_{X,G} = \sum_{v \in V} \|f_v\|_{X(\mathbb{T}^d(v))}.
\]

Thus, for example, \( G-W^* \) is the set of all \( G \) functions \( f = \{f_v\}_{v \in V} \), where each constituent function \( f_v \in X(\mathbb{T}^d(v)) \), and we write

\[
\|f\|_{W^*,G} = \sum_{v \in V} \|f_v\|_{W^*(\mathbb{T}^d(v))}.
\]

The symbol \( G-H_N \) denotes the set of \( G \) functions \( \{T_v\}_{v \in V} \), where each \( T_v \in H_N^d(e) \), and for a \( G \) function \( f = \{f_v\}_{v \in V} \),

\[
E_{N,G}(f) = \sum_{v \in V} E_N(d(v); f_v).
\]

To make precise the various inputs to the constituent functions, we introduce some conventions. We assume an enumeration of \( V \) such that \( S = \{v_1, \ldots, v_s\} \), \( q = \sum_{j=1}^s d(v_j) \), (i.e., the source nodes appear before other nodes). The input \( x \) can be viewed as a vector in \( \mathbb{R}^q \), but also as an element of \( \prod_{j=1}^s \mathbb{R}^{d(v_j)} \), i.e., \( x = ((x)_{v_1}, \ldots, (x)_{v_s}) \) so that \( (x)_{v_j} \in \mathbb{R}^{d(v_j)} \). Correspondingly, we define the sets

\[
C_{v_j} = \{(x)_{v_j} : x \in C\}.
\]

Thus, \( C_{v_j} \) is the training data “seen” by the source node \( v_j \). This notion is extended recursively to other nodes of \( G \). Let \( v \) not be a source node, \( u_1, \ldots, u_{d(v)} \) be the children of \( v \), \( C_{u_1}, \ldots, C_{u_{d(v)}} \) be the training data seen by these nodes. Thus, for any \( x \in C \), the components given by \( (x)_{u_j} \) are seen by \( u_j \), and

\[
C_v = \left\{ (f_{u_1}((x)_{u_1}), \ldots, f_{u_{d(v)}}((x)_{u_{d(v)}}) : x \in C \right\}.
\]

For example, in the DAG of Figure 1, the children of \( h_{14} \) are \( h_{10} \) and \( h_{11} \). For each \( x \in \mathbb{R}^9 \), \( h_{10} \) sees the components \( (x_1, x_2, x_3) \), while \( h_{11} \) sees the components \( (x_4, x_5) \). We have

\[
C_{h_{10}} = \{((x)_1, (x)_2, (x)_3) : x \in C\}, \quad C_{h_{11}} = \{((x)_4, (x)_5) : x \in C\}, \quad C_{h_{14}} = \{((h_{10}(x)_1, (x)_2, (x)_3), h_{11}(x)_4, (x)_5) : x \in C\}
\]

The analogue of Theorem 3.1 for deep networks naturally requires a condition on the constituent functions so as to be able to keep track of the minimal separations among the inputs to the different
nodes. A function \( f : \mathbb{T}^d \to \mathbb{R} \) is said to be bi-Lipschitz if there exists a positive constant \( c(f) > 0 \) such that
\[
\frac{1}{c(f)} |x - y| \leq |f(x) - f(y)| \leq c(f) |x - y|, \quad x, y \in \mathbb{T}^d. \tag{4.4}
\]

The analogue of Theorem 3.1 is the following.

**Theorem 4.1** Let \( \mathcal{G} \) be a DAG with source nodes \( S = \{v_1, \cdots, v_s\} \) and sink node \( v^* \). Let \( f = \{f_v\}_{v \in V} \) be a \( \mathcal{G} \)-function such that each of the constituent functions is bi-Lipschitz. Let \( \eta = \min_{1 \leq j \leq s} \eta_j(C_{v_j}). \) There exists \( C = C(f) > 0 \) with the following property: for \( N \geq C(f) \eta^{-1} \), there exists \( T^\#_N(D) \in \mathcal{G}_-\mathbb{H}_N \) such that
\[(T^\#_N(D))_{v^*}(x_j) = y_j, \quad j = 1, \cdots, M, \quad \text{(Zero training error)} \tag{4.5}\]
and
\[
\|f - T^\#_N(D)\| \leq c \left\{ \epsilon + E_{N/2, \mathcal{G}(f)} \right\}. \quad \text{(Good generalization error)} \tag{4.6}
\]

The analogue of Theorem 3.2 is similar; but one has to take into account the fact that one does not know the constituent functions. Nevertheless, knowing the DAG structure, one can construct a DAG trigonometric polynomial. For \( n > 0 \) and \( T \in \mathcal{G}_-\mathbb{H}_n \), let
\[
R_{n, \mathcal{G}}(T) = \max_{1 \leq j \leq M} |y_j - T_{v^*}(x_j)| + \frac{1}{n} \|T\|_{W^*, \mathcal{G}}. \tag{4.7}
\]
In this definition, it is understood that \( T_{v^*} \) is thought of as a function of the \( q \)-dimensional vector \( x \), but is computed using the all the constituent functions in \( T \) using DAG structure prescribed by \( \mathcal{G} \).

**Theorem 4.2** Let \( \mathcal{G} \) be a DAG with source nodes \( S = \{v_1, \cdots, v_s\} \) and sink node \( v^* \). Let \( f = \{f_v\}_{v \in V} \in \mathcal{G}_-\mathbb{W}^* \), and each of the constituent functions be bi-Lipschitz. Let \( N \) be as in Theorem 4.1. Then with the notation as in that theorem,
\[
\min_{T \in \mathcal{G}_-\mathbb{H}_N} R_{N, \mathcal{G}}(T) \leq c \left\{ \epsilon + \frac{1}{N} \|f\|_{W^*, \mathcal{G}} \right\}. \quad \text{(Good training error)} \tag{4.8}
\]

Let \( x \in \mathbb{T}^d \), and \( \delta = \min_{1 \leq j \leq M} |x - x_j| \), and \( T^*(D) = \arg \min_{\mathcal{G}_-\mathbb{H}_N} R_{N, \mathcal{G}}(T) \), then
\[
|f(x) - (T^*(D))_{v^*}(x)| \leq c N \delta \left\{ \epsilon + \frac{1}{N} \|f\|_{W^*} \right\}. \quad \text{(Good generalization error)} \tag{4.9}
\]

**Remark 4.1** The theorems in this section indicate that the superiority of deep learning comes from two factors. One is that the compositional structure of the target function allows us to study the problem in a cascade of low dimensional problems. The other is that this structure might allow us to sparsify the training data as we move up the cascade.

## 5 Proofs

### 5.1 Proof of Theorem 3.1

The proof depends upon the construction and properties of a highly localized trigonometric polynomial kernel.
Let \( h : \mathbb{R} \to [0, 1] \) be an infinitely differentiable, even function such that \( h(t) = 1 \) if \( |t| \leq 1/2 \), \( h(t) = 0 \) if \( |t| \geq 1 \). We define
\[
\Phi_N(x) = \sum_{k \in \mathbb{Z}^q} h\left(\frac{|k|^2}{N}\right) \exp(i k \cdot x), \quad x \in \mathbb{T}^q, \quad N > 0. \tag{5.1}
\]

For \( f \in C^* \), we define
\[
\sigma_N(f)(x) = \sum_{k \in \mathbb{Z}^q} h\left(\frac{|k|^2}{N}\right) \hat{f}(k) \exp(i k \cdot x), \quad x \in \mathbb{T}^q, \quad N > 0. \tag{5.2}
\]

We note that the sums in both (5.1) and (5.2) are finite sums, although they are written as infinite sums for convenience of notation.

The following proposition summarizes some essential properties of these kernels and operators.

**Proposition 5.1** Let \( S > q \) be an integer, \( 1 \leq p \leq \infty \).

(a) For \( N \geq 1 \),
\[
|\Phi_N(x)| \leq \frac{cN^q}{\max(1, (N|x|)^q)}, \quad x \in \mathbb{T}^q, \tag{5.3}
\]
and
\[
|\Phi_N(0)| \geq cN^q. \tag{5.4}
\]

(b) If \( C = \{x_1, \ldots, x_M\} \). There exists a constant \( B > 0 \) with the following property: if \( N \geq B \eta(C)^{-1} \) then for \( x \in \mathbb{T}^q \),
\[
\sum_{j=1}^M |\Phi_N(x - x_j)| \leq cN^q. \tag{5.5}
\]

and
\[
\sum_{j:|x_j - x| \geq \eta} |\Phi_N(x - x_j)| \leq (1/2)\Phi_N(0) = (1/2)\Phi_N(x - x) \leq cN^q. \tag{5.6}
\]

(c) If \( T \in \mathbb{H}^q_{N/2} \) then \( \sigma_N(T) = T \). Further,
\[
\|\sigma_N(f)\| \leq c\|f\|, \quad f \in C^*. \tag{5.7}
\]

Consequently,
\[
E_N(f) \leq \|f - \sigma_N(f)\| \leq cE_{N/2}(f), \quad f \in C^*. \tag{5.8}
\]

**Proof.** Part (a) is proved in [13 Theorem 6.1]. It is not difficult to verify (cf. [13 Lemma 5.3]) that for any \( x \in \mathbb{T}^q \) and \( r > 0 \),
\[
|\{\ell : |x_\ell - x| \leq r\}| \leq c\eta(C)^{-q}(r^q + \eta(C)^q).
\]

The estimate follows from this fact and [13 Proposition 5.1, Definition 4.1], taking into account that \( N \geq \eta^{-1} \). The estimate (5.6) follows from (5.5) and (5.4) taking into account the fact that there can be at most one \( x_j \) with \( |x - x_j| < \eta(C)/2 \). The estimate (5.7) is given in [3 Corollary 6.1] (The notation in [3] is different from the one used here). If \( T \in \mathbb{H}^q_{N/2} \), then \( \hat{T}(k) = 0 \) if \( |k|^2 \geq N/2 \), while \( h(t) = 1 \) if \( |t| \leq 1/2 \). It follows from the definition (5.2) that \( \sigma_N(T) = T \). Together with (5.7), this leads to (5.8).

A consequence of the above proposition is the following (cf. [13 Proposition 6.1]).

**Lemma 5.1** Let \( a, b \in \mathbb{R}^M \), and
\[
\sum_{j=1}^M a_j \Phi_N(x_\ell - x_j) = b_\ell, \quad \ell = 1, \ldots, M. \tag{5.9}
\]
Then
\[
\max_{1 \leq j \leq M} |a_j| \leq cN^{-q} \max_{1 \leq \ell \leq M} |b_\ell|. \tag{5.10}
\]
Proof of Theorem 3.1 In this proof, let \( N \) be an integer satisfying the conditions of Proposition 5.1(b), and for \( \ell = 1, \cdots, M \), \( z_\ell = f(x_\ell) - \sigma_N(f)(x_\ell) \). In view of (5.4) and (5.6), and a well known result in linear algebra (cf. \cite[Proposition 6.1]{13}), there exist \( a_j \in \mathbb{R} \) such that
\[
\sum_{j=1}^{M} a_j \Phi_N(x_\ell - x_j) = z_\ell = y_\ell - \sigma_N(f)(x_\ell), \quad \ell = 1, \cdots, M, \quad \text{(5.11)}
\]
and (cf. (5.8))
\[
\max_{1 \leq j \leq M} |a_j| \leq c N^{-q} \max_{1 \leq \ell \leq M} |z_\ell| = c N^{-q} \max_{1 \leq \ell \leq M} |y_\ell - \sigma_N(f)(x_\ell)| \\
\leq c N^{-q} \left\{ \max_{1 \leq \ell \leq M} |y_\ell - f(x_\ell)| + \max_{1 \leq \ell \leq M} |f(x_\ell) - \sigma_N(f)(x_\ell)| \right\} \\
\leq c N^{-q} \left\{ \epsilon + E_{N/2}(f) \right\}. \quad \text{(5.12)}
\]

We now define
\[
T_N^\#(D)(x) = \sigma_N(f)(x) + \sum_{j=1}^{M} a_j \Phi_N(x - x_j), \quad x \in \mathbb{T}^q. \quad \text{(5.13)}
\]
Clearly, \( T_N^\#(D) \in \mathbb{H}_N^q \), and \( T_N^\#(D)(x_\ell) = y_\ell, \ell = 1, \cdots, M \). This proves (3.1).

Moreover, for every \( x \in \mathbb{T}^q \), (5.13) and (5.8) lead to
\[
|f(x) - T_N^\#(D)(x)| \leq |f(x) - \sigma_N(f)(x)| + \left\{ \max_{1 \leq j \leq M} |a_j| \right\} \sum_{j=1}^{M} |\Phi_N(x - x_j)| \\
\leq c \left\{ E_{N/2,\infty}(f) + c N^{-q} \left\{ \epsilon + E_{N/2,\infty}(f) \right\} \sum_{j=1}^{M} |\Phi_N(x - x_j)| \right\}. \quad \text{(5.14)}
\]

In view of (5.5), this leads to (3.2). \( \blacksquare \)

5.2 Proof of Theorem 3.2

In order to prove Theorem 3.2 we need some preparation.

We recall a theorem from \cite[Theorem 1°]{5}.

**Theorem 5.1** Let \( q = 1, f \in W^*(\mathbb{T}), n \geq 1 \) be an integer, \( E > 0 \), and \( T \in \mathbb{H}^1_n \) satisfy
\[
\|f - T\|_1 \leq E. \quad \text{(5.15)}
\]

Then
\[
\|f' - T'\|_1 \leq c \left\{ nE + E_n(f') \right\}. \quad \text{(5.16)}
\]

In the multivariate case, we take the derivatives one variable at a time to deduce the following corollary of Theorem 5.1.

**Corollary 5.1** Let \( f \in W^*, n \geq 1 \) be an integer, \( E > 0 \), and \( T \in \mathbb{H}_N^q \) satisfy
\[
\|f - T\| \leq E. \quad \text{(5.17)}
\]

Then
\[
\|f - T\|_{W^*} \leq c \left\{ NE + \sum_{j=1}^{q} E_N(D_j f) \right\}. \quad \text{(5.18)}
\]
In particular,
\[ \|T\|_{W^*} \leq cN \left\{ E + \frac{1}{N} \|f\|_{W^*} \right\}. \] (5.19)

We note also the direct theorem of trigonometric approximation \[26, \text{Section 5.3}].

**Proposition 5.2** If \( f \in W^* \) then
\[ E_N(f) \leq cN \|f\|_{W^*}. \] (5.20)

We are now ready to prove Theorem 3.2.

**Proof of Theorem 3.2.** In this proof, let \( T^\# = T^\#_N(D) \) be as in Theorem 3.1, and \( E = \epsilon + E_{N/2}(f). \)

In view of (3.2), we may use Corollary 5.1 to deduce that
\[ \|f - T^\#\|_{W^*} \leq c \left\{ NE + \frac{1}{N} \sum_{j=1}^q E_N(D_j f) \right\} \leq cN \left\{ E + \frac{1}{N} \|f\|_{W^*} \right\}. \] (5.22)

and in particular,
\[ \|T^\#\|_{W^*} \leq cN \left\{ E + \frac{1}{N} \|f\|_{W^*} \right\}. \] (5.23)

Using (3.1), (5.21) and (5.23), we obtain:
\[ \min_{T \in H_N} R_N(T) \leq R_N(T^\#) \leq \max_{1 \leq j \leq M} |y_j - T^\#(x_j)| + \frac{1}{N} \|T^\#\|_{W^*}, \]
\[ = \frac{1}{N} \|T^\#\|_{W^*} \leq c \left\{ E + \frac{1}{N} \|f\|_{W^*} \right\}. \]

In view of Proposition 5.2
\[ E \leq c \left\{ \epsilon + \frac{1}{N} \|f\|_{W^*} \right\}. \]

Together with (5.23), this proves (3.6). Next, let \( x \in \mathbb{T}^q \), and \( \delta = \min_{1 \leq j \leq M} |x - x_j| = |x - x_\ell|. \) For brevity, we write
\[ \tilde{E} = \epsilon + \frac{1}{N} \|f\|_{W^*}. \]

Using (3.6) and Corollary 5.1 we deduce that
\[ |f(x) - T^*(x)| \leq |f(x) - f(x_\ell)| + |f(x_\ell) - T^*(x_\ell)| + |T^*(x_\ell) - T^*(x)| \]
\[ \leq |x - x_\ell| \|f\|_{W^*} + c\tilde{E} + |x - x_\ell| \|T^*\|_{W^*} \leq N \delta \frac{1}{N} \|f\|_{W^*} + c\tilde{E} + N \delta \tilde{E} \]
\[ \leq c(1 + N \delta) \tilde{E}. \]

This proves (3.7). \[\blacksquare\]

**Remark 5.1** An argument similar to that in the proof of Theorem 3.2 leads to the bound
\[ \left| f(x) - \frac{1}{\Phi_N(0)} \sum_{k=1}^M y_k \Phi_N(x - x_k) \right| \leq c \left\{ (1 + N \delta) \left\{ \epsilon + \frac{1}{N} \|f\|_{W^*} \right\} + N \delta \|f\| \right\}, \] (5.24)
and similarly with the polynomial obtained by solving the interpolation problem (3.3). \[\blacksquare\]
5.3 Proofs or the theorems in Section 4.

Proof of Theorem 4.1. Since each of the functions $f_v$ is bi-Lipschitz, $\eta(C_v) \geq c\eta$ for each $v \in V$. Therefore, Theorem 3.1 implies that for each non-sink node $v$, there is $T^\#_v \in H^\#_N$ satisfying

$$T^\#_v(x) = f_v(x), \quad x \in C_v, \quad \|f_v - T^\#_v\|_{d(v)} \leq cE_N/2(d(v); f_v).$$

(5.25)

Similarly, there is $T^\#_{v^*} \in H^\#_N$ that satisfies (thought of as a function of all the inputs to the network)

$$T^\#_{v^*}(x_j) = T^\#_{v^*}((x_j)_{v^*}) = y_j, \quad j = 1, \cdots, M,$$

(5.26)

and (thought of as a function on $T^{d(v^*)}$)

$$\|f_{v^*} - T^\#_{v^*}\|_{d(v^*)} \leq c\{\epsilon + E_N/2(d(v^*); f_{v^*})\}.$$

(5.27)

Then $T^\#_N = \{T^\#_v\} \in G-H_N$. The equation (5.26) is the same as (4.5). Since each $f_v$ is Lipschitz continuous, the estimate (4.6) follows from (5.25) and (5.27) by a repeated application of triangle inequality (good propagation property, cf. [19, Proof of Theorem 2.1]).

Proof of Theorem 4.2. This proof is essentially the same as that of Theorem 3.2. We point out some considerations required in the details which are different. Since $f \in G-W^*$, the simultaneous approximation theorem Corollary 5.1 holds for each $f_v$. We may assume that the perturbation exists only at the sink node, and the rest of the data is exact. Finally, we use the good propagation property.

6 Conclusions and open problems

We have explored the puzzle that deep networks (and sometimes also shallow ones) do not exhibit overfitting even though the number of parameters is very large and the training error is reduced to zero. We have initiated a rigorous study of this phenomenon from the point of view of function approximation, giving estimates on how many parameters are needed to exhibit a zero or good training error, which is also compatible with the generalization error. Our estimates are given in terms of the data characteristics and the smoothness of the target function.

One obvious problem is to reduce the number of parameters to be trained in the regularization functional (3.5). Expressing the trigonometric polynomials as linear combinations of the translates $\Phi_N(\circ - 2\pi j/N)$ ensures that the resulting solution will have coefficients that are small away from the training data. It is therefore reasonable to take only some of these translates that are close to the training data. However, it is not clear that the theory will work with the space defined by the span of only those translates which are kept. Also, there may be some numerical instability problems with this basis.

A deeper and wider area of theoretical investigation is the following. Theorems 3.2 and 4.2 suggest that approximation error given by the trigonometric polynomials constructed there gives an estimate on the support of the marginal distribution of the training and test data. In [4], the approximation errors of the convergent bounded interpolatory polynomials constructed in [3] were used for texture detection and segmentation of images. What would be the analogues for understanding the nature of the data using the approximation errors obtained here?

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