The gap between theory and practice in function approximation with deep neural networks

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Abstract. Deep learning (DL) is transforming whole industries as complicated decision-making processes are being automated by Deep Neural Networks (DNNs) trained on real-world data. Driven in part by a rapidly-expanding literature on DNN approximation theory showing that DNNs can approximate a rich variety of functions, these tools are increasingly being considered for problems in scientific computing. Yet, unlike more traditional algorithms in this field, relatively little is known about DNNs from the principles of numerical analysis, namely, stability, accuracy, computational efficiency and sample complexity. In this paper we introduce a computational framework for examining DNNs in practice, and use it to study their empirical performance with regard to these issues. We examine the performance of DNNs of different widths and depths on a variety of test functions in various dimensions, including smooth and piecewise smooth functions. We also compare DL against best-in-class methods for smooth function approximation based on compressed sensing. Our main conclusion is that there is a crucial gap between the approximation theory of DNNs and their practical performance, with trained DNNs performing relatively poorly on functions for which there are strong approximation results (e.g. smooth functions), yet performing well in comparison to best-in-class methods for other functions. Finally, we present a novel practical existence theorem, which asserts the existence of a DNN architecture and training procedure which offers the same performance as current best-in-class schemes. This result indicates the potential for practical DNN approximation, and the need for future research into practical architecture design and training strategies.

Key words. neural networks, deep learning, function approximation, compressed sensing, numerical analysis

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1. Introduction. The past decade has seen an explosion of interest in the field of machine learning, largely due to the impressive results achieved with Deep Neural Networks (DNNs). Breakthroughs have been obtained on large classes of historically-challenging problems, including: speech recognition [19, 45] and natural language processing [82], image classification [48,68], game intelligence [67], and autonomous vehicles [30]. As DNNs have shown such promise in these real-world applications, a trend has developed in the scientific computing community towards applying them to problems in mathematical modelling and computational science. Recent studies have focused on applications ranging from image reconstruction tasks in medical imaging [5], discovering underlying Partial Differential Equation (PDE) dynamics [64] and approximating solutions of PDEs [29,81] to complex mathematical modeling, prediction, and classification tasks in physics [13], biology [69,76,86], and engineering [52,75].

Simultaneously, the broader applied mathematics community has taken interest in the approximation capabilities of NNs [6,10,50,53,62,83,84]. The earliest results in this di-

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rection [18, 46] established that even a single hidden layer fully-connected NN has universal approximation capability: so long as the number of nodes in the hidden layer are allowed to grow unbounded, such architectures are able to approximate any Borel measurable function on a compact domain to arbitrary uniform accuracy. More recent works have studied the connection between expressiveness of DNNs and their depth, while others have established connections between DNNs and other methods of approximation, e.g., sparse grids [55], splines [78], polynomials [20, 21, 65], greedy strategies [24, 32], integral representations [25], and \(h, p\)-finite elements [60]. A plethora of results now exist concerning the approximation power of DNNs for different function spaces – e.g., Sobolev spaces [40], bandlimited functions [55], analytic functions [61], cartoon-like functions [39], Hölder spaces [66] – and tasks in scientific computing, such as approximation of high-dimensional functions [49, 65] and PDEs [11, 38], dimensionality reduction [85], and methods for DEs [54, 81]. Theoretically, these works establish best-in-class approximation properties of DNNs for many problems.

1.1. Challenges. Yet despite the impressive empirical and theoretical results achieved in the broader DL community, there is concern that methods based on DNNs do not currently meet the usual rigorous standards for algorithms in computational science [9]. While the aforementioned theoretical results assert the expressibility of the class of DNNs – that is, the existence of a DNN of a given architecture that achieves a desired rate of convergence for a given problem – they say little about their practical performance when trained by modern approaches in DL. If such techniques are to achieve widespread adoption in scientific computing, it is vital they be understood through the lens of numerical analysis, namely, (i) stability, (ii) accuracy, (iii) sample complexity, (iv) curse of dimensionality and (v) computational cost.

(i) Stability. Recently, researchers have begun to question the stability properties of DNNs [31, 56, 74]. A series of works have demonstrated that DNNs trained on tasks such as image classification are vulnerable to misclassification when provided images with small “adversarial” perturbations [57] and can even completely fail on image reconstruction tasks in the presence of small structural changes in the data [4, 37]. As deep learning is increasingly being applied towards critical problems in healthcare, e.g., DeepMind’s recent work on machine-assisted diagnostic imaging in retinal disease [22], many have questioned the ethics of applying tools whose stability properties are not fully understood to such problems.

(ii) Accuracy. Over the past 5 years, many works have been published on the classes of functions, e.g., analytic or piece-wise continuous, that can be approximated by DNNs of a given size with a certain rate of convergence. These results are constructive, often showing the existence of a DNN emulating another approximation scheme, e.g. polynomials, for which convergence rates have already been established. While such results provide a useful benchmark for DNN expressivity, they do not suggest methods for training DNNs that reliably achieve the tolerances required in computational science applications.

(iii) Sample complexity. Areas in which DL has seen the greatest success include problems in supervised learning such as image classification. In such settings, DNNs are trained on large sets of labeled images, yielding a model capable of predicting labels for unseen images. Popular datasets for DL competitions include the ImageNet database which contains 14 million hand-annotated images of more than 20,000 categories of subjects [23]. In contrast, problems in computational science are often relatively data-starved, e.g. applications in Un-
certainty Quantification (UQ) which involve computing a quantity of interest from sampled solutions of a parameterized PDE [41]. As each sample involves the discretization and solution of a PDE, which may require thousands of degrees of freedom to accurately resolve, there is great attention paid in such problems to minimizing the required number of samples [3, 27].

(iv) **Curse of dimensionality.** Many modern problems in scientific computing involve high dimensionality. High-dimensional PDEs occur in numerous applications, and parametrized PDEs in UQ applications often involve tens to hundreds of variables. Recent works have show that certain DNNs have the expressive capabilities to mitigate the curse of dimensionality to the same extent as current best-in-class schemes [11, 38, 55, 61, 65]. Yet, as noted, this does not assert these rates can be achieved via training. Moreover, the curse of dimensionality is an important consideration in the sample complexity.

(v) **Computational cost.** By far, the largest barrier to entry for DL research is the cost of training. DNNs are typically trained on graphics processing units (GPUs), and a single GPU can cost thousands of US dollars. In many industry applications, models are trained on hundreds of these specialized cards. In addition, the training process itself is very energy-intensive, and can produce a large amount of excess CO\(_2\) emissions\(^1\). Even a small reduction in computational cost can yield large cost savings and greater access to resources for researchers.

In the near term, it seems likely that any DL implementation will pay a price in computational cost. Hence there needs to be a clear understanding of the benefits vis-a-vis properties (i)–(iv) above. The study of these concerns is the broad purpose of this paper.

1.2. **Contributions.** Our main objective is to examine practical DNN approximation on problems motivated by scientific computing. In many applications in computational science, the core task involves approximating a function \(f : U \to \mathbb{R}\), with domain \(U \subset \mathbb{R}^d\) where \(d \geq 1\) (often \(d \gg 1\)). Hence our main aim is to examine the performance of DL on practical function approximation through the five considerations (i)–(v). Our main contributions are:

1. We propose a computational framework for examining the practical capabilities of DNNs in scientific computing, based on the rigorous testing principles of numerical analysis. We provide clear practical guidance on training DNNs for function approximation problems.

2. We conduct perhaps the first comprehensive empirical study of the performance of training DNN approximations on standard function classes considered in numerical analysis, namely, (piecewise) smooth functions on bounded domains. We compare performance over a range of dimensions, examining the capability of DL for mitigating the curse of dimensionality.

3. We examine the effect of network architecture (depth and width) on both ease of training and approximation performance of the trained DNNs.

4. We make a clear empirical comparison between DL and current best-in-class approximation schemes for smooth function approximation. The latter is based on polynomial approximation via Compressed Sensing (CS) [3], which (as we also show) achieves exponential rates of convergence for analytic functions in arbitrarily-many dimensions.

5. We provide a novel theoretical insight comparing the performance of CS with DL for smooth function approximation. In particular, we develop a **practical existence theorem**, which

\(^1\)A recent study estimated the cost of training a natural language processing model for 274,000 GPU hours at between $942,000-$3,300,000 USD, meanwhile producing an excess of 626,000 lbs of CO\(_2\), or the equivalent of 5 cars output over their expected lifespan [73].
asserts the existence of a DNN architecture and training procedure (based on minimizing a certain cost function) that attains the same exponential rate of convergence as CS for analytic function approximation. In particular, this result points towards the potential for DL to eventually outperform current best-in-class methods in practical settings.

1.3. Conclusions. The primary conclusion of this work is the following. While it is increasingly well understood that DNNs have substantial expressive power for problems relevant to scientific computing, there remains a large gap between expressivity and practical performance. Surprisingly, trained DNNs can perform very badly on functions for which there are strong expressivity results, such as smooth functions in high dimensions and piecewise smooth functions. Yet, on other examples, they are competitive with current best-in-class schemes based on CS. We also draw several further conclusions:

1. The accuracy of trained DNNs is limited by the precision used, but is typically nowhere near machine epsilon despite training to such tolerances in the loss. In this work, we perform experiments in both single and double precision. Yet, in both cases, it is typically impossible to get beyond four digits of accuracy.

2. On successful training runs, the resulting DNNs appear to be numerically stable. We use a high-accuracy sparse grid quadrature rule to numerically evaluate the trained DNNs. Conversely, while failure during training is a rare occurrence with the setup we have chosen, when failed training runs do occur the resulting DNNs are often numerically unstable. Such networks exhibit spikes and other artefacts, even when the weights remain small.

3. Getting a setup that works for DNNs across a range of architectures and functions is challenging, and naive implementations are destined to fail. After extensive testing, we chose the Adam optimizer with exponentially decaying learning rate over a variety of optimizers including standard SGD. While we present clear implementation details, including choice of software, architecture, optimizer and hyperparameter settings, training can be slow and can sometimes fail to converge within the time budget.

4. Generally speaking, deeper architectures (which are sufficiently wide) are both easier to train and perform better than shallower architectures. However, this depends on the function and the amount of training data. Shallower networks may perform better with less training data. The width of the network also plays an important role; we find networks with width 5-10 times larger than the depth perform better. While this trend appears to be general, some of our results indicate that it is not universal.

5. Development of numerical instabilities during training is more common for very deep and wide networks. Such networks easily achieve machine epsilon tolerance during training, but exhibit poor accuracy, i.e. overfitting to the data.

6. While much of the success of DL has been in the field of classification, surprisingly performance of trained DNNs on simple piecewise constant functions is relatively poor in comparison to smooth functions, and adversely affected by the curse of dimensionality. Yet, DNNs do approximate such functions to some accuracy, unlike polynomial-based CS techniques. This highlights the flexibility of the DL approach.

7. Existence results on networks which achieve a given error in approximating piecewise continuous functions employ large weights in approximating the discontinuity. On the other hand, many common initialization and training strategies suggest weights should be initialized
with small variance and trained with a small learning rate in order to prevent failure. Empirically we find such strategies prevent networks from achieving the theoretical error estimates, as networks trained under these strategies have relatively small weights.

1.4. Outlook. This paper raises and seeks to answer the following question: is DL a useful tool for problems in scientific computing? The above conclusions may appear rather negative in this regard, certainly in comparison to the positive impression given by the plethora of expressivity results on DNNs. Let us raise several caveats. First, this study considers one particular setup: namely, fully-connected, ReLU networks of constant hidden layer widths, in combination with the $\ell^2$-loss function. There are almost countless variations on this setup, some of which will undoubtedly perform better. These variations include different activation functions (e.g. sigmoid, hyperbolic tangent), different architectures (e.g. ResNets, sparsely-connected layers, convolutional layers) and different loss functions (e.g. those incorporating regularization). We elected to use this setup based on standards in the literature; for instance, most expressibility results consider ReLU activations. Given difficulties and intense computational resources required for training, it is beyond the scope of this first work to methodically compare all possible setups. Second, the practical existence theorem we prove shows that a careful choice of architecture and cost function can allow DNNs to offer similar performance to state-of-the-art techniques. While it is not clear whether the approach can lead to a practical algorithm (as discussed in §5), it indicates that theory-inspired architecture and cost function design is a possible route towards enhancing performance in the future.

1.5. Outline. The outline of the remainder of this paper is as follows. In §2 we introduce the approximation problem, DNNs, DL and CS. In §3 we describe the experimental setup, including details of the training procedure used. Our numerical results are found in §4. Finally, in §5 we present our theoretical results. Additional information for this paper is contained in the Appendices. Code accompanying the computational framework is available at https://github.com/ndexter/MLFA.

2. Framework. In this section, we first describe the function approximation problem, and then introduce DNNs, DL, polynomial approximation and CS.

2.1. Problem formulation. Throughout this paper, we consider the unit cube in $d$ dimensions, $\mathcal{U} = (-1,1)^d$, equipped with the uniform probability measure $d\varrho = 2^{-d} dx$, where $dx$ is the Lebesgue measure and $x = (x_1, \ldots, x_d)$ is the $d$-dimensional variable. Let $L^2(\mathcal{U})$ denote the space of real-valued square-integrable functions on $\mathcal{U}$ with respect to $\varrho$. Our objective is to approximate an unknown function $f \in L^2(\mathcal{U})$ from samples. These samples are generated by simple Monte Carlo sampling: we draw $x_1, \ldots, x_m$ randomly and independently from the measure $\varrho$. Hence the approximation problem we aim to solve is

(AP) \quad \text{Given the measurements } \{(x_i, f(x_i))\}_{i=1}^m, \text{ approximate } f.

We note in passing that much of what follows in this paper can be extended to more general domains, sampling strategies and to functions taking values in other vector spaces (for instance, complex-valued functions, vector-valued functions, or even Hilbert-valued functions, as arise commonly in UQ applications [27]). We assume the above setup for ease of presentation.
We require several further pieces of notation. We write \( \| \cdot \|_{L^2} \) for the \( L^2 \)-norm with respect to \( \rho \). The space of essentially bounded functions on \( U \) is denoted by \( L^\infty(U) \) and its norm by \( \| \cdot \|_{L^\infty} \). We use \( \nu = (\nu_1, \ldots, \nu_d) \) to denote a (multi)index of length \( d \). If \( 0 < p < \infty \) and \( F \subseteq \mathbb{N}_0^d \) is a finite or countable (multi)index set, we write \( \ell^p(F) \) for the space of \( \ell^p \)-summable sequences \( c = (c_\nu)_{\nu \in F} \subseteq \mathbb{R} \), i.e. those satisfying \( \|c\|_p := (\sum_{\nu \in F} |c_\nu|^p)^{1/p} < \infty \). When \( p = \infty \), we define \( \ell^\infty(F) \) and \( \| \cdot \|_{\infty} \) in the usual way.

2.2. Deep Learning. We now introduce DL. First, we recall the definition of a DNN:

**Definition 2.1 (Neural network).** Let \( L \in \mathbb{N}_0 \) and \( N_0, \ldots, N_{L+2} \in \mathbb{N} \). A map \( \Phi : \mathbb{R}^{N_0} \to \mathbb{R}^{N_{L+2}} \) given by

\[
\Phi(x) = \begin{cases} 
A_1(\rho(A_0(x))), & L = 0 \\
A_{L+1}(\rho(A_L(\rho(\cdots \rho(A_0(x)) \cdots))), & L \geq 1
\end{cases}
\]

with affine linear maps \( A_l : \mathbb{R}^{N_l} \to \mathbb{R}^{N_{l+1}}, l = 0, \ldots, L + 1 \), and the activation function \( \rho \) acting component-wise (i.e., \( \rho(x) := (\rho(x_1), \ldots, \rho(x_d)) \) for \( x = (x_1, \ldots, x_d) \)) is called a Neural Network (NN). The map \( \Phi \) corresponding to layer \( l \) is given by \( A_l(x) = W_l x + b_l \), where \( W_l \in \mathbb{R}^{N_{l+1} \times N_l} \) is the \( l \)th weight matrix and \( b_l \in \mathbb{R}^{N_{l+1}} \) the \( l \)th bias vector. We refer to \( L \) as the depth of the network and \( \max_{1 \leq l \leq L+1} N_l \) as its width.

Informally, we consider a Deep Neural Network (DNN) as any NN with \( L \geq 1 \) hidden layers. Definition 2.1 pertains to feedforward DNNs. We do not consider more exotic constructions such as recurrent networks or ResNet in this paper. We also consider so-called fully connected networks, meaning that the weights and biases can take arbitrary real values. The layers \( l = 1, \ldots, L \) are referred to as hidden layers. In our experiments later, we set their widths to be equal, \( N_1 = \ldots = N_{L+1} \). Note that \( N_0 \) and \( N_{L+2} \) are specified by the problem. In our case, \( N_0 = d \) and \( N_{L+2} = 1 \).

There are numerous choices for the activation function \( \rho \), and moreover, one may also choose different activation functions in different layers. Since it is popular both in theory and in practice, we use the Rectified Linear Unit (ReLU), defined by \( \rho(x) = \max\{0, x\} \).

The architecture of a network is the specific choice of activation \( \rho \) and parameters \( L \) and \( N_1, \ldots, N_{L+1} \). We denote the set of neural networks of a given architecture by \( \mathcal{N} \). Note that this family is parametrized by the weight matrices and biases. Selecting the right architecture for a given problem is a significant challenge. We discuss this topic further in §3 and §4.

Given an unknown function \( f \in L^2(U) \), training is the process of computing a neural network \( \Phi \) that approximates \( f \) from the data \( \{(x_i, f(x_i))\}_{i=1}^m \). This is normally achieved by minimizing a loss function \( \mathcal{L} : \mathcal{N} \to \mathbb{R} \), i.e., we solve

\[
\min_{\Phi \in \mathcal{N}} \mathcal{L}(\Phi),
\]

where \( \mathcal{N} \) is the family of neural networks of the chosen architecture. Note that this is equivalent to a minimization problem for the weights \( W_l \) and biases \( b_l \). A typical choice is the \( \ell^2 \)-loss (also known as empirical risk, mean squared loss):

\[
\mathcal{L}(\Phi) := \frac{1}{m} \sum_{i=1}^m (\Phi(x_i) - f(x_i))^2.
\]
We primarily use this loss function in this paper. However, many other choices are possible. For instance, it is common to add a regularization term to the loss function, e.g.

\[ \mathcal{L}(\Phi) := \frac{1}{m} \sum_{i=1}^{m} (\Phi(x_i) - f(x_i))^2 + \mathcal{J}(\Phi). \]

Here \( \mathcal{J} : \mathcal{N} \to \mathbb{R} \) is chosen to promote some desirable features of the network. For instance, it may be a norm of the weight matrices, thus promoting small and/or sparse weights.

### 2.3. Polynomial approximation of smooth functions.

We now introduce the polynomial approximation schemes against which we compare DL for function approximation. Polynomial approximation is a vast and classical topic. Yet, it has received renewed attention in the last several decades, motivated by applications in UQ where one seeks to approximate a smooth quantity of interest of a parametric PDE [17]. The particular scheme we consider is based on orthogonal expansions in orthonormal polynomials in \( L^2(U) \), i.e. multivariate Legendre polynomials. The univariate, orthonormal Legendre polynomials on the \([-1, 1]\) are defined by

\[ \psi_\nu(x) = \sqrt{2\nu + 1} P_\nu(x), \quad \nu \in \mathbb{N}_0, \]

where \( P_\nu \) is the classical Legendre polynomial with normalization \( P_\nu(1) = 1 \). The functions \( \psi_\nu \) form an orthonormal basis of \( L^2(-1, 1) \). When \( d > 1 \), we define the tensor orthonormal Legendre polynomials as

\[ \Psi_\nu(x) = \prod_{i=1}^{d} \psi_{\nu_i}(x_i), \quad \nu = (\nu_1, \ldots, \nu_d) \in \mathbb{N}_0^d, \quad x = (x_1, \ldots, x_d) \in U. \]

The set \( \{\Psi_\nu\}_{\nu \in \mathbb{N}_0^d} \) forms an orthonormal basis of \( L^2(U) \). Hence any function \( f \in L^2(U) \) has a convergent expansion

\[ f = \sum_{\nu \in \mathbb{N}_0^d} c_\nu \Psi_\nu, \tag{2.3} \]

where \( c_\nu = \int_U f(x) \Psi_\nu(x) \, d\rho(x) \) is the coefficient of \( f \) with respect to \( \Psi_\nu \). Note that the sequence \( c = (c_\nu)_{\nu \in \mathbb{N}_0^d} \) is an element of \( \ell^2(\mathbb{N}_0^d) \), the space of square-summable sequences with indices in \( \mathbb{N}_0^d \).

By Parseval’s identity, \( \|f\|_{L^2(U)} = \|c\|_2 \).

When \( d = 1 \), approximating a smooth function in the Legendre basis is typically achieved by truncating the expansion (2.3) after its first \( s \) terms, then using, for instance, least-squares to approximately recover the coefficients \( c_0, \ldots, c_{s-1} \) from the measurements \( \{(x_i, f(x_i))\}_{i=1}^{m} \).

In \( d \geq 2 \) dimensions, the situation becomes more complicated, since there are many different choices of index set \( S \) of cardinality \( s \) one might employ to truncate the expansion (2.3):

\[ f \approx f_S = \sum_{\nu \in S} c_\nu \Psi_\nu. \]

By Parseval’s identity, the error \( \|f - f_S\| = \sqrt{\sum_{\nu \in \mathbb{N}_0^d \setminus S} |c_\nu|^2} \) depends on the coefficients outside \( S \). Hence, an \textit{a priori} choice of \( S \) may have limited effectiveness, since it may fail to capture any anisotropic behaviour of \( f \). This naturally motivates the concept of \textit{best} \( s \)-term approximation [17]. In best \( s \)-term approximation, the index set \( S \)
is chosen so that it contains the multi-indices corresponding to the large $s$ coefficients $c_\nu$ in absolute value. This is a type of nonlinear approximation scheme [26]. If $\tilde{f}_s$ denotes the best $s$-term approximation, the error satisfies

$$\|f - \tilde{f}_s\|_{L^2} = \inf \left\{ \sqrt{\sum_{\nu \in S} |c_\nu|^2} : S \subset \mathbb{N}_0^d, |S| \leq s \right\}.$$ 

Under appropriate conditions (e.g. $f$ is analytic), this approximation converges exponentially fast in $s$ (see Theorem 5.2). In high dimensions this significantly improves over any linear approximation scheme based on a fixed, isotropic choice of $S$. We discuss this further in §5.1.

2.4. Polynomial approximation with compressed sensing. Computing the best $s$-term approximation is on the face of it a daunting task. In theory, it involves computing all infinitely-many of the coefficients $c_\nu$, then selecting the largest $s$. This is of course intractable, and generally still computationally infeasible even if one limits oneself to computing a large, but finite number of coefficients.

A solution is to use Compressed Sensing (CS). Here one first selects a large, but finite multi-index set $\Lambda \subset \mathbb{N}_0^d$. This set is generally assumed to contain the coefficients of some quasi-best $s$-term approximation, if not the coefficients of the true best $s$-term approximation itself. For reasons that will be made clear in §5.2, a reasonable choice is $\Lambda = \Lambda_{HC}^s$, where

$$\Lambda_{HC}^s = \left\{ \nu = (\nu_1, \ldots, \nu_d) \in \mathbb{N}_0^d : \prod_{j=1}^d (\nu_j + 1) \leq s + 1 \right\},$$

is the hyperbolic cross index set of degree $s$.

Having chosen $\Lambda$, the finite vector $c_\Lambda = (c_\nu)_{\nu \in \Lambda}$ can now be assumed to be approximately sparse. Next, one formulates the normalized measurement matrix and vector of measurements

$$A = \left( \frac{\Psi_\nu(x_i)}{\sqrt{m}} \right)_{1 \leq i \leq m, \nu \in J}, \quad f = \left( \frac{f(x_i)}{\sqrt{m}} \right)_{1 \leq i \leq m}.$$ 

Then one searches for an approximately sparse solution of the linear system $Az = f$. A standard means to do this is to solve the quadratically-constrained basis pursuit problem

$$\minimize_{z \in \mathbb{R}^n} \|z\|_1 \quad \text{s.t.} \quad \|Az - f\|_2 \leq \eta,$$

for suitably chosen $\eta \geq 0$, or the unconstrained LASSO problem

$$\minimize_{z \in \mathbb{R}^n} \|z\|_1 + \mu \|Az - f\|_2^2,$$

for appropriately chosen $\mu > 0$. A solution $\hat{c} = (\hat{c}_\nu)_{\nu \in \Lambda}$ of either problem yields an approximation $\hat{f} = \sum_{\nu \in \Lambda} \hat{c}_\nu \Psi_\nu$ of $f$.

Unfortunately, simply promoting the sparsity of the polynomial coefficients via the $\ell^1$-norm is not sufficient to achieve favourable sample complexity bounds. Bounds on $m$ for $\ell^1$-norm based approaches can be exponential in the dimension $d$ [3]. Fortunately, as considered
in [1, 14, 63], this issue can be overcome by replacing the \( \ell^1 \)-norm with a certain weighted \( \ell^1 \)-norm. For instance, instead of (2.6) one now solves

\[
\text{minimize}_{z \in \mathbb{R}^N} \|z\|_{1,u} \quad \text{s.t.} \quad \|Az - f\|_2 \leq \eta.
\]

(2.8)

Here \( u = (u_\nu)_{\nu \in \Lambda} \) is a vector of weights and \( \|z\|_{1,u} = \sum_{\nu \in \Lambda} u_\nu |z_\nu| \). As shown in [1], an appropriate choice of weights is

\[
u_\nu = \|\Psi_\nu\|_{L^\infty} = \prod_{j=1}^d \sqrt{2\nu_j + 1}, \quad \nu = (\nu_1, \ldots, \nu_d).
\]

(2.9)

For the remainder of this paper, we consider the CS polynomial approximation scheme \( \hat{f} = \sum_{\nu \in \Lambda} \hat{c}_\nu \Psi_\nu \), where \( \hat{c} \) is either a solution of (2.8) or for the sake of comparison, (2.6).

3. Testing setup. We now describe the testing setup for our experiments. Training DNNs requires careful choices of the optimization solver, initialization and optimization parameters. This section describes the choices we made to deliver consistent performance across a range of DNN architectures. In summary, we find Adam optimizer with exponentially-decaying learning rate and a specific random initialization to deliver this performance, whereas other solvers such as SGD and other learning rate schedules perform less consistently.

3.1. Setup. We first summarize the main methodology:

(i) Implementation. Our framework has been implemented in a package called MLFA (Machine Learning Function Approximation) in version 1.13 of Google’s TensorFlow software library https://www.tensorflow.org/, and is available on GitHub at https://github.com/ndexter/MLFA. Details about the set of features supported by MLFA and data recorded by the code can also be found on the GitHub page.

(ii) Hardware. In the course of testing our DNN models, we observed improved accuracy on some of our test problems by initializing and training the networks in double precision. Modern GPUs often support half, single, and double precision arithmetic, though many commonly-available GPUs are optimized to perform single precision computations much more quickly (see §A.1). The majority of our computations were performed in single precision using the Tesla P100 GPUs on Compute Canada’s Cedar compute cluster at Simon Fraser University, though for some of our test problems we provide double precision results for a subset of the architectures considered for comparison.

(iii) Choice of architectures and initialization. We consider fully-connected ReLU networks. This choice is inspired by the many theoretical existence results on such networks (see §1). There is a vast literature suggesting various strategies for designing architectures and initializing neural networks. For an introduction to these topics see, e.g., [36, §5.2 & 8.4]. We recall the work [42] focusing on which DNN architectures result in exploding and vanishing gradients, a common problem in backpropagation which can result in failure during training. Our empirical results confirm that choosing DNN architectures with a fixed number of nodes per layer \( N \) and depth \( L \) such that the ratio \( \beta := L/N \) is small, e.g., \( \beta \in (0.025, 0.5) \), is an
effective choice for training. In §3.3, we study several popular strategies for initializing DNNs. Our results show that initializing the weights and biases to be normal random variables with mean 0 and variance 0.01 is an effective choice for many of the architectures and problems considered herein. We note that for the range of architectures studied, this choice results in weights and biases with variance smaller than many other popular choices, e.g., the strategies from [35, 44], and is sufficiently small to avoid the failure modes analyzed in [43]. We also note that setting the variances smaller than 0.01 can result in networks which are more difficult to train, which can be attributed to the exponentially decaying length scales described in [43, Theorem 1]. The seed used for the random number generators can also have an important effect on the initialization. In this study, we initialize all of our networks from the same seed 0 for both TensorFlow and NumPy, in order to reduce the complexity of our experiments. A more comprehensive study of the average performance of DL would require averaging over a large set of seeds used in initialization. We leave such a study to a future work.

(iv) Optimizers for training and parameterization. §3.4 compares the performance of a variety of solvers and learning rate schedules on the function approximation problem. In practice, we find the Adam optimizer [47] with an exponentially decaying learning rate yields the most accurate results of the solvers tested in the least amount of training time. See §A.2 for implementation details. In single precision, the DNNs are trained for 50,000 epochs or to a tolerance of $\varepsilon_{\text{tol}} = 5 \times 10^{-7}$, while in double precision DNNs are trained for 200,000 epochs or to a tolerance of $\varepsilon_{\text{tol}} = 5 \times 10^{-16}$. Due to the non-monotonic convergence of minimizing the non-convex loss (2.2) with respect to the weights and biases, we checkpoint our partially trained networks once the training loss has been reduced to 1/8th of the previous checkpoint’s training loss, saving the best result at the end of training. We then average our testing results over the final trained networks.

(v) Training data and design of experiments. To understand the average performance of DL on a variety of reconstruction tasks, we run 20 trials of solving (AP) with each of our DNN architectures and CS over a range of data sets of increasing size. We then average the testing error and run statistics over all trials for each data set in plotting. We define a trial as one complete run of training a DNN, initialized as above, or solving a CS problem on a set of training data consisting of the values $\{(x_i, f(x_i))\}_{i=1}^{m_k}$. To generate each data set of size $m_k$, with $0 < m_1 < m_2 < \cdots < m_{k_{\text{final}}}$, we sample 20 i.i.d. sets of points $\{x_i\}_{i=1}^{m_k}$ from the uniform distribution on $(-1,1)^d$ and evaluate our target function $f$ at these points to form our training data. Since we are interested in the sample complexity of the DL problem, for most of our examples we choose $m_{k_{\text{final}}}$ to be a relatively small number $O(10^3)$.

(vi) Testing data and error metric. To study the generalization capabilities of DL, we use a common error metric for numerical analysis, the relative $L^2$ error

$$\varepsilon_{\text{rel}} = \|f - \tilde{f}\|_{L^2}/\|f\|_{L^2},$$

where $\tilde{f}$ is an approximation obtained using either DL or CS. As we run multiple trials of our experiments, we compute the average of (3.1) over all of our trials in testing. In contrast to the training data, we use deterministically generated points and function data for testing the relative $L^2$ errors. More specifically, we compute an approximation to the $L^2$ integrals using a high order isotropic Clenshaw Curtis sparse grid quadrature [34] rule, see, e.g., [59]
for more details. As opposed to the training data, we use a large set of testing points, e.g.,
\((d = 1)\ 65,537,\ (d = 2)\ 311,297,\ (d = 4)\ 643,073,\ \text{and}\ (d = 8)\ 1,863,937\ \text{points, to ensure a good covering of our parameter space} \mathcal{U}\ \text{in computing these statistics. For such moderate dimensional problems an isotropic rule is sufficient to study the generalization performance of both CS and DL. For higher-dimensional instances of (AP), the points and weights can be pre-computed and re-used in testing multiple functions. We rely on the TASMANIAN sparse grid toolkit [70,71,72] for the generation of these rules.}

(vii) Compressed sensing. We solve the problems (2.6) and (2.8) (with weights (2.9)) using the MATLAB solver SPGL1 [79,80] in double precision. The parameter \(\eta\) is chosen as

\[
\eta = \|A\mathbf{c}_\Lambda - \mathbf{f}\|_2, \quad \mathbf{c}_\Lambda = (c_\nu)_{\nu \in \Lambda},
\]

To compute \(\mathbf{c}_\Lambda\) we use the same sparse grid rule described above in evaluating each coefficient

\[c_\nu = \int_{\mathcal{U}} f(x) \Psi_\nu(x) \, d\rho(x).\]

See §A.5 for further discussion. We set \(\Lambda\) as in (2.4) to be the hyperbolic cross index set of degree \(s\) chosen so that \(\#(\Lambda^\text{HC}_s) \approx 3,000\).

3.2. Solvers. The choice of solver and parameterization of the solver are important factors in training DNN models to a desired tolerance in a reasonable amount of time. A common choice in many computational science applications is the Adam (adaptive moments) optimizer, a variant of SGD (stochastic gradient descent) incorporating moment estimates of the gradient. In the course of testing our implementation of the MLFA package, we studied the effect of the solvers on the generalization error and time to train given a fixed budget of 50,000 epochs in single precision. Fig. 1 displays results for a variety of solvers and learning rate schedules. There we observe comparable performance for the Adam and RMSProp algorithms in terms of accuracy, with Adagrad, SGD, and PGD (proximal gradient descent) performing the worst in both accuracy and computational cost. When comparing run times and accuracy for all methods tested, the Adam optimizer achieves the best accuracy with the least computational cost. We also include results obtained with the AdamW optimizer [51], which implements a decoupled weight decay (a form of \(\ell^2\)-regularization) on the weights and biases. In Fig. 1 we observe that smaller values of the weight decay parameter \(\lambda\) allow the AdamW optimizer to achieve identical performance to Adam with minimal overhead, but do not outperform standard Adam, while larger values of \(\lambda\) both decrease accuracy and increase run time.

For certain solvers, it is often the case that some of the trials of a given test may fail to achieve the desired loss tolerance before arriving at the final epoch. An example of this can be seen in the left plot of Fig. 2 where none of the trials of SGD with a constant learning rate of \(10^{-3}\) were able to achieve the desired tolerance in 50,000 epochs of training. The middle plot of Fig. 2 displays the effect of using an exponentially decaying learning rate with SGD, though we also observe there that none of trials trained with this learning rate schedule were able to achieve the tolerance in 50,000 epochs of training. On the other hand the right plot shows that, on the same problem, all 20 trials trained with the Adam optimizer with the exponentially decaying learning rate were able to converge to the \(5 \times 10^{-7}\) loss tolerance in under 14,000 epochs of training. We also compared learning rate schedules for the Adam optimizer, but found the exponentially decaying learning rate to give consistently good results. See §A.3.

Previous studies on training DNNs suggest that the batch size can affect the convergence of the algorithms. Due to the small data set sizes considered herein over those in, e.g. computer
vision, we have found that setting the batch size too small can result in longer training times (due to the increased transfer time between the CPU and GPU) and only marginal performance benefit. See §A.4. We leave a more detailed study of the affects of batch size on the performance of trained DNNs in higher-dimensional problems to a future work.

3.3. Initialization and Precision. The strategy used to initialize NNs can have a large effect on the success or failure of training. In all cases tested, we initialized our NNs using symmetric uniform or normal distributions with small variance, finding that larger variance values tend to result in failure during training. Fig. 3 presents three different initialization strategies for training three different architectures with Adam, namely normal with mean 0 and variance 0.01, normal with mean 0 and variance $2/N$, and uniform on $(-2/N, 2/N)$. For the majority of our results, we focused on architectures with a small ratio $\beta = L/N$ (with $L$ the number of layers and $N$ the number of nodes per layer). However, we also note that setting $\beta$ too small can result in DNNs which exhibit numerical instabilities after training, see Fig. 5. We also remark that this can occur for networks with relatively small weights, see the right plot of Fig. 14 which shows the weights and biases for the $20 \times 800$ network remain on average bounded by 2 as we increase the samples.

We also observed that for some problems, initializing and training our DNN models in double precision can lead to improved accuracy in testing the generalization performance, and that the improvement is more pronounced for deeper networks, see Fig. 4. Due to the massive
increase in computation time associated with training in double precision, a result of needing to train for more epochs to achieve the tolerance $5 \times 10^{-16}$ and the increased time of double precision arithmetic, see item (ii) on Hardware in §3.1, we limit our comparisons of single vs. double precision results to a handful of problems and architectures.

![Figure 3](image)

**Figure 3.** Comparison of strategies for initializing ReLU DNNs with $L$ hidden layers and $N$ nodes per hidden layer with (left) $L = 2$ and $N = 20$, (middle) $L = 3$ and $N = 30$, and (right) $L = 5$ and $N = 50$. Results were obtained by training with the Adam optimizer and an exponentially decaying learning rate schedule on function data generated from $f(x)$ from (4.4) with $d = 2$.

![Figure 4](image)

**Figure 4.** Comparison of (a) & (b) average relative $L^2$ error and (c) & (d) average training time for DNNs initialized and trained in single vs. double precision on a (a) & (c) one dimensional smooth function $f(x) = \log(\sin(10x) + 2) + \sin(x)$ and (b) & (d) eight-dimensional smooth function $f(x)$ from (4.3).

### 3.4. Convergence of Adam on function approximation problems

We now discuss the convergence of the Adam optimizer. Our stopping criteria for testing the convergence depends only on the $\ell_2$ loss with respect to the training data and the current number of epochs of training. During the course of training, the process outlined above may result in networks which exhibit numerical instabilities or provide poor performance, see Fig. 5. In §3.2, we noted that some trials may not achieve the desired accuracy tolerance within our budget of 50,000 epochs in single precision and 200,000 epochs in double precision. This can also occur for some of the trials with the Adam optimizer, see Fig. 6. Despite these issues, when viewing the average performance of the Adam optimizer on such problems we often find that the majority of networks are numerically stable and approximate the function well, see Fig. 6 which displays
boxplots of the average relative $L^2$ error of trained ReLU DNNs with 10 layers and 100 nodes per layer on a discontinuous two-dimensional function. We also remark that the observed performance improves with depth, see Fig. 7 which displays the outputs of all 20 trials of a variety of ReLU DNN architectures trained on a smooth, one-dimensional function.

![Figure 5](image1.png)

**Figure 5.** Unstable ReLU networks with 20 hidden layers, trained in single precision to a loss tolerance of $5 \times 10^{-7}$ on noiseless data. The (left) network has 200 nodes per layer and exhibits a numerical instability (a spike) near $x = 0.2334$, while the (right) network has 800 nodes per layer and exhibits multiple instabilities throughout the domain, providing poor pointwise estimation of the target function.

![Figure 6](image2.png)

**Figure 6.** Training a 10 layer DNN with 100 nodes per layer with Adam on the function (4.4) with $d = 2$. (left) An example where one out of 20 trials is unable to complete within 50,000 epochs. (middle) Boxplot of the average relative $L^2$ errors of 20 trials. For the boxplot, the tops and bottoms of the boxes represent the 25th and 75th percentiles, with the whiskers covering the most extreme datapoints and outliers (red plusses) plotted individually, see boxplot from MATLAB for more details.

![Figure 7](image3.png)

**Figure 7.** Comparison of outputs of a variety of ReLU DNN architectures trained with Adam on 750 samples of the function $f(x) = \log(\sin(100x) + 2) + \sin(10x)$ (plotted in black).

4. Numerical experiments. We now present our numerical experiments. We test on smooth functions of one or more variables, as well as piecewise continuous functions. The
results presented in this section elaborate on the main conclusions in §1.3.

4.1. Smooth one-dimensional functions. We first consider problems where the target function has analytic dependence on only one variable. Specifically, we consider

\begin{equation}
    f(x) = \log(\sin(10Kx) + 2) + \sin(Kx)
\end{equation}

for values of $K = 1$ (sparse) and $K = 10$ (less sparse). Fig. 8 displays results in the case of $K = 1$, where we see the coefficients of the expansion of $f$ in the Legendre basis rapidly decay in magnitude with increasing index. Such functions are ideal for approximation with CS techniques. The right plot of Fig. 8 compares the average relative $L^2$ errors of the CS and DL approaches with respect to the number of samples $m$ used in training. There we see shallower networks fail to achieve a good approximation. We also observe increasing depth and width leads to networks which are competitive with the unweighted and weighted CS approaches. However, comparing the results obtained with the 10 hidden layer deep and 20 hidden layer deep networks, we note that increasing the size of the networks has diminishing returns on their performance. This could be due, e.g., to the increased difficulty of training larger networks and the development of numerical instabilities associated with the accumulation of errors from standard sources including roundoff, overflow, and underflow. We remark that improved results have been obtained on this function by training some of our networks in double precision, see Fig. 4. However we also observe that training the 20 hidden layer DNN in double precision did not improve, but actually decreased its accuracy.

Fig. 9 displays the results of approximating the function $f$ when $K = 10$. There we see the coefficients of the Legendre expansion now decay much more slowly, leading to a less accurate resolution of the target function by both approaches. We again observe improved accuracy by increasing depth and width as in the previous example. We also again observe the diminishing returns increasing the size of the network architectures from 10 hidden layers with 100 nodes per layer to 20 hidden layers with 200 nodes per layer, although the 20 hidden layer network provides the best accuracy of all tested DNNs after approximately 600 samples and achieves the same accuracy as the weighted CS approximations around 700 samples.
Fig. 9. Legendre coefficients of \( f(x) = \log(\sin(100x) + 2) + \sin(10x) \) sorted (left) lexicographically and (center) by decreasing magnitude. (right) Average relative \( L^2 \) error v.s. number of samples used in training. CS approximations were computed with the Legendre basis of cardinality \( n = 3,000 \).

Fig. 10 displays the effect of choosing wider networks in approximating \( f \) with \( K = 10 \). There we see wider counterparts of the network architectures generally outperform narrower architectures with the same number of hidden layers. However, here we also observe diminishing returns going from 10 hidden layers to 20 hidden layers, and in the right plot we see the ReLU \( 20 \times 800 \) DNN diverges due to lack of stability of the trained networks, see, e.g., Fig. 5 for a typical example of a trained network of this architecture on this problem.

Fig. 11 compares the average absolute maximum of the weights and biases for ReLU DNNs trained on (4.1). There we see that to approximate the more oscillatory version of this function, corresponding to \( K = 10 \), the trained DNN architectures on average have larger weights and biases in magnitude compared to those trained on the same function with \( K = 1 \).

4.2. Smooth higher-dimensional functions. In Fig. 12, we present results for the function

\[
 f(x_1, \ldots, x_d) = \exp\left(-\left(\cos(x_1) + \ldots + \cos(x_d)\right)/(8d)\right),
\]
Figure 11. Average absolute maximum of weights and biases v.s. number of samples of \( f(x) = \log(\sin(10Kx) + 2) + \sin(Kx) \) for (left) \( K = 1 \) and \( \beta = 0.1 \), (middle) \( K = 10 \) and \( \beta = 0.1 \), and (right) \( K = 10 \) and \( \beta = 0.025 \).

studied in [14]. Despite the analytic dependence of \( f \) on its parameters and rapidly decaying coefficients in the Legendre basis, the DNNs are unable to obtain an approximation accurate beyond 3 digits while both CS approaches achieve nearly 8 digits of accuracy.

Figure 12. Legendre coefficients of \( f \) from (4.2) with \( d = 8 \) sorted (left) lexicographically and (center) by decreasing magnitude. (right) Average relative \( L^2 \) error v.s. number of samples used in training. CS approximations were computed with the Legendre basis of cardinality \( n = 3,023 \).

Fig. 13 displays the results of approximating \( f \) from (4.2) with both narrower and wider networks. In the small width regime, i.e., for the narrower DNN architectures corresponding to \( \beta \in \{0.1, 0.2, 0.5\} \), we observe deeper networks perform better. In the large width regime, i.e., the wider architectures corresponding to \( \beta \in \{0.025, 0.05\} \), we observe the shallower networks perform better. In all cases, the best performing networks had between \( 10^3 \) and \( 10^5 \) total trainable parameters. We also observe divergence of the 20 hidden layer networks in all plots.

Fig. 14 displays the average absolute maximum of the weights and biases for each architecture. There we observe that the weights and biases of narrower network architectures, e.g. \( \beta \in \{0.1, 0.2, 0.5\} \), remain relatively small as we increase the number of samples. However, as we increase the width of the networks to values corresponding to \( \beta = 0.05 \) and \( \beta = 0.025 \), we begin to see the weights growing with depth as we train on larger sample sets. This growth
Figure 13. Comparison of average relative $L^2$ errors w.r.t. number of samples of $f$ from (4.2) with $d = 8$ used in training ReLU architectures parameterized with $\beta = L/N$ (hidden layers/nodes per hidden layer) for values (top-left) $\beta = 0.5$, (top-middle) $\beta = 0.2$, (top-right) $\beta = 0.1$, (bottom-left) $\beta = 0.05$, and (bottom-middle) $\beta = 0.025$. (bottom-right) Table of best-performing architectures for each choice of $\beta$ and number of parameters. CS approximations were computed with the Legendre basis of cardinality $n = 3,023$.

in the weights and biases can lead to numerical instabilities for deeper architectures, as seen in the one-dimensional example in Fig. 5.

Fig. 15 displays the average run time of the Adam optimizer in training our DNNs as we increase the number of training samples. For the narrower and shallower DNN architectures, we see the transfer time bottleneck between the CPU and GPU is yielding an effective linear scaling with respect to samples in the average training time. This effect is also present in the deeper and wider networks, though at a diminished amount due to the fast convergence of the Adam optimizer on larger networks.

Next we present results on the function

$$f(x) = \left( \prod_{k=1}^{[d/2]} \left( 1 + 4^k x_k^2 \right) \prod_{k=[d/2]+1}^{d} (100 + 5x_k) \right)^{1/d},$$

also from [14]. Fig. 16 displays the Legendre coefficients, and the average relative $L^2$ error obtained by both the CS and DL approaches. Due to the slower coefficient decay, the CS approximations only achieve error of roughly $10^{-1}$. The best performing ReLU DNNs achieve an error that is roughly five times smaller.
Figure 14. Comparison of average absolute maximum of weights and biases w.r.t. number of samples of \( f \) from (4.2) with \( d = 8 \) used in training ReLU architectures parameterized with \( \beta = L/N \) (hidden layers/nodes per hidden layer) for values (top-left) \( \beta = 0.5 \), (top-middle) \( \beta = 0.2 \), (top-right) \( \beta = 0.1 \), (bottom-left) \( \beta = 0.05 \), and (bottom-right) \( \beta = 0.025 \).

Fig. 17 displays the effect of increasing the width of the DNNs as before. There, as in the previous example, we observe best performance is achieved by networks that are both wide and deep, e.g. the ReLU 5 × 25 and 10 × 20 networks. We also again observe that for wider networks, architectures with fewer hidden layers perform the best. Nonetheless, comparing the results between the ReLU 1 × 20 and 1 × 40 DNNs and those achieved by the 10 × 20, 5 × 25, and 2 × 20 DNNs, we see that far better performance is achieved with fewer samples by the deeper and narrower DNN architectures.

Figure 18 compares the average absolute maximum of the weights and biases of the trained DNNs. There, as in the one-dimensional examples, we observe that the weights and biases of DNNs trained on function data from the less smooth function (4.3) are on average larger than those obtained after training on the smoother function (4.2).

Fig. 19 again displays the average run time of the Adam optimizer in training the DNNs as we increase the number of samples. There we observe similar patterns to the timing results obtained on function (4.2), e.g., linear scaling in the runtimes for narrower architectures due to the CPU-GPU transfer bottleneck. However, we also observe longer training time in general in approximating the function (4.3) compared to Fig. 15, suggesting the difficulty of approximating less smooth functions can impact training time.
4.3. Piecewise continuous functions. In this section, we present results on approximating piecewise continuous functions. We consider the function

\[ f(x_1, \ldots, x_d) = \mathbb{1}_K(x_1, \ldots, x_d), \quad \text{with} \quad K = \{ z \in \mathbb{R}^d : z_1 + \ldots + z_d \geq 0 \}. \]

where \( \mathbb{1}_K(x_1, \ldots, x_d) = 1 \) if \((x_1, \ldots, x_d) \in K\) and 0 otherwise. In one dimension \( K = \{ x \in \mathbb{R} : x \geq 0 \} \), so that \( f(x) = \mathbb{1}_{\{x \geq 0\}}(x) \). We note this simple discontinuous function equally splits the data between values in \( \{0, 1\} \) in arbitrary dimension \( d \), and that the separating hyperplane between the sets \( K \) and \( K^c \) is not aligned to any particular axis. In \( d > 1 \) dimensions, the CS approximation fails to converge since the coefficients are not sufficiently summable. On the other hand, the work [62] shows the Heaviside function in \( d \) dimensions given by \( H(x) = \mathbb{1}_{(0, \infty) \times \mathbb{R}^{d-1}}(x) \) can be approximated to \( L^2 \) accuracy \( \varepsilon^{1/2} \) by a 2-layer ReLU network with five nonzero weights taking value in \( \{\varepsilon^{-1}, 1, -1\} \). As the function (4.4) is a rotation of the \( d \)-dimensional Heaviside function, the result holds in this case as well.

Fig. 20 displays the results of approximating this function in 1, 2, and 4 dimensions. There we observe the lack of convergence of the CS approximations in \( d > 1 \). While the DNNs perform better than the CS approximations for this problem, none of the achieved results obtain more than 2 digits of accuracy. In the right plot of Fig. 20, we see the double descent behavior that has been observed in other works, see, e.g., [58, §7].
The gap between theory and practice.

Fig. 16. Legendre coefficients of $f$ from (4.3) with $d = 8$, sorted (left) lexicographically and (center) by decreasing magnitude. (right) Average relative $L^2$ error w.r.t. number of samples used in training. CS approximations were computed with the Legendre basis of cardinality $n = 3,023$.

Fig. 21 displays the average absolute maximum of the weights and biases in training the DNNs. There we observe that while on average the maximum weights are larger than those found for the smooth functions of the previous section, they remain bounded for the trained DNNs. Comparing to the aforementioned existence results, we note the weights never grow large enough in our experiments to obtain such high accuracy approximations in practice. Due to the initialization strategy chosen in this work to prevent failure during training, all of our networks start from an initial point corresponding to weights and biases close to 0. Combined with the training process which uses an initial learning rate of $10^{-3}$ which decays exponentially with the number of epochs, the algorithms may never reach a minimizer corresponding to higher-accuracy approximations of the halfspace function with larger weights.

5. Theoretical insights. We conclude this paper with some theoretical insights. Specifically, we first establish convergence rates for polynomial approximation via CS (Theorem 5.4) and then show a practical existence theorem for DL which demonstrates the existence of an architecture and training procedure that achieves the same rates (Theorem 5.5). Proofs in this section can be found in the Appendices.

5.1. Exponential convergence of polynomial approximations. In §2.3 we introduced the best $s$-term Legendre polynomial approximation. We first establish exponential rates of convergence of such approximations. To this end, let $E_\rho = \{(z + z^{-1})/2 : z \in \mathbb{C}, |z| \leq \rho \}$ be the Bernstein ellipse with parameter $\rho > 1$ and define the Bernstein polyellipse $B_\rho = \otimes_{j=1}^d E_{\rho_j}$, where $\rho = (\rho_1, \ldots, \rho_d) \geq 1$. This inequality is understood componentwise, i.e. $\rho \geq 1$ if and only if $\rho_j \geq 1$ for all $j$. We now make the following assumption:

Assumption 5.1. For some $\rho > 1$, the function $f : \mathcal{U} \to \mathbb{R}$ admits a holomorphic extension to an open set $\mathcal{O}$ containing $\mathcal{E}_\rho$.

Note that this is a reasonable assumption in practice: it is known that functions that arise as quantities of interest for a range of parametric PDEs admit holomorphic extensions [16,17].
Under Assumption 5.1, it is known that the Legendre polynomial coefficients satisfy

\[ |c_\nu| \leq \|u\|_{L^\infty(\xi_\rho)} \rho^{-\nu} \prod_{j=1}^d (1 + 2\nu_j)^{1/2}, \]

where \( \|u\|_{L^\infty(\xi_\rho)} = \sup_{z \in \xi_\rho} |f(z)| \) (see, for instance, the proof of Theorem 3.5 in [61]). When \( d = 1 \) this is a classical result in polynomial approximation, and guarantees convergence of the truncated expansion at an exponential rate \( \rho^{-s} \). When \( d > 1 \), it also clarifies why best \( s \)-term approximation is a suitable strategy; namely, unless the parameter \( \rho \) is known, it is difficult to make an \textit{a priori} choice of coefficients which lead to a fast rate of exponential convergence.

On the other hand, the following theorem shows favourable exponential rates of convergence for the best \( s \)-term approximation. It also reveals another important property; namely, that the prescribed rate can be achieved using an index set that is \textit{lower}. We recall that a set \( \Lambda \) of multi-indices is lower if, for any \( \nu \in \Lambda \) one has \( \mu \in \Lambda \) whenever \( \mu \leq \nu \) (this inequality is understood componentwise, i.e. \( \mu_j \leq \nu_j, \forall j \)). As discussed later, the lower set property is crucial for obtaining approximations using CS that attain the same rates.

For convenience, from now on we consider the \( s \)-term approximation error in the \( L^\infty \)-norm

\[ \text{Table of best-performing architectures for each choice of } \beta \text{ and number of parameters. CS approximations were computed with the Legendre basis of cardinality } n = 3,023. \]
on $U$. This is slightly more convenient for the subsequent analysis, although $L^2$-norm bounds could also be proved with some additional technicalities.

**Theorem 5.2.** Let $s \geq 1$ and $f$ satisfy Assumption 5.1 for some $\rho > 1$. Then there exists a lower set $\Lambda \subset \mathbb{N}_0^d$ of size at most $s$ for which

$$\|f - p\|_{L^\infty(U)} \leq C \exp \left( -\gamma s^{1/d} \right),$$

where $p = \sum_{\nu \in \Lambda} c_{\nu} \Psi_{\nu}$ and $C > 0$ depends on $d$, $\rho$, $\gamma$ and $f$ only, for any $\gamma$ satisfying

$$0 < \gamma < (d + 1)^{-1} \left( d! \prod_{j=1}^d \log(\rho_j) \right)^{1/d}. $$

This result asserts exponential convergence of the best $s$-term approximation at a rate depending on the product of $\log(\rho_j)$, as opposed to $\log(\rho_{\min})$, $\rho_{\min} = \min_j \{\rho_j\}$, which would arise if some fixed isotropic index set were used.

**Remark 5.3.** There are numerous results on the convergence rate of the best $s$-term polynomial approximation of holomorphic functions. Algebraic rates of convergence can be found

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**Figure 18.** Comparison of average absolute maximum of weights and biases w.r.t. number of samples of $f$ from (4.3) with $d = 8$ used in training ReLU architectures parameterized with $\beta = L/N$ (hidden layers/nodes per hidden layer) for values (top-left) $\beta = 0.5$, (top-middle) $\beta = 0.2$, (top-right) $\beta = 0.1$, (bottom-left) $\beta = 0.05$, and (bottom-right) $\beta = 0.025$. 
Figure 19. Comparison of training time vs. number of samples of $f(x)$ from (4.3) used in training for ReLU architectures parameterized with $\beta = L/N$ for values (left) 0.1, (middle) 0.05, and (right) 0.025.

Figure 20. Average relative $L^2$ error w.r.t. number of samples used in training ReLU DNNs and solving the CS problem with Legendre basis of cardinality $n$ in $d$ dimensions with (left) $d = 1$ and $n = 3,000$, (center) $d = 2$ and $n = 3,001$, and (right) $d = 4$ and $n = 3,079$.

in, for instance, [15, 16], for not only Legendre, but also Chebyshev and Taylor expansions. Notably, these results also extend to the case $d = \infty$, which theoretically permits the approximation of functions of infinitely-many variables. However, the constants in the error bounds may be large in practice [77]. The rates shown above – which are based on [17, Sec. 3.9] and [61] – possess the advantage of always being attained in lower sets. However, they may
also exhibit a poor scaling with $d$ in the constant $C$. For quasi-optimal error bounds and rates, see [7, 8, 77]. The results shown in [77] are asymptotically sharp as $s \to \infty$, hence they provide the optimal rate in the finite-dimensional setting.

5.2. Exponential convergence via compressed sensing. Theorem 5.2 prescribes exponential rates of convergence for the best $s$-term approximation. We now show that these rates can be achieved via CS. To do so, following [2], we now suppose that the CS approximation $\hat{f} = \sum_{\nu \in \Lambda} \hat{c}_\nu \Psi_\nu$ is computed by solving the so-called weighted square-root LASSO problem

$$\minimize_{z \in \mathbb{R}^n} \|z\|_1 + \mu \|Az - f\|_2,$$

rather than (2.8). The reasons for doing this are explained in §A.5.

**Theorem 5.4.** There exist universal constants $C_1, C_2 > 0$ such that the following holds. Suppose that $0 < \varepsilon < 1$, $m \geq C_1 L_{m,d,\varepsilon}$, where

$$L_{m,d,\varepsilon} = \log(2m) \left( \log^2(2m) \log(2d) + \log(2\varepsilon^{-1} \log(2m)) \right),$$

$x_1, \ldots, x_m$ are drawn independently from the uniformly measure on $U$,

$$1 \leq s \leq \sqrt{\frac{m}{C_1 L_{m,d,\varepsilon}}},$$

and $\Lambda = \Lambda_{s}^{HC}$ is as in (2.4). Then the following holds with probability at least $1 - \varepsilon$. Let $f : U \to \mathbb{R}$ satisfy Assumption 5.1 for some $\rho > 1$ and let $\hat{f} = \sum_{\nu \in \Lambda} \hat{c}_\nu \Psi_\nu$, where $\hat{c} = (\hat{c}_\nu)_{\nu \in \Lambda}$ is any minimizer of (5.3) with $\mu = \frac{12\sqrt{32}}{35}s$ and weights $u$ given by (2.9). Then

$$\|f - \hat{f}\|_{L^\infty(U)} \leq C_2 \cdot C \cdot \exp(-\gamma s^{1/d}),$$

for all $\gamma$ satisfying (5.2), where $C > 0$ is as in Theorem 5.2.

This theorem asserts that CS achieves the same rates as those guaranteed in Theorem 5.2, with a sample complexity that is (up to the logarithmic factor) quadratic in $s$. In particular,
scaling implied by (5.4) depends only on logarithmically on the dimension $d$. Hence, this estimate scales particularly well in higher dimensions.

It is important to note the key role the lower set property plays in this result. First, the union of all lower sets $S$ of cardinality at most $s$ is $\bigcup\{S : S \text{ lower, } |S| \leq s\} = \Lambda_{s}^{HC}$, i.e. the hyperbolic cross set of degree $s$. This is the rationale for choosing $\Lambda$ in this way. Second, much like how sparse sets are promoted by the $\ell^1$-norm, sparse and lower sets are promoted by the weighted $\ell^1$-norm, with the weights taken to be $u$ (these weights penalize high indices). Had one considered the unweighted $\ell^1$-norm in the above result, the sample complexity would have scaled with a higher algebraic power of $s$ [3].

5.3. Existence of good training for DNN approximation. We now give our main result:

Theorem 5.5. Let $0 < \delta, \varepsilon < 1$, $C_1 > 0$ and $L_{m,d,\varepsilon}$ be as in Theorem 5.4 and suppose that $m \geq C_1 L_{m,d,\varepsilon}$ and $s$ satisfies (5.4). Let $x_1, \ldots, x_m$ be drawn independently from the uniform measure on $\mathcal{U}$. Then the following holds with probability at least $1 - \varepsilon$. Let $f : \mathcal{U} \to \mathbb{R}$ satisfy Assumption 5.1 for some $\rho > 1$. Then there exists a family of neural networks $\mathcal{N}$ with $n = |\Lambda_{s}^{HC}|$ trainable parameters and of size and depth

$$\begin{align*}
\text{depth}(\Phi) &\leq C (1 + d \log(d))(1 + \log(s)) (s + \log(\sqrt{n}s)) \\
\text{size}(\Phi) &\leq C (d^2 s^3 + d^2 s^2 \log(2\sqrt{n}s) + d^2 n (1 + \log(s) + \log(\sqrt{n}s)))
\end{align*}$$

$\Phi \in \mathcal{N}$,

and a regularization functional $\mathcal{J} : \mathcal{N} \to \mathbb{R} \_+$ such that any minimizer $\tilde{\Phi}$ of the regularized loss function $\mathcal{L}(\Phi) := \sqrt{\frac{1}{m} \sum_{i=1}^{m} |\Phi(y_i) - f(y_i)|^2 + \mathcal{J}(\Phi)}$, satisfies

$$\|f - \tilde{\Phi}\|_{L^\infty(\mathcal{U})} \leq C_2 \cdot C \cdot \exp(-\gamma s^{1/4}),$$

for all $\gamma$ satisfying (5.2), where $C > 0$ is as in Theorem 5.4 and $C_2 > 0$ is a universal constant. The functional $\mathcal{J}$ is a weighted $\ell^1$-norm penalty of the weights in the output layer.

Note that in this result the size of an architecture refers to the number of nonzero weights and biases. The number of trainable parameters in an architecture refers to the number of weights and biases that are trainable, as opposed to those that are fixed. The proof of this theorem uses a result of [61] (see Proposition B.6), which states that a finite set of Legendre polynomials can be uniformly approximated by a neural network of a given depth and size. Theorem 5.5 is obtained by rewriting the CS recovery using the weighted square-root LASSO as a neural network training problem. See §B for the details.

Theorem 5.5 asserts the existence of a DNN architecture, with relatively few training parameters, and a training procedure for which the resulting DNN approximations are guaranteed to perform as well as CS, up to a constant, in terms of sample complexity and convergence rates. Of course, the specific procedure suggested by the proof would not be expected to lead to any superior performance over CS. We make no claim that this approach is either practical or numerically stable (indeed, its proof relies on monomials). This is analogous to how standard existence theorems in DNN approximation theory (see §1), while constructive, do not lead to superior approximations over the classical approximations on which they are based. However, it does indicate that with sufficiently careful architecture design and training, one may achieve superior performance with DNNs over CS. The extent to which this can be done is a largely open problem, requiring further theoretical and empirical investigation.
6. Conclusions. In this work we have presented results highlighting the key issues of accuracy, stability, sample complexity and computational efficiency of practical function approximation with DNNs. Our theoretical contribution on the existence of a DL procedure which performs as well as CS suggests that DL can, in theory, enjoy the same accuracy and sample complexity properties as CS. However, our numerical results comparing current methods of training DNNs with CS techniques suggest that current methods are generally unable to achieve these theoretical convergence rates. On the other hand, while DNNs perform relatively badly on sparser functions, their performance on more challenging problems, such as non-sparse functions or functions with jump discontinuities is rather more promising. Certainly the fact that the same DNN architectures can be used on quite different problems sets them apart from traditional methods in scientific computing, e.g. polynomial-based methods, which are usually tied to a specific class of function (e.g. smooth functions). Hence there is ample scope and need for future work along the lines of investigation initiated in this paper. This includes both empirical investigations into architecture and cost function design, as well as algorithms for training, and further novel theoretical insights into practical existence theory; that is, the existence of not only effective DNN architectures, but also training procedure and sampling strategies which realize them efficiently. The hope is that, with these further efforts, DNNs may develop into effective tools for scientific computing that can consistently outperform current best-in-class approaches for a range of challenging problems.

Appendix A. Testing setup – further information.

In this section, we give further details of the testing and training setup for the DNNs and numerical experiments with CS. Section A.1 describes the hardware used in training and testing our DNN models in single and double precision. Section A.2 describes further aspects of training our DNNs with the Adam solver. Section A.3 presents results on training DNNs with Adam under a variety of learning rate schedules. Section A.4 discusses the importance of batch size on the convergence of the Adam optimizer. Section A.5 describes the selection of truncation parameters in our CS experiments.

A.1. Single versus double precision. Double precision calculations using GPUs a generally more computationally demanding and hence we conducted a limited number of such studies. For example, the NVIDIA Tesla P100 GPUs operate at 4.7 TFLOPS (trillion floating point operations per second) in double precision vs. 9.3 TFLOPS in single precision, implying a 1:2 ratio for single vs. double precision computation time. On the other hand, common off-the-shelf consumer GPUs such as the NVIDIA GeForce GTX 1080 Ti operate at 0.355 TFLOPS in double precision vs. 11.5 TFLOPS in single precision, implying a 1:32 ratio for single vs. double precision computation time.

A.2. The Adam optimizer. We use the Adam optimizer [47] as follows. We use the default values $\beta_1 = 0.9$, $\beta_2 = 0.999$ and $\delta = 10^{-7}$, and set the initial learning rate $\tau_{\text{init}} = 10^{-3}$. Then at epoch $k \in \mathbb{N}$ we set the learning rate

$$\tau_k = \tau_{\text{init}} \times b^{k/K_{uf}},$$

where $K_{uf} = 10^3$ is the update frequency and $b := (\tau_{\text{final}}/\tau_{\text{init}})^{K_{uf}/K_{final}}$ is the base, so that at the final epoch $k = K_{\text{final}}$, $\tau_k = \tau_{\text{final}}$ the desired final learning rate. We allow the learning
rate \( \tau_k \) to vary continuously between \( \tau_{\text{init}} \) and \( \tau_{\text{final}} \), using the constants above only as scaling factors. In single precision, the DNNs are trained for \( K_{\text{final}} = 50,000 \) epochs or to a tolerance of \( \varepsilon_{\text{tol}} = 5 \times 10^{-7} \), while in double precision DNNs are trained for \( K_{\text{final}} = 200,000 \) epochs or to a tolerance of \( \varepsilon_{\text{tol}} = 5 \times 10^{-16} \). We set the final stepsize \( \tau_{\text{final}} = \varepsilon_{\text{tol}} \), so that these choices ensure that the base \( b \) is approximately 0.85, implying the learning rate is reduced by 15% every \( K_{\text{uf}} \) iterations.

A.3. Learning rate schedules for Adam. In Fig. 22 we compare learning rate schedules for the Adam optimizer on a discontinuous 2-dimensional function. The schedules compared are the exponentially decaying learning rate from (A.1), a constant learning rate of \( 10^{-3} \), and a linearly decaying learning rate, i.e., at each iteration setting \( \tau_k = (1 - k/K_{\text{final}})10^{-3} + k\tau_{\text{final}}/K_{\text{final}} \), over a range of DNN architectures. We observe that shallower networks tend to perform marginally better under the exponentially-decaying learning rate schedule, while the effect is insignificant for deeper networks. In testing a range of values of the base parameter \( b \), we found values smaller than \( b = 0.85 \) result in a learning rate that can decrease too quickly to achieve the desired tolerance with the error stagnating, while larger values of \( b \) can result in a learning rate not decreasing fast enough to quickly train larger models.

A.4. Batch size comparison. In many standard computer vision tasks, networks are trained on batches of images consisting of a small subset of the overall training set. Due to the lower dimension of the problems and smaller data set sizes considered herein, we find empirically that setting the batch size too small can result in the transfer time between the CPU and GPU contributing to a large portion of overall run time. Fig. 23 displays the effect of training four different architectures with batch sizes ranging from full-batch to quarter-batch on the generalization performance of the DNNs on a smooth 8-dimensional function. There we observe that decreasing the batch size leads to a marginal improvement in the overall error. Nonetheless for such moderate dimensional problems we find the increase in training time associated with smaller batches is not proportional to the improvement in the overall error. We leave a more detailed study of the affects of batch size on generalization performance of trained ReLU DNNs in higher-dimensional problems to a future work.

A.5. Truncation parameters in compressed sensing. In our numerical experiments, we solve the weighted (2.8) or unweighted (2.6) quadratically-constrained basis problems with truncation parameter chosen as in (3.2).
It is well-known that the accuracy of the quadratically-constrained basis pursuit is affected by the choice of \( \eta \), with it declining if \( \eta \) is too large or too small [12]. In (3.2), we chose \( \eta \) as small as possible such that the exact coefficients \( c_\Lambda \) are feasible for (2.6), which is in some sense an optimal choice. See [2] for further information. In practice, when the coefficients \( c_\nu \) cannot be feasibly computed, an alternative is to use cross validation, see, e.g., [28].

In our theoretical analysis in §5 we consider the weighted square-root LASSO problem (5.3). As discussed above, the choice of \( \eta \) in (3.2) depends on the unknown expansion coefficients \( c_\Lambda \), and more precisely, the expansion tail since \( f - Ac_\Lambda = e \), where \( e = \frac{1}{\sqrt{m}} (\sum_{\nu \in \Lambda} c_\nu \Psi_{\nu}(x_i))^{m} \). Hence, previous theoretical error estimates for polynomial approximations via CS often involve unrealistic assumptions on the size of this term [3, 14]. Much the same is true of the unconstrained LASSO (2.7), or its weighted variant. This problem was studied in [12], and in [2] the weighted square-root LASSO (5.3) was proposed as a solution. While far less well known than the LASSO, the square-root LASSO has the beneficial property that the optimal choice of its parameter \( \mu \) is independent of the noise term (i.e. the expansion tail), and depends only on the parameter \( s \) (this can be seen in Theorem 5.4). Hence, as shown in Theorem 5.4, it allows for explicit convergence rate estimates for CS, without unrealistic assumptions being imposed on the expansion tail.

On the other hand, in our experiments we continue to use (weighted) quadratically-constrained basis pursuit because it is the standard approach in the literature.

Appendix B. Proofs.
In this section, we present the proofs of Theorems 5.2, 5.4 and 5.5.

B.1. Proof of Theorem 5.2. The proof is based on techniques from [61, Sec. 3].

Proof of Theorem 5.2. It is clear from (5.1) that \( c \in \ell^1_u(N_d) \). Notice the following straightforward inequality

\[ \left\| f - \sum_{\nu \in \Lambda} c_\nu \Psi_{\nu} \right\|_{L^\infty} \leq \sum_{\nu \notin \Lambda} u_\nu |c_\nu|. \]

Hence it suffices to consider the right-hand side. Without loss of generality \( s \geq 2 \). Choose
0 < \epsilon < 1 such that

\[ s = \prod_{j=1}^{d} \left( \frac{\log(\epsilon^{-1})}{\log(\rho_j)} + 1 \right), \]

and define the lower set \( \Lambda = \{ \nu : \rho^{-\nu} \geq \epsilon \} \). In the proof of Theorem 3.5 in [61] it is shown that

\[ \sum_{\nu \notin \Lambda} u_\nu |c_\nu| \leq C \exp \left( -\beta |\Lambda|^{1/d} \right), \]

for any \( \beta \) satisfying

\[ 0 < \beta < \left( d! \prod_{j=1}^{d} \frac{\log(\rho_j)}{\log(\rho_j)} \right)^{1/d}, \]

where \( C > 0 \) depends on \( d, \rho, \beta \) and \( f \) only. We now derive upper and lower bounds for |\( \Lambda \)| in terms of \( s \). First, observe that

\[ \Lambda = \left\{ \nu \in \mathbb{N}_0^d : \sum_{j=1}^{d} \nu_j \frac{\log(\rho_j)}{\log(\rho_j) - \log(\epsilon^{-1})} \leq |\Lambda| \right\}, \]

and therefore

\[ \prod_{j=1}^{d} \left( 1 + \left\lfloor \frac{\log(\epsilon^{-1})}{d \log(\rho_j)} \right\rfloor \right) \leq |\Lambda| \leq \prod_{j=1}^{d} \left( 1 + \left\lfloor \frac{\log(\epsilon^{-1})}{\log(\rho_j)} \right\rfloor \right). \]

Hence

\[ s \geq \prod_{j=1}^{d} \left( \left\lfloor \frac{\log(\epsilon^{-1})}{\log(\rho_j)} \right\rfloor + 1 \right) \geq |\Lambda|, \]

and

\[ s \leq \prod_{j=1}^{d} \left( d \left\lfloor \frac{\log(1/e)}{d \log(\rho_j)} \right\rfloor + d + 1 \right) = \prod_{j=1}^{d} \left( \left\lfloor \frac{\log(1/e)}{d \log(\rho_j)} \right\rfloor + 1 \right) \prod_{j=1}^{d} \left( d + \frac{1}{\left\lfloor \frac{\log(1/e)}{d \log(\rho_j)} \right\rfloor + 1} \right), \]

which gives \( s \leq |\Lambda| (d + 1)^d \). Therefore

\[ s(d + 1)^{-d} \leq |\Lambda| \leq s. \]

Returning to (B.1), we deduce that

\[ \sigma_{s(\epsilon)}(c)_{1, \eta} \leq C \exp \left( -\beta |\Lambda|^{1/d} \right) \leq C \exp \left( -\beta s^{1/d} / (d + 1) \right) = C \exp \left( -\gamma s^{1/d} \right). \]

This completes the proof.
B.2. Compressed sensing for lower set recovery. The proofs of Theorem 5.4 and 5.5 require some elements of compressed sensing theory, which we now introduce. We note that many of the constructions developed below apply more generally (for instance, to other measures \( \varrho \) and other orthonormal systems). However, for simplicity, we focus only on the case of Legendre polynomials. What follows is based primarily on \([2,3,14,63]\).

Since our focus is on lower set recovery, the setup differs to the standard compressed sensing framework (see, e.g., \([33]\)) for the recovery of arbitrary \( s \)-sparse vectors. Let \( s \geq 1 \) and recall that the union of all lower sets of cardinality at most \( s \) is the hyperbolic cross index set \( \Lambda = \Lambda^\text{HC}_s \), defined by (2.4). Write \( n = |\Lambda^\text{HC}_s| \). Throughout this section, we consider vectors in \( \mathbb{C}^n \) indexed over \( \Lambda \).

Define intrinsic lower sparsity of order \( s \) by

\[
K(\cdot) := \max \left\{ |S|_u : S \subseteq \Lambda, |S| \leq s, S \text{ lower} \right\},
\]

where

\[
|S|_u := \sum_{\nu \in S} u_\nu^2
\]

is the weighted cardinality of a subset \( S \) with respect to the weights \( u \) \([63]\). Note that \( K(s) \) is bounded, and satisfies

\[
s^2/4 \leq K(s) \leq s^2,
\]

for weights \( u \) as in (2.9). See, for example, \([2, \text{Lem. 2.2}]\). Given this, we define the best \( s \)-term and lower approximation error as

\[
\sigma_{s,L}(c) = \inf \left\{ \|c - c_S\|_{1,u} : S \subset \mathbb{N}_0^n, |S|_u \leq K(s) \right\}.
\]

Note that here and henceforth, we use \( c_S \) to denote either the vector \( c_S \in \mathbb{C}^n \) with \( \nu \)-th entry equal to \( c_\nu \) if \( \nu \in S \) and zero otherwise, or the vector \( c_S = (c_\nu)_{\nu \in \Lambda} \in \mathbb{C}^{|\Lambda|} \). The precise meaning will be clear from the context.

We now require the following (see \([14]\) or \([2, \text{Defn. 5.3}]\)):

**Definition B.1 (Lower robust null space property).** Given \( 0 < \rho < 1 \) and \( \tau > 0 \), a matrix \( A \in \mathbb{C}^{m \times n} \) is said to have the lower robust null space property (lower rNSP) of order \( s \) if

\[
\|z_S\|_2 \leq \frac{\rho}{\sqrt{K(s)}} \|z_{S^c}\|_{1,u} + \tau \|Az\|_2, \quad \forall z \in \mathbb{C}^n,
\]

for any \( S \subseteq \Lambda \) such that \( |S|_u \leq K(s) \), where \( K(s) \) is defined as in (B.2).

The lower rNSP is sufficient to provide a recovery guarantee for the weighted square-root LASSO decoder (5.3). In fact, although we shall not do it, this property also provides recovery guarantees for the decoders (2.6) and (2.7); see \([2]\).

**Theorem B.2.** Suppose that \( A \in \mathbb{C}^{m \times n} \) satisfies the lower rNSP of order \( s \) with constants \( 0 < \rho < 1 \) and \( \tau > 0 \). Let \( c \in \mathbb{C}^n \) and \( y = Ac + e \in \mathbb{C}^m \) for some \( e \in \mathbb{C}^m \) and consider the
the weighted square-root LASSO problem (5.3) with parameter $$\mu \geq \frac{2\tau}{1 + \rho} \sqrt{K(s)}.$$

Then

$$\|c - \hat{c}\|_{1,u} \leq \frac{1 + \rho}{1 - \rho} \sigma_{s,L}(c)_{1,u} + \left(\frac{1 + \rho}{1 - \rho} \mu + \frac{2\tau\sqrt{K(s)}}{1 - \rho}\right) \|e\|_2.$$ 

Proof. By [2, Thm. 5.6], we have

$$\|c - \hat{c}\|_{1,u} \leq \frac{1 + \rho}{1 - \rho} \sigma_{s,L}(c)_{1,u} + \left(\frac{1 + \rho}{1 - \rho} \mu + \frac{2\tau\sqrt{K(s)}}{1 - \rho}\right) \|e\|_2.$$ 

Since $$\hat{c}$$ is a minimizer, we obtain

$$\|c - \hat{c}\|_{1,u} \leq \frac{1 + \rho}{1 - \rho} \sigma_{s,L}(c)_{1,u} + \left(\frac{1 + \rho}{1 - \rho} \mu + \frac{2\tau\sqrt{K(s)}}{1 - \rho}\right) \|e\|_2,$$

and by assumption on $$\mu$$ we deduce that

$$\|c - \hat{c}\|_{1,u} \leq \frac{1 + \rho}{1 - \rho} \sigma_{s,L}(c)_{1,u} + \left(\frac{1 + \rho}{1 - \rho} \mu + \frac{2\tau\sqrt{K(s)}}{1 - \rho}\right) \|e\|_2,$$

as required. \qed

We note in passing one can also provide recovery guarantees in the 2-norm. See, for instance, [2]. In practice, it is difficult to work directly with the lower rNSP. Hence we consider the following (see [14] or [2, Defn. 5.3]):

Definition B.3 (Lower restricted isometry property). A matrix $$A \in \mathbb{C}^{m \times n}$$ is said to have the lower restricted isometry property of order $$s$$ if there exists a constant $$0 < \delta < 1$$ such that

$$(1 - \delta)\|z\|_2^2 \leq \|Az\|_2^2 \leq (1 + \delta)\|z\|_2^2, \quad \forall z \in \mathbb{C}^n, |\text{supp}(z)|_u \leq K(s),$$

where $$\text{supp}(z) := \{\nu \in \Lambda : z_\nu \neq 0\}$$ and $$|\text{supp}(z)|_u$$ is its weighted cardinality defined as in (B.3). The smallest constant such that this property holds is called the $$s$$th lower restricted isometry constant of $$A$$ and it is denoted as $$\delta_{s,L}$$.

The following result, see [14] or [2, Lem. 5.4], asserts that the lower restricted isometry property is a sufficient condition for the lower rNSP:

Lemma B.4. Let $$s \geq 2$$ and suppose $$A \in \mathbb{C}^{m \times n}$$ satisfies the lower restricted isometry property (with $$K(s)$$ as in (B.2) for weights (2.9)) of order $$2s$$ with constant $$\delta_{2s,L} < 1/5$$. Then $$A$$ has the lower rNSP of order $$s$$ with constants $$\rho = \frac{4\delta}{1 - \delta}$$ and $$\tau = \frac{\sqrt{1 + \delta}}{2(1 - \delta)}$$. 

Finally, we also need a result asserting the lower restricted isometry property for the measurement matrix (2.5). The following result was first proved in [14]. See, for example, [2, Thm. 5.5]:

**Theorem B.5.** Let $0 < \delta, \varepsilon < 1$ and suppose that

$$m \geq C \cdot K(s) \cdot L(s, \delta, \varepsilon),$$

where $K(s)$ is as in (B.2), $C > 0$ is a universal constant,

$$L(s, \delta, \varepsilon) = \frac{1}{\delta^2} \ln \left( \frac{K(s)}{\delta^2} \right) \max \left\{ \frac{1}{\delta^4} \ln \left( \frac{K(s)}{\delta^2} \right), \frac{1}{\delta} \ln \left( \frac{1}{\delta \varepsilon} \ln \left( \frac{K(s)}{\delta^2} \right) \right) \right\},$$

and $n = |\Lambda^{HC}|$. Let $x_1, \ldots, x_m$ be drawn independently according to the uniform measure on $U$ and consider the matrix $A$ defined in (2.5), where $\{\Psi_\nu\}_{\nu \in \Lambda}$ is the orthonormal Legendre polynomial basis. Then, with probability at least $1 - \varepsilon$, $A$ satisfies the lower RIP of order $s$ with constant $\delta s, L \leq \delta$.

**B.3. Proof of Theorem 5.4.** We now give the proof of Theorem 5.4. First, we recall the following inequality for the cardinality of the hyperbolic cross index set:

$$n = |\Lambda^{HC}| \leq \min\{2s^34^d, e^2s^2+\log_2(d)\}$$

See, for example, [2, Eqn. (17)].

**Proof of Theorem 5.4.** We claim that, with probability at least $1 - \varepsilon$, the matrix $A$ has the lower restricted isometry property of order $2s$ with constant $\delta \leq \delta_{2s,L} = 1/6$. Suppose this claim is true. Then Lemma B.4 gives that it satisfies the lower rNSP with constants $\rho = 4/5$ and $\tau = \sqrt{42}/5$. Also, by this and (B.4),

$$\frac{2\tau}{1 + \rho} \sqrt{K(s)} \leq \frac{12\sqrt{42}}{35} s = \mu.$$

Hence Theorem B.2 gives

$$\|f - \hat{f}\|_{L^\infty(U)} \leq \|c - \hat{c}\|_{1,u} \leq C_2 (\sigma_{s,L}(c)_{1,u} + s\|e\|_2).$$

Recall by definition that

$$\|e\|_2 = \sqrt{\frac{1}{m} \sum_{i=1}^{m} \left| f(x_i) - \sum_{\nu \in \Lambda} c_\nu \Psi_\nu(x_i) \right|^2} \leq \left\| f - \sum_{\nu \in \Lambda} c_\nu \Psi_\nu \right\|_{L^\infty(U)} \leq \|c - \hat{c}\|_{1,u} \leq \sigma_{s,L}(c)_{1,u}.$$}

Hence, by Theorem 5.2,

$$\|f - \hat{f}\|_{L^\infty(U)} \leq C_2 (1 + s)C \exp \left(-\gamma s^{1/d}\right).$$
Since this holds for all \( \gamma \) satisfying (5.2), and since the exponential term dominates as \( s \to \infty \), we deduce (after possible change of \( C \)) that
\[
\| f - \tilde{f} \|_{L^\infty(U)} \leq C_2 C \exp\left( -\gamma s^{1/d} \right).
\]

To complete the proof, it remains to prove the claim. Let \( L(2s, \delta_{2s,L}, \varepsilon) \) be the log factor in Theorem B.5. Then, since \( \delta_{2s,L} = 1/6 \) and \( K(s) \leq s^2 \) by (B.4), we have
\[
L(2s, \delta_{2s,L}, \varepsilon) \leq C_1 \log(2s) \max\{ \log(2s) \log(n), \log(2\varepsilon^{-1} \log(2s)) \}.
\]

Note that \( \log(2s) \log(2s) \leq \log(4s^2) = 2 \log(2s) \). Using this and the estimate (B.5) for \( n = |\Lambda_{HC}^s| \) we obtain
\[
L(2s, \delta_{2s,L}, \varepsilon) \leq C_1 \log(2s) \left( \log(2m) + \log(2\varepsilon^{-1} \log(2m)) \right) = C_1 L_{m,d,\varepsilon},
\]
for possibly different constant \( C_1 > 0 \). Hence
\[
m \geq C_1 \cdot s^2 \cdot L_{m,d,\varepsilon} \geq C_1 \cdot s^2 \cdot L(2s, \delta_{2s,L}, \varepsilon).
\]
The claim now follows immediately from Theorem B.5.

### B.4. Proof of Theorem 5.5

We make use of the following result, which can be found in [61, Prop. 2.10]:

**Proposition B.6.** For every finite subset \( \Lambda \subset \mathbb{N}_0^d \) and every \( 0 < \delta < 1 \) there exists a ReLU neural network \( \Phi_{\Lambda,\delta}: \mathbb{R}^d \to \mathbb{R}^{|\Lambda|} \) such that, if \( \Phi_{\nu,\delta} = (\Phi_{\nu,\delta})_{\nu \in \Lambda} \), then
\[
\| \Psi_{\nu} - \Phi_{\nu,\delta} \|_{L^\infty(U)} \leq \delta.
\]

The depth and size of this network satisfy
\[
\text{depth}(\Phi_{\Lambda,\delta}) \leq C \left( 1 + d \log(d) \right) \left( 1 + m(\Lambda) \log(\Lambda) \right) \text{ log}(\log(\log(\log(\log(\log(\log(\log(n))))))),
\]
\[
\text{size}(\Phi_{\Lambda,\delta}) \leq C \left( d^2 m(\Lambda)^3 + d^2 m(\Lambda)^2 \text{ log}(\log(\log(\log(\log(\log(\log(\log(\log(n)))))))) \right) + d^2 |\Lambda| \left( 1 + m(\Lambda) \log(\log(\log(\log(\log(\log(\log(\log(n)))))))) \right).
\]

where \( m(\Lambda) = \max_{\nu \in \Lambda} \| \nu \|_1 \).

The general idea of the proof is to use Proposition B.6 to approximately express matrix-vector multiplication \( Az \) as a neural network \( \Phi \) evaluated at the sample points \( x_i \) and then use the compressed sensing results to establish an error bound. Since this process commits an error, we first require the following result, which shows that the lower rNSP is robust to small matrix perturbations:
Lemma B.7. Suppose that $A \in \mathbb{C}^{m \times n}$ satisfies the lower rNSP of order $s$ with constants $0 < \rho < 1$ and $\tau > 0$ and let $A' \in \mathbb{C}^{m \times n}$ satisfy

$$
\|A - A'\|_2 \leq \sigma, \quad \sigma < \frac{1 - \rho}{\tau(\sqrt{K(s)} + 1)}.
$$

Then $A'$ satisfies the lower rNSP of order $s$ with constants $0 < \rho' < 1$ and $\tau$, where

$$
\rho' \leq \rho + \tau\sigma\sqrt{K(s)}.
$$

Proof. Let $z \in \mathbb{C}^n$ and $S$ satisfy $|S|_u \leq K(s)$. Then

$$
\|zS\|_2 \leq \frac{\rho}{\sqrt{K(s)}} \|zS_c\|_{1,u} + \tau\|Az\|_2
\leq \frac{\rho}{\sqrt{K(s)}} \|zS_c\|_{1,u} + \tau\|A'z\|_2 + \tau\sigma\|z\|_2
\leq \frac{\rho}{\sqrt{K(s)}} \|zS_c\|_{1,u} + \tau\|A'z\|_2 + \tau\sigma\|z\|_2 + \tau\sigma\|zS_c\|_2.
$$

Hence

$$
(1 - \tau\sigma)\|zS\|_2 \leq \left(\frac{\rho}{\sqrt{K(s)}} + \tau\sigma\right) \|zS_c\|_{1,u} + \tau\|A'z\|_2.
$$

The result now follows immediately.

Proof of Theorem 5.5. Let $\Lambda = \Lambda_s^{HC}$ and $\Phi_{\Lambda,\delta}$ be as in Proposition B.6, where

$$
\delta = \frac{5/\sqrt{42}}{\sqrt{n}(9 + 10s)}.
$$

Notice that

$$
\|
u\|_1 \leq \prod_{j=1}^d (\nu_j + 1) - 1 \leq s, \quad \nu \in \Lambda,
$$

and therefore $m(\Lambda) \leq s$, which gives

$$
\text{depth}(\Phi_{\Lambda,\delta}) \leq C(1 + d \log(d))(1 + \log(s))(s + \log(\delta^{-1}))
$$

and

$$
\text{size}(\Phi_{\Lambda,\delta}) \leq C \left( d^2 s^3 + d^2 s^2 \log(\delta^{-1}) + d^2 n \left( 1 + \log(s) + \log(\delta^{-1}) \right) \right).
$$

Now define the family of neural networks

$$
\mathcal{N} = \left\{ \Phi : x \mapsto z^\top \Phi_{\Lambda,\delta}(x), \ z \in \mathbb{R}^n \right\}.
$$
Notice that this family has \( n \) trainable parameters, and \( \text{depth}(\Phi) = \text{depth}(\Phi_{\Lambda,\delta}) + 1 \) and \( \text{size}(\Phi) = \text{size}(\Phi_{\Lambda,\delta}) + n \) for \( \Phi \in \mathcal{N} \). For \( \Phi \in \mathcal{N} \), let \( \mathcal{J}(\Phi) = \mu^{-1}\|z\|_{1,u} \), where \( \mu = \frac{5\sqrt{42}}{9+10s} \).

Then observe that
\[
\Phi(x) = \sum_{\nu \in \Lambda} z_{\nu} \Psi_{\nu,\delta}(x).
\]
and therefore
\[
\mathcal{L}(\Phi) = \|A'z - f\|_2 + \mu^{-1}\|z\|_{1,u}, \quad A' = \frac{1}{\sqrt{m}} (\Psi_{\nu}(x_i))_{1 \leq i \leq m}.
\]

Hence \( \hat{\Phi} = c^\top \Phi_{\Lambda,\delta} \) is a minimizer of \( \mathcal{L} \) over \( \mathcal{N} \) if and only if \( c \) is a minimizer of
\[
\min_{z \in \mathbb{R}^n} \|z\|_{1,u} + \mu\|A'z - f\|_2.
\]

We seek to use Lemma B.7 and relate \( A' \) to the matrix \( A \). Observe that
\[
\| (A - A')z \|_2^2 = \frac{1}{m} \sum_{i=1}^m \left| \sum_{\nu \in \Lambda} z_{\nu} (\Psi_{\nu}(x_i) - \Psi_{\nu,\delta}(x_i)) \right|^2 \leq \sum_{\nu \in \Lambda} \|\Psi_{\nu} - \Psi_{\nu,\delta}\|_{L^\infty(\mathcal{U})}^2 \|z\|_2^2 \leq n\delta^2 \|z\|_2^2.
\]

Hence, by the conditions on \( \delta \),
\[
\|A - A'\|_2 \leq \sqrt{n}\delta \leq \sigma := \frac{5\sqrt{42}}{9+10s}.
\]

As in the proof of Theorem 5.4, the conditions on \( m \) assert that \( A \) has the lower rNSP of order \( s \) with constants \( \rho = 4/5 \) and \( \tau = \sqrt{42}/5 \). Therefore, by Lemma B.7, \( A' \) has the lower rNSP of order \( s \) with constants \( \rho' \) and \( \tau = \sqrt{42}/5 \), where
\[
\rho' \leq \frac{\rho + \tau \sigma s}{1 - \tau \sigma} \leq 9/10.
\]

For the remainder of the proof, we follow the same arguments as in proof of Theorem 5.4. \( \blacksquare \)

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