A PRIORI ANALYSIS OF STABLE NEURAL NETWORK SOLUTIONS TO NUMERICAL PDEs

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May 11, 2021

ABSTRACT

Methods for solving PDEs using neural networks have recently become a very important topic. We provide an a priori error analysis for such methods which is based on the \( \mathcal{H}_1(D) \)-norm of the solution. We show that the resulting constrained optimization problem can be efficiently solved using a greedy algorithm, which replaces stochastic gradient descent. Following this, we show that the error arising from discretizing the energy integrals is bounded both in the deterministic case, i.e. when using numerical quadrature, and also in the stochastic case, i.e. when sampling points to approximate the integrals. In the later case, we use a Rademacher complexity analysis, and in the former case we use standard numerical quadrature bounds. This extends existing results to methods which use a general dictionary of functions to learn solutions to PDEs and importantly gives a consistent analysis which incorporates the optimization, approximation, and generalization aspects of the problem. In addition, the Rademacher complexity analysis is simplified and generalized, which enables application to a wide range of problems.

1 Introduction

Recently, due to the dramatic success of deep learning, neural networks have been studied for their potential in solving high-dimensional partial differential equations [16, 27, 39, 41]. Despite remarkable empirical success in using neural networks for solving PDEs [32, 49, 52], there are many open theoretical questions concerning the numerical analysis of the resulting methods. There has been much recent work on these problems, see for instance [4, 10, 17, 19, 23, 31, 33, 35, 36, 38, 42, 46, 50, 51]. In these papers, different aspects of the problem are addressed, specifically the approximation, generalization, and optimization theory behind these methods. However, as far as we know, no rigorous analysis is able to take into account all of these aspects simultaneously. In this work, we provide the first consistent analysis which takes into account all three aspects of the problem: approximation, generalization, and optimization. Our analysis relies heavily upon the notions developed in [44], specifically the \( \mathcal{H}_1(D) \)-space. It depends upon the exact solution lying in \( \mathcal{H}_1(D) \), and also on the solution of a optimization problems of fixed dimension (see equation (31) below), which we argue are more tractable than optimizing the whole network (for instance via gradient descent), and which can provably be solved for shallow neural networks [25].

We consider solving 2m-th order elliptic PDEs using finite combinations of dictionary elements for a dictionary \( D \subset H^m(\Omega) \). Our approach combines the approximation theory developed in [1, 22, 43] with a Rademacher complexity analysis [3] to obtain error bounds on the discrete solution when Monte Carlo quadrature is used. We only require the true solution to be bounded in the \( \mathcal{H}_1(D) \)-norm, and when high-order numerical quadrature is used, we require the dictionary elements and the coefficients of the PDE to be sufficiently smooth. We use such a non-standard smoothness assumption because this is the only way to overcome the ‘curse of dimensionality.’ Indeed, in high dimensions the metric entropy of classical smoothness spaces, i.e. spaces defined by \( L^p \)-norm bounds on derivatives, decay very slowly [30]. However, in order to obtain methods which scale well with dimension, we must assume our solution is bounded in space whose entropy decays at a rate independent of dimension, which rules out classical smoothness
We follow here largely the setting in \[53\]. Let \(\Omega\) be a bounded domain with a sufficiently smooth boundary \(\partial \Omega\). For any integer \(m \geq 1\), we consider the following model 2\(m\)-th order partial differential equation with certain boundary conditions:

\[
\begin{aligned}
Lu &= f \quad \text{in } \Omega, \\
B^k(u) &= 0 \quad \text{on } \partial \Omega \quad (0 \leq k \leq m-1),
\end{aligned}
\]

(1)

where \(B^k(u)\) denotes the Dirichlet, Neumann, or mixed boundary conditions which will be discussed in detail in the following. Here \(L\) is the partial differential operator defined as follows

\[
Lu = \sum_{|\alpha| = m} (-1)^{m} \partial^\alpha (a_\alpha(x) \partial^\alpha u) + a_0(x)u,
\]

(2)

where \(\alpha\) denotes \(n\)-dimensional multi-index \(\alpha = (\alpha_1, \cdots, \alpha_n)\) with

|\(\alpha| = \sum_{i=1}^{n} \alpha_i, \quad \partial^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}}.

For simplicity, we assume that \(a_\alpha\) are strictly positive and bounded on \(\Omega\) for \(|\alpha| = m\) and \(\alpha = 0\), namely, \(\exists a_0 > 0, \alpha_1 < \infty\), such that

\[
a_0 \leq a_\alpha(x), a_0(x) \leq a_1 \quad \forall x \in \Omega, \quad |\alpha| = m.
\]

(3)

Further, when considering deterministic numerical quadrature in Section \(5\) we will make the additional assumption that \(a_\alpha \in C^\infty(\Omega)\).

Given a nonnegative integer \(k\) and a bounded domain \(\Omega \subset \mathbb{R}^d\), let

\[
H^k(\Omega) := \{ v \in L^2(\Omega), \partial^\alpha v \in L^2(\Omega), |\alpha| \leq k \}
\]

(4)

be standard Sobolev spaces with norm and seminorm given respectively by

\[
||v||_k := \left( \sum_{|\alpha| \leq k} ||\partial^\alpha v||_0^2 \right)^{1/2}, \quad |v|_k := \left( \sum_{|\alpha| = k} ||\partial^\alpha v||_0^2 \right)^{1/2}.
\]
For $k = 0$, $H^0(\Omega)$ is the standard $L^2(\Omega)$ space with the inner product denoted by $(\cdot, \cdot)$. Similarly, for any subset $K \subset \Omega$, $L^2(K)$ inner product is denoted by $(\cdot, \cdot)_{0,K}$. We note that, by a well-known property of Sobolev spaces, the assumption (3) implies that

$$a(v, v) \geq \|v\|^2_{m, \Omega}, \forall v \in H^m(\Omega). \tag{5}$$

Next, we discuss the boundary conditions in detail. A popular type of boundary conditions are Dirichlet boundary condition when $B^k = B^k_D$ are given by the following Dirichlet type trace operators

$$B^k_D(u) := \frac{\partial^k u}{\partial \nu^k}|_{\partial \Omega} \quad (0 \leq k \leq m - 1), \tag{6}$$

with $\nu$ being the outward unit normal vector of $\partial \Omega$.

For the aforementioned Dirichlet boundary condition, the elliptic boundary value problem (1) is equivalent to

Minimization Problem M: Find $u \in H^m_0(\Omega)$ such that

$$J(u) = \min_{v \in H^m_0(\Omega)} J(v), \tag{7}$$

with the energy function $J$ defined by

$$J(v) = \frac{1}{2}a(v, v) - \int \Omega fvdx, \tag{8}$$

and

$$a(u, v) := \sum_{|\alpha| = m} (a_{\alpha} \partial^\alpha u, \partial^\alpha v)_{0, \Omega} + (a_0 u, v). \tag{9}$$

Enforcing the boundary conditions for $H^m_0(\Omega)$ in (7), while relatively easy for finite element methods, is difficult or impossible when using neural networks. As a result, we consider first the pure Neumann boundary conditions, which is equivalent to the minimization problem (7) over the whole space $H^m(\Omega)$:

Minimization Problem N: Find $u \in H^m(\Omega)$ such that

$$u = \arg\min_{v \in H^m(\Omega)} J(v), \tag{10}$$

with energy function $J$ defined by (8).

In this sense, the pure Neumann boundary conditions are the most natural and easiest to enforce, especially when optimizing over the class of neural network functions. It remains to be determined which form the pure Neumann boundary conditions, which we denote by $B^k_N$, take when $m \geq 2$. This is given by the following result, which applies to any PDE operator (2).

**Lemma 1.** [53, Lemma 5.1] For each $k = 0, 1, \ldots, m - 1$, there exists a bounded linear differential operator of order $2m - k - 1$:

$$B^k_N : H^{2m}(\Omega) \mapsto L^2(\partial \Omega) \tag{11}$$

such that the following identity holds

$$(Lu, v) = a(u, v) - \sum_{k=0}^{m-1} \langle B^k_N(u), B^k_D(v) \rangle_{0, \partial \Omega}. \tag{12}$$

Namely

$$\sum_{|\alpha| = m} (-1)^m (\partial^\alpha (a_{\alpha} \partial^\alpha u), v)_{0, \Omega} = \sum_{|\alpha| = m} (a_{\alpha} \partial^\alpha u, \partial^\alpha v)_{0, \Omega} - \sum_{k=0}^{m-1} \langle B^k_N(u), B^k_D(v) \rangle_{0, \partial \Omega} \tag{12}$$

for all $u \in H^{2m}(\Omega), v \in H^m(\Omega)$. Furthermore,

$$\sum_{k=0}^{m-1} \|B^k_D(u)\|_{L^2(\partial \Omega)} + \sum_{k=0}^{m-1} \|B^k_N(u)\|_{L^2(\partial \Omega)} \lesssim \|u\|_{2m, \Omega}. \tag{13}$$
We are now in a position to state the pure Neumann boundary value problems for the PDE operator (2):

\[
\begin{aligned}
& Lu = f \quad \text{in } \Omega, \\
& B_k^N(u) = 0 \quad \text{on } \partial \Omega \quad (0 \leq k \leq m - 1).
\end{aligned}
\]

(14)

In light of the previous result, we note that problem (14) is equivalent to the optimization (10).

In order to handle Dirichlet boundary conditions, we consider the mixed boundary value problem:

\[
\begin{aligned}
& Lu_\delta = f \quad \text{in } \Omega, \\
& B_k^D(u_\delta) + \delta B_k^N(u_\delta) = 0 \quad (0 \leq k \leq m - 1).
\end{aligned}
\]

(15)

It is well-known that (15) is equivalent to the following optimization problem:

\[
\begin{aligned}
u_\delta = \arg \min_{v \in H^m(\Omega)} J_\delta(v)
\end{aligned}
\]

where

\[
J_\delta(v) = \frac{1}{2} a_\delta(v, v) - (f, v)
\]

(17)

and

\[
a_\delta(u, v) = a(u, v) + \delta^{-1} \sum_{k=0}^{m-1} (B_k^D(u), B_k^D(v))_{0, \partial \Omega}.
\]

(18)

In order to handle the Dirichlet conditions, we will let \( \delta \to 0 \) and use the theory developed in [53], specifically Lemma 5.4.

The further analysis in this paper will require that the solution \( u \) of the above problem be bounded in the \( K_1(D) \)-norm (recall the \( \mathcal{X}_1(D) \) space studied in [44]). We note that the results in [44] combined with the standard regularity theory for linear elliptic problems implies this if the coefficients \( a_\alpha \) and \( a_0 \) are smooth (see Lemma 5.5 and 5.6 in [53]).

### 2.2 Convex Dictionary Spaces

In order to approximate the solutions of (14) and (16), we aim to minimize the objective defined in (8) over a parameterized class of functions with finitely many parameters, i.e. to solve

\[
\begin{aligned}
u_n = \arg \min_{u \in V_n} J(u),
\end{aligned}
\]

where \( V_n \subset H^m(\Omega) \) is the set of functions parameterized by finitely many parameters. For instance, in the traditional conforming finite element method, \( V_n \) is taken to be a finite element space. We note that the minimizer above may not be unique, but we write equality by abuse of notation.

In our approach, we take the set of functions parameterized by finite expansions with respect to a dictionary \( D \subset H^m(\Omega) \). Specifically, we consider the set

\[
\Sigma_{n,M}(D) = \left\{ \sum_{i=1}^n a_i d_i, d_i \in D, \sum_{i=1}^n |a_i| \leq M \right\}.
\]

(20)

Note that here we restrict the \( \ell^1 \)-norm of the coefficients \( a_i \) in the expansion. This is necessary when we approximate the integrals in (8) by random sampling in order to control the random errors which are incurred. This means that

\[
\bigcup_{n=1}^\infty \Sigma_{n,M}(D) = \{ f \in H^m(\Omega) : \| f \|_{\mathcal{X}_1(D)} \leq M \},
\]

(21)

where \( \mathcal{X}_1(D) \) is the space introduced in [7] and studied further in [44], which for the dictionary of rectified linear ridge functions is equivalent to the Barron space introduced in [11, 34]. For a traditional conforming finite element method, this closure would be \( H^m(\Omega) \). In our method, \( M \) is a parameter which must be adjusted depending upon the number of sample points used to approximate the integrals in (8). This is analogous to a regularization parameter in statistical learning.
2.2.1 A counterexample to a Bernstein-type inequality for neural networks

Here we give a counterexample to a Bernstein-type inequality for the spaces $\Sigma_{n,M}(\mathbb{D})$ for $\mathbb{D} = \{\text{ReLU}(x+b), b \in [-2,2]\}$. Bernstein’s inequality shown that for polynomials or trigonometric polynomials, higher order derivatives can be bounded in terms of lower order derivatives, with a constant depending upon the degree of the polynomial. For example, if $T_d$ is a trigonometric polynomial of degree $d$, then
\[
\|T_d\|_{L^2} \leq n \|T_d\|_{L^2}.
\]
Bernstein-type inequalities, i.e. inequalities which bound higher order derivatives in terms of lower order derivatives for certain classes of functions are an important tool in characterizing approximation spaces (see [8], Chapter 7, for instance). Consequently, a natural question is whether or not a Bernstein-type inequality can hold for the class of functions $\Sigma_{n,M}(\mathbb{D})$, with a constant potentially depending upon both $n$ and $M$. The following proposition shows that such an inequality cannot exist.

**Proposition 1.** For each $\epsilon > 0$, there exists a $u_\epsilon \in \Sigma_{3,4}(\mathbb{D})$ for $\mathbb{D} = \{\text{ReLU}(x+b), b \in [-2,2]\}$ which satisfies
\[
\|u_\epsilon\|_{L^2([-1,1])} \geq \sqrt[3]{\epsilon^{-1}} \|u_\epsilon\|_{L^2([-1,1])},
\]

**Proof.** Consider the function
\[
 u_\epsilon(x) = \text{ReLU}(x+\epsilon) - 2\text{ReLU}(x) + \text{ReLU}(x-\epsilon), \quad x \in [-1,1].
\]
Clearly $u_\epsilon \in \Sigma_{3,4}(\mathbb{D})$ for $\mathbb{D} = \{\text{ReLU}(x+b), b \in [-2,2]\}$ and a direct calculation shows that
\[
\|u_\epsilon\|_{L^2([-1,1])} = \sqrt[3]{\epsilon^{-1}}, \quad \|u_\epsilon\|_{L^2([-1,1])} = \frac{\sqrt[3]{\epsilon}}{\sqrt{3}},
\]
which completes the proof.

\[\square\]

3 Monte Carlo Sampling

In this section, we describe and analyze a procedure for approximating the integrals in (8) and (16) in high dimensions $d$.

We consider first the case of the pure Neumann boundary conditions (8). In this case, we sample points $\partial \nu$ which completes the proof.

For the case of mixed boundary conditions (16) we sample $\partial \nu$, which is compact by the Heine-Borel Theorem. Thus the optimization is effectively over a bounded set in a finite dimensional space, which is compact by the Heine-Borel Theorem.

Some result that says under which circumstances to have an estimate of $\|u\|_{\mathcal{X}(\mathbb{D})}$ can be found in [53] (see Theorem 5.6) and [51] (See Theorem 2.5 and Theorem 2.6). We note that the minimizer above is achieved as long as the $\sup_{\mathbb{D}} \|d\|_{H^m}(\partial \nu) < \infty$. For in this case the optimization is over a bounded set and $J_N$ only depends upon the values and derivatives at finitely many points. Thus the optimization is effectively over a bounded set in a finite dimensional space, which is compact by the Heine-Borel Theorem.

For the case of mixed boundary conditions (16) we sample $N$ points $x_1, \ldots, x_N \in \partial \Omega$ uniformly at random and also sample $N_0$ points $y_1, \ldots, y_{N_0} \in \partial \Omega$ uniformly at random from the boundary. We then approximate the integrals in (16) by
\[
 J_{N,\delta}(u) = \frac{1}{2N} \sum_{i=1}^{N} \sum_{|\alpha| = m} a_\alpha(x_i)(\partial^\alpha u(x_i))^2 + \frac{1}{2N} \sum_{i=1}^{N} a_0(x_i)u(x_i)^2 - \frac{1}{N} \sum_{i=1}^{N} f(x_i)u(x_i) + \delta^{-1} \sum_{i=1}^{N_0} \sum_{k=0}^{m-1} \left| \frac{\partial^k}{\partial y^k} u(y_i) \right|^2.
\]
Forming the loss function (29) requires being able to calculate normal derivatives of functions \( u \) and to sample points uniformly from the boundary. This is possible for many important domains, such as the sphere or cube. We note that if the above sampling is not possible, then it suffices to be able to sample from a non-uniform distribution on \( \Omega \) and \( \partial \Omega \) with mass function \( \rho \) if we weight each of the sums above by \( \rho^{-1} \). We then propose to solve the following optimization problem to approximate solutions to (16)

\[
    u_{n,M,N,\delta} = \arg\max_{v \in \mathcal{B}(\mathbb{D})} J_{N,\delta}(v). \tag{30}
\]

The optimization problems (27) and (30) can be efficiently approximately solved using greedy algorithms \([2, 20, 25, 26, 54]\). Specifically, the algorithm we use is the following

\[
    u_0 = 0, \ g_k = \arg\max_{g \in \mathbb{D}} \langle \nabla J_N(u_{k-1}), g \rangle, \ u_k = (1-s_k) u_{k-1} - M s_k g_k, \tag{31}
\]

where \( s_k = \min(1, \frac{1}{2}) \). Importantly, we have that \( u_k \in \Sigma_{k,M}(\mathbb{D}) \), so that this algorithm produces neural networks with finite width. Note that this algorithm requires the computation of an argmin over the dictionary \( \mathbb{D} \), which may be a complicated step for certain dictionaries. We assume in what follows that this step can be efficiently calculated, which we argue is a reasonable assumption in practice for a wide range of dictionaries. For instance, when using the dictionary \( \mathbb{P}^d_K \) corresponding to ReLU\(^d\), this corresponds to an optimization over a compact \( d \)-dimensional set. Solving this problem for shallow neural network training was considered in \([25]\) and numerical experiments demonstrating the application to PDEs can be found in \([18]\).

The algorithm (31) was first introduced in \([20]\) for the quadratic least-squares objective. It was analyzed in the context of neural networks for least squares fitting in \([25]\) and for density estimation \([26]\), and for general activation functions in \([54]\). Further extensions, such as the orthogonal greedy algorithm, relaxed greedy algorithm, and pure greedy algorithm, which however do not ensure that their iterates have bounded \( \mathcal{X}(\mathbb{D}) \)-norm, are studied in \([29, 28, 29, 45, 47]\).

In what follows, we provide a convergence analysis which is applicable to our problem of interest. More generally, we assume in our convergence analysis that the argmax in (31) is not solved exactly, but rather is approximated in the following sense

\[
    \langle \nabla J_N(u_{k-1}), g_k \rangle \geq \frac{1}{R} \max_{g \in \mathbb{D}} \langle \nabla J_N(u_{k-1}), g \rangle \tag{32}
\]

for some \( R > 1 \). This is a more tractable problem for most dictionaries. However, we only consider the case of \( R = 1 \) in the convergence analysis given in this section. In later sections, we assume for simplicity that \( R = 1 \) in the analysis of the quadrature error.

For our analysis we will need that the objectives \( J_N \) and \( J_{N,\delta} \) are convex and \( K \)-smooth with respect to a Hilbert space norm \( H \). Recall that a function \( L : H \to \mathbb{R} \) is \( K \)-smooth if

\[
    J_N(g) \leq J_N(f) + \langle \nabla J_N(f), g - f \rangle + \frac{K}{2} \| g - f \|_H^2. \tag{33}
\]

In the following analysis, we will let \( H \) be the discrete \( \mathcal{H}^k \) norm corresponding to the sample points \( x_1, \ldots, x_N \) and \( y_1, \ldots, y_{N_0} \), i.e. \( H \) is given by

\[
    \langle u, v \rangle_H = \frac{1}{N} \sum_{i=1}^{N} \sum_{|\alpha|=m} (\partial^\alpha u(x_i))(\partial^\alpha v(x_i)) + \frac{1}{N} \sum_{i=1}^{N} u(x_i)v(x_i) + \frac{1}{N_0} \sum_{i=1}^{N_0} \sum_{k=0}^{m-1} \| \partial^k \partial^\alpha u(y_i) \|_H^2. \tag{34}
\]

With respect to the norm \( H \) above, the smoothness parameter \( K \) in the pure Neumann case \([26]\) is the maximum of the coefficient functions \( a_{\alpha} \) and \( a_0 \). In the case of mixed boundary conditions \([29]\) the smoothness parameter is bounded by \( K \leq \max(\| a_{\alpha} \|_{L^\infty}, \| a_0 \|_{L^\infty}) + \delta^{-1} \).

We have the following convergence result for the algorithm (31).

**Theorem 1.** Suppose that the dictionary \( \mathbb{D} \) is symmetric and satisfies \( \sup_{d \in \mathbb{D}} \| d \|_H \leq C < \infty \). Let the iterates \( u_n \) be given by the relaxed greedy algorithm (31) with \( s_k = \max(1, \frac{1}{2}) \), where the loss function \( L \) is convex and \( K \)-smooth (on the Hilbert space \( H \)). Suppose that the argmax in (31) is approximated up to a factor \( R \) as in (32). Then we have

\[
    \| u_n \|_{\mathcal{X}(\mathbb{D})} \leq M \quad \text{and} \quad \inf_{v \in \mathcal{X}(\mathbb{D})} L(v) \leq \frac{32((CM)^2K)^2}{R^2 M}. \tag{35}
\]
In particular, if $M \geq \|u\|_{\mathcal{X}_f(\mathcal{D})}$ where $u = \arg\min_L L(v)$ is the global minimizer, then the objective converges to the optimal value in the above theorem.

We note that applying this theorem to the squared error loss $L(f) = \frac{1}{2}\|f - f^*\|_H^2$ implies an approximation rate of

$$\inf_{f_n \in \mathcal{D}_M} \|f_n - f^*\|_H \lesssim Mn^{-\frac{1}{2}}, \tag{36}$$

for any $f^* \in B_M(\mathcal{D})$. This is essentially the method of proof used in [20]. In fact, for special dictionaries $\mathcal{D}$, the above rate can be improved. For instance, when $\mathcal{D} = \mathcal{D}_k^{\text{sp}}$ the optimal rate was determined in [44] to be $n^{-1 - \frac{2(k - m) + 1}{d}}$. Further, for more general activation functions it was shown that these rates can also be moderately improved in [43].

**Proof.** Since $u_0 = 0$ and $u_k$ is a convex combination of $u_{k-1}$ and $-Mg_k$, we see by induction that $\|u_k\|_{\mathcal{X}_f(\mathcal{D})} \leq M$.

The $K$-smoothness of the objective $L$ implies that

$$L(u_k) \leq L(u_{k-1}) + \langle \nabla L(u_{k-1}), u_k - u_{k-1} \rangle + \frac{K}{2} \|u_k - u_{k-1}\|_H^2. \tag{37}$$

Using the iteration (31), we see that $u_k - u_{k-1} = -s_k u_{k-1} - M s_k g_k$. Plugging this into the above equation, we get

$$L(u_k) \leq L(u_{k-1}) - s_k \langle \nabla L(u_{k-1}), u_k - u_{k-1} + M g_k \rangle + \frac{K s_k^2}{2} \|u_k - u_{k-1} + M g_k\|_H^2. \tag{38}$$

Since the dictionary elements $g_k$ satisfy $\|g_k\|_H \leq C$ and $\|u_{k-1}\|_{\mathcal{X}_f(\mathcal{D})} \leq M$, we see that $\|u_{k-1}\|_H \leq CM$ as well. Plugging this into the previous equation implies the bound

$$L(u_k) \leq L(u_{k-1}) - s_k \langle \nabla L(u_{k-1}), u_k - u_{k-1} + M g_k \rangle + 2(CM)^2 K s_k^2. \tag{39}$$

Now let $z$ with $\|z\|_{\mathcal{X}_f(\mathcal{D})} \leq R^{-1}M$ be arbitrary. Then also $\|z\|_{\mathcal{X}_f(\mathcal{D})} \leq R^{-1}M$ and the arg max characterization of $g_k$ (32) implies that

$$\langle \nabla L(u_{k-1}), -z \rangle \leq \langle \nabla L(u_{k-1}), Mg_k \rangle. \tag{40}$$

Using this in equation (39) gives

$$L(u_k) \leq L(u_{k-1}) - s_k \langle \nabla L(u_{k-1}), u_k - u_{k-1} - z \rangle + 2(CM)^2 K s_k^2. \tag{41}$$

The convexity of $L$ means that $L(u_{k-1}) - L(z) \leq \langle \nabla L(u_{k-1}), u_{k-1} - z \rangle$. Using this and subtracting $L(z)$ from both sides of the above equation gives

$$L(u_k) - L(z) \leq (1 - s_k) (L(u_{k-1}) - L(z)) + 2(CM)^2 K s_k^2. \tag{42}$$

Expanding the above recursion (using that $s_k \leq 1$), we get that

$$L(u_n) - L(z) \leq \left( \prod_{k=1}^n (1 - s_k) \right) (L(u_0) - L(z)) + 2(CM)^2 K \sum_{i=1}^n \left( \prod_{k=i+1}^n (1 - s_k) \right) s_i^2. \tag{43}$$

Using the choice $s_k = \max\left(1, \frac{1}{K}\right)$, for which $s_1 = 1$, we get

$$L(u_n) - L(z) \leq 2(CM)^2 K \sum_{i=1}^n \left( \prod_{k=i+1}^n (1 - s_k) \right) s_i^2. \tag{44}$$

Finally, we bound the product $\prod_{k=i+1}^n (1 - s_k)$ using that $\log(1 + x) \leq x$ as

$$\log \left( \prod_{k=i+1}^n (1 - s_k) \right) \leq - \sum_{k=i+1}^n s_k = - \sum_{k=i+1}^n \frac{2}{K} \leq - \int_{i+1}^{n+1} \frac{2}{x} dx \leq 2 \left( \log(i + 1) - \log(n + 1) \right), \tag{45}$$

for $i \geq 1$. Thus, $\prod_{k=i+1}^n (1 - s_k) \leq \left( \frac{i+1}{n+1} \right)^2$. Using this in equation (44), we get

$$L(u_n) - L(z) \leq 2(CM)^2 K \sum_{i=1}^n \left( \frac{i+1}{n+1} \right)^2 s_i^2 \leq 8(CM)^2 K \frac{1}{(n+1)^2} \sum_{i=1}^n \left( \frac{i+1}{n+1} \right)^2. \tag{46}$$

Crudely bounding $\frac{(i+1)^2}{i^2} \leq 4$ for $i \geq 1$, we get

$$L(u_n) - L(z) \leq 32(CM)^2 K \frac{n}{(n+1)^2} \leq \frac{32M^2 K}{n}, \tag{47}$$

Taking the infemum over $z$ with $\|z\|_{\mathcal{X}_f(\mathcal{D})} \leq R^{-1}M$ gives the result. \qed

Our goal in what follows will be to analyze the numerical error in solving (27) and (50).
3.1 Relationship with Statistical Learning Theory

The relationship between solving differential equations and statistical learning theory comes from the discretization of the integrals in (8) using Monte Carlo quadrature. Specifically, letting \( \mu \) denote the uniform measure on the set \( \Omega \), the energy can be written as

\[
J(u) = \mathbb{E}_{x \sim \mu} \left( \sum_{|\alpha|=m} a_\alpha(x) [\partial^\alpha u(x)]^2 dx + a_0(x)u(x)^2 - f(x)u(x) \right). \tag{48}
\]

In this way, the energy function \( J(u) \) plays the role of the (true) risk function in statistical learning theory \[40\]. However, an important difference is that here we know the probability distribution \( \mu \) explicitly, while in statistical applications the distribution \( \mu \) is usually not known. Rather, there is a dataset consisting of samples drawn from the distribution \( \mu \). In our case, we know \( \mu \) and generate this ‘training data’ artificially. In high-dimensions, this Monte Carlo quadrature is necessary since deterministic quadrature is very inefficient for evaluating high-dimensional integrals.

The minimization problem (27) then corresponds to the empirical risk function in statistical learning theory. In order to ensure that the true risk, or energy, of the minimizer of the empirical risk is small, it is necessary to obtain a law of large number which is uniform in the class of functions we are optimizing over. This is done in the remainder of this section using the well-known tool of Rademacher complexity.

Finally, note that the optimization problem (27) incorporates the a priori bound \( \|u_{n,M,N}\|_{\mathcal{X}_1(D)} \leq M \). We will see later that our error bounds depend upon the true solution \( u \) also satisfying the bound \( \|u\|_{\mathcal{X}_1(D)} \leq M \). The parameter \( M \) controls what is called the bias-variance trade-off in statistical learning. If we choose \( M \) too small, we won’t be able to capture the true solution \( u \) and both the empirical (27) and true (8) energy will be large. This represents the high bias regime. On the other hand, if \( M \) is very large, although we capture the true solution, which means that the empirical energy is small, we may overfit the ‘data points,’ and the true energy will be large. This represents the high variance regime.

In statistical learning, the amount of data is fixed and the hyperparameters of the model, which control the bias-variance trade-off, must be tuned using a validation dataset. Finally, the resulting model is tested once and for all on a test dataset. In the application to PDEs, however, we know the distribution \( \mu \) and can thus generate as much training data as we need. Consequently, once we have determined a suitable value of the parameter \( M \) in (27), we can generate as many datapoints \( N \) as we need to guarantee a good ‘generalization accuracy,’ i.e. to guarantee that the true energy will be comparable to the empirical, or discrete, energy. Thus, for PDE applications, there is no need for a validation or test dataset since we can always ensure that there is enough ‘training data’ to validate the assumptions of our model.

The problem of how to determine a suitable parameter \( M \) remains. In order to solve this problem, we propose to solve the problem (27) for a given value \( M_0 \) and then to adaptively increase \( M \) until the optimal energy determined in (27) stops decreasing. Each time we increase \( M \), we must sample more points \( N \) to ensure that we are not overfitting.

3.2 Rademacher Complexity

In order to bound the error incurred by approximating the true energy function (8) by the empirical energy function (26), we use the Rademacher complexity \[31\]. For more information on the Rademacher complexity and related concepts, we refer the reader to \[40\].

Given a class of functions \( \mathcal{F} : \Omega \to \mathbb{R} \), and a collection of sample points \( x_1, \ldots, x_N \in \Omega \), the empirical Rademacher complexity of \( \mathcal{F} \) is defined by

\[
\hat{R}_N(\mathcal{F}) = \mathbb{E}_{\xi_1, \ldots, \xi_N} \left[ \sup_{h \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^N \xi_i h(x_i) \right], \tag{49}
\]

where \( \xi_1, \ldots, \xi_N \) are Rademacher random variables, i.e. uniformly distributed signs. The Rademacher complexity is obtained by averaging over the samples \( x_i \), which we take to be uniformly distributed over \( \Omega \), i.e. we have

\[
R_N(\mathcal{F}) = \mathbb{E}_{x_1, \ldots, x_N \sim \mu} \mathbb{E}_{\xi_1, \ldots, \xi_N} \left[ \sup_{h \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^N \xi_i h(x_i) \right], \tag{50}
\]

where \( \mu \) is the uniform distribution on \( \Omega \). For the mixed boundary value problem, we will also need the Rademacher complexity with respect to the uniform distribution on the boundary \( \partial \Omega \), which we denote by \( R_{2,N}(\mathcal{F}) \).

The utility of the Rademacher complexity is its role in giving a law of large numbers which is uniform over the class \( \mathcal{F} \), detailed by the following theorem.
Theorem 2. [48 Proposition 4.11] Let $\mathcal{F}$ be a set of functions. Then
\[\mathbb{E}_{x_1,\ldots,x_N} \sup_{h \in \mathcal{F}} \left|\frac{1}{N} \sum_{i=1}^{N} h(x_i) - \int h(x) d\mu\right| \leq 2R_N(\mathcal{F}).\] (51)

3.3 Bounding the Integral Discretization Error

Our next step will be to apply the Rademacher complexity to bound the Monte Carlo discretization error in equations (26) and (29) uniformly over the class $B_m(\Omega)$.

To this end, we introduce the class of functions
\[\mathcal{F}_{n,M} = \left\{ \frac{1}{2} \sum_{|\alpha|=m} a_\alpha(x)(\partial^\alpha u(x))^2 + \frac{1}{2} a_0(x)u(x)^2 - f(x)u(x) : u \in \Sigma_{n,M}(\Omega) \right\}.\] (52)

and proceed to bound the Rademacher complexity $R_N(\mathcal{F}_{n,M})$. For this we will utilize the following fundamental lemma.

Lemma 2. Let $\mathcal{F} , \mathcal{I}$ be classes of functions on $\Omega$. Then the following bounds hold.

- $R_N(\text{conv}(\mathcal{F})) = R_N(\mathcal{F})$.
- Define the set $\mathcal{F} + \mathcal{I} = \{ h(x) + g(x) : h \in \mathcal{F}, g \in \mathcal{I} \}$. We have $R_N(\mathcal{F} + \mathcal{I}) = R_N(\mathcal{F}) + R_N(\mathcal{I})$.
- Suppose that $\phi : \mathbb{R} \to \mathbb{R}$ is $L$-Lipschitz. Let $\phi \circ \mathcal{F} = \{ \phi(h(x)) : h \in \mathcal{F} \}$. Then $R_N(\phi \circ \mathcal{F}) \leq LR_N(\mathcal{F})$.
- Suppose that $f : \Omega \to \mathbb{R}$ is a fixed function. Let $f \cdot \mathcal{F} = \{ f(x)h(x) : h \in \mathcal{F} \}$. Then $R_N(f \cdot \mathcal{F}) \leq \|f(x)\|_{L^\infty(\Omega)} R_N(\mathcal{F})$.

Proof. The first, second, and third of these statements are well-known facts, see [40 Lemma 26.7] for the first, [37 Page 56] for the second and [40 Lemma 26.9] for the third, so we only prove the fourth. Suppose that $\|f(x)\|_{L^\infty(\Omega)} \leq 1$, the general results follows by a scaling argument. Let $x_1, \ldots, x_N \in \Omega$ and consider the empirical Rademacher complexity
\[\hat{R}_N(f \cdot \mathcal{F}) = \mathbb{E}_{\xi_1,\ldots,\xi_N} \left[ \sup_{h \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^{N} \xi_i f(x_i)h(x_i) \right].\] (56)

We observe that the right-hand side of the above equation, being an average of a supremum of linear functions, is a convex function of $\hat{f} = (f(x_1), \ldots, f(x_N))$. Consequently, its maximum must be achieved at the extreme points of the set $\{ \hat{y} : \|\hat{y}\|_\infty \leq 1 \}$, which correspond to the points where each component is $\pm 1$. Thus we only need to consider the case where $f(x_i) = \epsilon_i \in \{ \pm 1 \}$. But then
\[\mathbb{E}_{\xi_1,\ldots,\xi_N} \left[ \sup_{h \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^{N} \xi_i \epsilon_i h(x_i) \right] = \mathbb{E}_{\xi_1,\ldots,\xi_N} \left[ \sup_{h \in \mathcal{F}} \frac{1}{N} \sum_{i=1}^{N} \xi_i h(x_i) \right] = \hat{R}_N(\mathcal{F}),\] (57)
since the $\epsilon_i$ simply permute the choices of sign $\xi_i$ in the expectation. Taking an average over the sample points $x_1, \ldots, x_N$ completes the proof.

Utilizing this lemma, we prove the following bound on the Rademacher complexity of the set $\mathcal{F}_{n,M}$ in (52).

Theorem 3. Suppose that $\|a_\alpha\|_{L^\infty(\Omega)}, \|a_0\|_{L^\infty(\Omega)} \leq K$ and $\sup_{d \in \mathbb{D}} \|d\|_{W^{m,\infty}} \leq C$. Then the Rademacher complexity of the set $\mathcal{F}_{n,M}$ in (52) is bounded by
\[R_N(\mathcal{F}_{n,M}) \leq CKM \sum_{|\alpha|=m} R_N(\partial^\alpha \mathbb{D}) + CKMR_N(\mathbb{D}) + \|f\|_{L^\infty(\Omega)} MR_N(\mathbb{D}),\] (58)
where $\partial^\alpha \mathbb{D} = \{ \partial^\alpha d : d \in \mathbb{D} \}$. 


For the mixed boundary conditions, we have

\[ W\text{ are primarily interested in the following corollary of this result, which uniformly bound the Monte Carlo discretization error in both the pure Neumann and Dirichlet cases.}

\textbf{Corollary 1.} Under the assumptions of Theorem 4 we have for the pure Neumann boundary conditions that

\[ \mathbb{E}_{x_1,\ldots, x_N} \sup_{u_{m} \in \mathcal{B}M(\mathcal{D})} |J_N(u_{m}) - J(u_{m})| \leq 2\text{CKM} \sum_{|a|=m} R_N(\partial^a \mathcal{D}) + 2C\text{KMRN}(\mathcal{D}) + 2 \|f\|_{L^\infty}(\Omega) \text{MRN}(\mathcal{D}). \] (62)

For the mixed boundary conditions, we have

\[ \mathbb{E}_{x_1,\ldots, x_N, y_1,\ldots, y_{N_0}} \sup_{u_{m} \in \mathcal{B}M(\mathcal{D})} |J_N,\delta(u_{m}) - J(\delta(u_{m}))| \leq 2\text{CKM} \sum_{|a|=m} R_N(\partial^a \mathcal{D}) + 2C\text{KMRN}(\mathcal{D}) \]

\[ + 2 \|f\|_{L^\infty}(\Omega) \text{MRN}(\mathcal{D}) + 2\delta^{-1}M \sum_{|a|<m} R_{\delta, N}(\partial^a \mathcal{D}). \] (63)

\textbf{Proof.} This follows immediately by combining Theorem 3 with Theorem 2 and using Lemma 2 for the boundary terms in the case of mixed boundary conditions. \(\square\)

### 3.4 Rademacher Bounds for Neural Networks

In this section, we show how the Rademacher complexity can be bounded for dictionaries corresponding to shallow neural networks. Specifically, we consider dictionaries of the form

\[ \mathcal{D}_\sigma = \{ \sigma(\omega \cdot x + b) : (\omega, b) \in \Theta \} \subset H^m(\Omega), \] (64)

where the parameter set \( \Theta \subset \mathbb{R}^{d+1} \) is compact. Of particular importance are the dictionaries corresponding to ReLU activation functions, \( \mathbb{P}_k^d \), which were introduced in [14]. Our main result is the following bound on the Rademacher complexity. This generalizes the results of [11], which calculate the Rademacher complexity of the unit ball in the Barron space for ReLU neural networks (see also [15], Theorem 2 and [21], Theorem 3).

\textbf{Theorem 4.} Suppose that \( \sigma \in W^{m+1, \infty} \). Then for any \( \alpha \) with \( |\alpha| \leq m \), we have

\[ R_N(\partial^\alpha \mathcal{D}) \lesssim N^{-\frac{1}{2}}, \quad R_{\delta, N}(\partial^\alpha \mathcal{D}) \lesssim N^{-\frac{1}{2}} \] (65)

where the implied constant is independent of \( N \).

\textbf{Proof.} This results follows immediately upon noting that

\[ \partial^\alpha \mathcal{D} = \{ \omega^\alpha \sigma(\delta) : (\omega, b) \in \Theta \}. \] (66)

Since \( \Theta \) is a compact set, \( |\omega^\alpha| \) is bounded. Further, since \( \sigma \in W^{m+1, \infty} \), we have that \( \sigma(\delta) \) is Lipschitz. Using the third point in Lemma 2 we obtained

\[ R_N(\partial^\alpha \mathcal{D}) \lesssim R_N(\{ \omega \cdot x + b : (\omega, b) \in \Theta \}), \] (67)

and likewise for \( R_{\delta, N}(\partial^\alpha \mathcal{D}) \).

It is well-known that the Rademacher complexity of the set of linear functions is bounded by \[ \mathbb{H} \] Section 26.2 [40] for any distribution on \( x \) which is bounded almost surely. This applies both to the uniform distribution on \( \Omega \) as well as to the uniform distribution on \( \delta \Omega \), which completes the proof. \(\square\)
4 Monte Carlo Sampling Error Analysis

Finally, in this section, we collect the previous results to derive a rigorous error analysis for the approximate solution given in (27) and (30). We have the following convergence result in the pure Neumann case.

**Theorem 5.** Suppose that the conditions of Theorem 3 are satisfied, i.e. that in (25) we have \( \|a\|_{L^\infty(\Omega)}, \|a_0\|_{L^\infty(\Omega)} \leq K \). In addition, assume that the dictionary \( D \) satisfies \( \sup_{d \in D} \|d\|_{W^{\infty,\infty}(\Omega)} < \infty \) and the Rademacher complexity bound

\[
R_N(\partial^2 D), R_N(D), R_{\partial^2 D}(\partial^2 D) \lesssim N^{-\frac{1}{2}}.
\]

Assume that the true solution \( u \in X_1(D) \) satisfies \( \|u\|_{X_1(D)} \leq M \) and let the numerical solution \( u_{n,M,N} \in \Sigma_{n,M}(D) \) be obtained by optimizing (27) using the algorithm (31) for \( n \) steps. Then we have

\[
E_{x_1,\ldots,x_N}(J(u_{n,M,N}) - J(u)) \leq M \left(C_1(K + \|f\|_{L^\infty(\Omega)})N^{-\frac{1}{2}} + C_2KMn^{-1}\right),
\]

where the constants \( C_1 \) and \( C_2 \) depend only upon the dictionary \( D \), the dimension \( d \) and the order \( m \). Using the assumption that the coefficients \( a_{\alpha} \) are bounded away from 0, this implies in particular that

\[
E_{x_1,\ldots,x_N}(\|u_{n,M,N} - u\|_{H^m(\Omega)})^2 \leq M \left[C_1'N^{-\frac{1}{2}} + C_2'Mn^{-1}\right],
\]

where \( C_1' \) and \( C_2' \) depend only upon the dictionary and the differential operator.

Note that we have here an a priori bound which depends upon the \( X_1(D) \)-norm \( M \) of the true solution \( u \).

**Proof.** We write

\[
E_{x_1,\ldots,x_N}(J(u_{n,M,N}) - J(u)) \leq E_{x_1,\ldots,x_N}(J_N(u_{n,M,N}) - J_N(u))
+ E_{x_1,\ldots,x_N}(J_N(u_{n,M,N}) - J(u_{n,M,N}))
+ E_{x_1,\ldots,x_N}(J_N(u) - J(u)).
\]

Using Theorem 2 the last two terms on the right are both bounded via the Rademacher complexity by

\[
CM(K + \|f\|_{L^\infty(\Omega)})N^{-\frac{1}{2}}
\]

for an appropriate constant \( C \) since \( u_{n,M,N}, u \in B_M(D) \).

The first term on the right hand side of equation (72) is bounded by \( C'KM^2n^{-1} \) using Theorem 1 for another constant \( C' \). Specifically, see the remarks about the \( K \)-smoothness of \( J_N \) preceding Theorem 1 and use the assumption that \( \sup_{d \in D} \|d\|_{W^{\infty,\infty}(\Omega)} < \infty \) to conclude that \( D \) is uniformly bounded in the discrete \( H^m \) norm (34).

Collecting these bounds completes the proof.

\[\square\]

Next, we give the convergence result in the case of mixed boundary conditions (16).

**Theorem 6.** Suppose that the conditions of Theorem 3 are satisfied, i.e. that in (25) we have \( \|a\|_{L^\infty(\Omega)}, \|a_0\|_{L^\infty(\Omega)} \leq K \). In addition, assume that the dictionary \( D \) satisfies \( \sup_{d \in D} \|d\|_{W^{\infty,\infty}(\Omega)} < \infty \) and the Rademacher complexity bound

\[
R_N(\partial^2 D), R_N(D), R_{\partial^2 D}(\partial^2 D) \lesssim N^{-\frac{1}{2}}.
\]

Assume that the true solution \( u_\Sigma \in X_1(D) \) of (16) satisfies \( \|u_\Sigma\|_{X_1(D)} \leq M \) and let the numerical solution \( u_{n,M,N,\Sigma} \in \Sigma_{n,M}(D) \) be obtained by optimizing (30) using the algorithm (31) for \( n \) steps. Then we have

\[
E_{x_1,\ldots,x_N,\Sigma_1,\ldots,\Sigma_N}(J_\Sigma(u_{n,M,N,\Sigma}) - J_\Sigma(u_\Sigma)) \leq M \left[C_1(K + \|f\|_{L^\infty(\Omega)} + \delta^{-1})N^{-\frac{1}{2}} + C_2(K + \delta^{-1})Mn^{-1}\right],
\]

where the constants \( C_1 \) and \( C_2 \) depend only upon the dictionary \( D \), the dimension \( d \) and the order \( m \). Using the assumption that the coefficients \( a_{\alpha} \) are bounded away from 0, this implies in particular that

\[
E_{x_1,\ldots,x_N}(\|u_{n,M,N,\Sigma} - u_\Sigma\|_{H^m(\Omega)})^2 \leq M(1 + \delta^{-1}) \left[C_1'N^{-\frac{1}{2}} + C_2'Mn^{-1}\right],
\]

where \( C_1' \) and \( C_2' \) depend only upon the dictionary and the differential operator.
We proceed to apply the deterministic numerical quadrature form (80) to approximate $T$. We collect the quadrature points for each of the elements using the algorithm for $n$ steps. Then we have

$$
E_{\alpha_1 \ldots \alpha_N} (\| u_{n,M,N,\delta} - u \|^2_{H^m(\Omega)}) \leq M(1 + \delta^{-1}) \left[ C_1^\prime N^{-\frac{d}{2}} + C_2^\prime M n^{-1} \right] + C^\prime_R \delta \| u \|^2_{2m,\Omega},
$$

where $\delta$ depend only upon the dictionary and the differential operator. In particular, with the choice $N = O(n^2)$ and $\delta = O(n^{-\frac{d}{2}})$, we obtain the convergence rate

$$
E_{\alpha_1 \ldots \alpha_N} (\| u_{n,M,N,\delta} - u \|^2_{H^m(\Omega)}) \lesssim n^{-\frac{d}{2}}.
$$

### 5 Numerical Quadrature Analysis

Let $\mathcal{T}_h = \{ T \}$ be a uniform partition of $\Omega$ with mesh size $h$ and $P_r(\mathcal{T}_h)$ denote the piecewise degree $r$ polynomials on $\mathcal{T}_h$, i.e.

$$
P_r(\mathcal{T}_h) = \{ p \in L^2(\Omega) : p(x)|_T \in P_r(T), \forall T \in \mathcal{T}_h \},
$$

where $P_r(T)$ is the set of degree $r$ polynomials on $T$.

On each element $T \in \mathcal{T}_h$ and any given function $g$, we use numerical quadrature to approximate $\int_T g(x)dx$, namely

$$
\int_T g(x)dx \approx \sum_{i=1}^{n_T} w_{T,i} g(x_{T,i}),
$$

where the points $x_i$ and weights $w_{T,i}$ and chosen so the above approximation is exact for polynomials of degree $r$.

We collect the quadrature points for each of the elements $T$ to obtain the the deterministic numerical quadrature with quadrature points $x_i$ and weights $w_i$,

$$
\int_{\Omega} g(x)dx = \sum_{T \in \mathcal{T}_h} \int_T g(x)dx \approx \sum_{T \in \mathcal{T}_h} \sum_{i=1}^{n_T} w_{T,i} g(x_{T,i}) = \sum_{i=1}^{N} w_i g(x_i).
$$

Note that $n_T = n$ is a fixed number for each element $T$ by the quadrature formula given in (79), so that $N = O(N_T)$, where $N_T$ is the number of elements of $\mathcal{T}_h$. From this we see that $N = O(h^{-d})$.

We proceed to apply the deterministic numerical quadrature form (80) to approximate $J(v)$ defined in (8), namely

$$
J_N(v) = \sum_{i=1}^{N} w_i \left( \frac{1}{2} \sum_{|a|=m} a_\alpha(x_i) (\partial^a v(x_i))^2 + \frac{1}{2} a_0(x_i) (v(x_i))^2 - f(x_i)v(x_i) \right).
$$

Let $u_{n,M,N} \in \Sigma_{n,M}(\Omega)$ be obtained by applying algorithm (51) to solve

$$
u_{n,M,N} = \arg \min_{v \in B_M(\Omega)} J_N(v)
$$

for $n$ steps, where $J_N(\cdot)$ is defined by (81).

### Theorem 8

Let $u$ be the solution of (19). Suppose that $u \in \mathcal{K}^1(\Omega)$ and let $u_{n,M,N} \in \Sigma_{n,M}$ be obtained by solving (82) using the algorithm (51) with $M \geq \| u \|_{\mathcal{K}^1(\Omega)}$. Suppose that

- the coefficients and $f$ in (8) satisfy $\| a_\alpha \|_{W^{r-1,p}(\Omega)}, \| a_0 \|_{W^{r-1,p}(\Omega)}$, $\| f \|_{W^{r-1,p}(\Omega)} \leq K$, and
- the dictionary $\mathcal{D}$ satisfies $\sup_{d \in \mathcal{D}} \| d \|_{W^{r-1,p}(\Omega)} = C < \infty$. 

The proof is completely analogous to the proof of Theorem 5 and we omit it for brevity.

We note that by Theorem 4 both Theorem 5 and 6 apply to the case when $\mathcal{D} = \mathcal{D}_\sigma$ corresponds to shallow neural networks. Further, the difference between $u$ and $u_\delta$ is given by the following lemma.

### Lemma 3

**Lemma 5.4** Let $u$ be the solution of (7) and $u_\delta$ be the solution of (16). Then

$$
\| u - u_\delta \|_{H^m(\Omega)} \lesssim \sqrt{\delta} \| u \|_{2m,\Omega}.
$$

By applying Lemma 3 and choosing $\delta$ appropriately, Theorem 8 can be used to obtain a result for the pure Dirichlet boundary conditions as well.
Then, if we choose the number of quadrature points as \( N = O(n^{\frac{d}{d+1}}) \), we get the estimate
\[
\|u_{n,M,N} - u\|_a \lesssim n^{-\frac{1}{2}}.
\] (83)

**Proof.** By the assumption the quadrature points \( x_i \) and weights \( w_i \) satisfy
\[
\int_{\Omega} g(x)dx - \sum_{i=1}^{N} w_i g(x_i) = 0, \quad \forall g(x) \in P_r(\mathcal{T}_h).
\] (84)

Using the Bramble-Hilbert Lemma [5], we get
\[
\left| \int_{\Omega} h(x)dx - \sum_{i=1}^{N} w_i h(x_i) \right| \leq C_n N^{-\frac{d+1}{2}} \|h\|_{r+1,\infty} \quad \forall h \in W^{r+1,\infty}(\Omega).
\] (85)

For any \( v \in W^{m+r+1,\infty}(\Omega) \), letting \( h(x) = \frac{1}{2} \sum_{|\alpha|=m} a_\alpha(x)(\partial^\alpha v(x))^2 + \frac{1}{2} a_0(x)(v(x))^2 - f(x)v(x) \), we have
\[
|J_N(v) - J(v)| \leq C_m C_n r N^{-\frac{d+1}{2}} \|v\|_{m+r+1,\infty}.
\] (86)

We now calculate
\[
\frac{1}{2} \|u_{n,M,N} - u\|_a^2 = J(u_{n,M,N}) - J(u) \leq J_N(u_{n,M,N}) - J_N(u) + |J(u_{n,M,N}) - J_N(u_{n,M,N})| + |J(u) - J_N(u)|.
\] (87)

The last two terms above are bounded by equation (86) since we have \( u_{n,M,N}, u \in B_M(\mathcal{D}) \) and thus \( \|u_{n,M,N}\|_{W^{m+r+1,\infty}(\Omega)}, \|u\|_{W^{m+r+1,\infty}(\Omega)} \leq CM \). The first term is bounded by \( C'KM^2n^{-1} \) for some constant \( C' \). Putting this together, we get
\[
\frac{1}{2} \|u_{n,M,N} - u\|_a^2 \lesssim N^{-\frac{d+1}{2}} + n^{-1}.
\] (88)

Choosing \( N = O(n^{\frac{d}{d+1}}) \) completes the proof. \( \square \)

Now we proceed to apply the deterministic numerical quadrature to approximate \( J_\delta(v) \) defined in (17), namely
\[
J_{N,\delta}(v) = \sum_{i=1}^{N} w_i \left( \frac{1}{2} \sum_{|\alpha|=m} a_\alpha(x_i)(\partial^\alpha v(x_i))^2 + \frac{1}{2} a_0(x_i)(v(x_i))^2 - f(x_i)v(x_i) \right) + \delta^{-1} \sum_{i=1}^{N_0} \sum_{k=1}^{m-1} w_{i,j} \left( \frac{\partial^k}{\partial v^k} v(y_i) \right)^2,
\] (89)

here \( w_{i,j}, 1 \leq i \leq N_0 \) are the quadrature weights and points for approximating the integral \( \sum_{k=0}^{m-1} (B^k_D(\hat{u}), B^k_D(v))_{0,\partial\Omega} \).

Let \( u_{n,M,N,\delta} \in \Sigma_{n,M}(\mathcal{D}) \) be obtained by solving
\[
u_{n,M,N,\delta} = \arg \min_{\nu \in \Sigma_{n,M}(\mathcal{D})} J_{N,\delta}(\nu)
\] (90)

using the greedy algorithm (31), where \( J_{N,\delta}(\cdot) \) is defined by (89).

**Theorem 9.** Let \( u_\delta \) be the solution of (16). Suppose that \( u_\delta \in \mathcal{K}_1(\mathcal{D}) \) and let \( u_{n,M,N,\delta} \in \Sigma_{n,M} \) be obtained by solving (90) using the algorithm (31) with \( M \geq \|u_\delta\|_{\mathcal{K}_1(\mathcal{D})} \). Suppose that

- the coefficients and \( f \) in (17) satisfy \( \|a_\alpha\|_{W^{r,\infty}(\Omega)}, \|a_0\|_{W^{r,\infty}(\Omega)}, \|f\|_{W^{r,\infty}(\Omega)} \leq K_r \), and
- the dictionary \( \mathcal{D} \) satisfies \( \sup_{d \in \mathcal{D}} \|d\|_{W^{m+r+1,\infty}(\Omega)} = C < \infty \).

Then, we have
\[
\|u_{n,M,N,\delta} - u_\delta\|_a \lesssim N^{-\frac{d+1}{2}} + (1 + \delta^{-\frac{1}{2}})(N_0^{-\frac{d+1}{2}} + n^{-\frac{1}{2}}).
\] (91)

The proof of Theorem 9 is similar to the proof of 8 and we omit it for brevity.

Further, by applying Lemma 3 and choosing \( \delta \) appropriately, Theorem 9 can be used to obtain a result for the pure Dirichlet boundary conditions as well.
Theorem 10. Suppose that the conditions of Theorem 9 are satisfied. Assume that the true solution \( u_\delta \in \mathcal{H}_1(D) \) of (16) satisfies \( \| u_\delta \|_{\mathcal{H}_1(D)} \leq M \) for all \( \delta > 0 \). Let \( u \) be the solution of (7) and the numerical solution \( u_{n,M,\delta} \in \Sigma_{n,M}(D) \) be obtained by solving (90) using the algorithm (31) with \( M \geq \| u_\delta \|_{\mathcal{H}_1(D)} \). Then, if we choose \( \delta = O(n^{-1/2}) \) and the number of quadrature points as \( N = O(n^{-d/2}) \) and \( N_0 = O(n^{-d+1}) \), we get the estimate

\[
\| u_{n,M,\delta} - u \|_a \lesssim n^{-1/4}.
\]

6 Conclusion

We have provided an analysis of the finite neuron method for both Monte Carlo and numerical quadrature. The key is to constrain the \( \mathcal{H}_1(D) \)-norm of the numerical solution, which enables an a priori Rademacher complexity analysis. This is made possible by using a greedy algorithm instead of the commonly used stochastic gradient descent algorithm.

Similar to the analysis of many numerical methods in scientific computing, our analysis is based on an a priori assumption, namely on the \( \mathcal{H}_1(D) \)-norm of the solution, which determines the choice of \( M \). For example the convergence analysis of Newton’s method requires the initial iterate to be close enough to the minimizer. In addition, a priori error analysis for finite element methods relies on an a priori bound on the solution in an appropriate norm. Similar to the adaptive finite element method, developing a fully adaptive method with an a posteriori error analysis is a topic of ongoing work.

Another interesting further research direction is the study of more efficient algorithms for solving the argmax subproblem which occurs in equation (31). In addition, it would also be interesting to extend this analysis to more general PDEs, such as parabolic and hyperbolic equations.

7 Acknowledgements

We would like to thank Professors George Karniadakis, Jason Klusowski, Yulong Lu, Yeonjong Shin and Haizhao Yang for helpful discussions which inspired this work. This work was supported by the Verne M. Willaman Chair Fund at the Pennsylvania State University, and the National Science Foundation (Grant No. DMS-1819157).

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