ERROR ESTIMATES OF RESIDUAL
MINIMIZATION USING NEURAL
NETWORKS FOR LINEAR PDES

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We propose an abstract framework for analyzing the convergence of least-squares methods based on residual minimization when feasible solutions are neural networks. With the norm relations and compactness arguments, we derive error estimates for both continuous and discrete formulations of residual minimization in strong and weak forms. The formulations cover recently developed physics-informed neural networks based on strong and variational formulations.

KEY WORDS: least-squares method, subdomain least-squares, a priori and a posteriori estimates, linear well-posed problems

1. INTRODUCTION

Deep learning algorithms using neural networks (NNs) have been employed to solve forward and inverse problems for partial differential equations (PDEs). Many works have shown their effectiveness in various applications (Berg and Nyström, 2018; E and Yu, 2018; Khoo et al., 2019; Lagaris et al., 1998, 2000; Li et al., 2019; Liao and Ming, 2021; Mao et al., 2020; Nabian and Meidani, 2019; Pang et al., 2019; Raissi and Karniadakis, 2018; Raissi et al., 2017, 2019, 2020; Samaniego et al., 2020; Sirignano and Spiliopoulos, 2018; Zhang et al., 2019). Empirical studies (Raissi and Karniadakis, 2018; Raissi et al., 2020) have found that deep learning algorithms are particularly effective in solving inverse problems for PDEs with a few data points. Such inverse problems are known to be challenging for existing classical methods. However, the mathematical theory of deep learning algorithms for PDEs is far from being complete at the moment.

Due to the nonlinear and compositional nature of NNs, deep learning for PDEs is often recast as highly nonconvex and nonlinear optimization problems. A critical step in deep learning is
the formulation of an appropriate loss functional. A least-squares type loss is a common choice when it comes to regression or supervised learning. The least-squares finite element methods (LS-FEM) (Bochev and Gunzburger, 2016; Bramble and Schatz, 1970) are classic examples of using such loss functionals. The LS-FEM uses a linear finite element space for feasible solutions and solves linear systems for linear problems. In contrast, deep learning methods use NNs as surrogate models for solutions and solve nonlinear optimization problems even for linear problems. While NNs are universal approximators, a collection of NNs does not form a linear space. Thus, the error estimates and convergence of deep learning methods will significantly differ from those of the LS-FEM. The analysis of the least-squares with a linear space (e.g., LS-FEM in Bochev and Gunzburger, 2016; Bramble and Schatz, 1970) cannot be applied directly.

There are two sources of errors for the deep learning algorithms for PDEs: mathematical formulation and optimization/training. The present work focuses on analyzing the errors from mathematical formulations. The analysis of optimization/training errors is deferred to future work. Specifically, we study the problem of the error estimates of NN solutions that minimize the least-squares type loss functionals. This problem has been investigated in Mishra and Molinaro (2023) and Mishra and Molinaro (2022) for both linear and nonlinear equations from fluid dynamics, in Shin et al. (2020a) for a discrete loss functional for linear elliptic and parabolic equations, and in Sirignano and Spiliopoulos (2018) for a continuous loss functional for quasilinear parabolic PDEs. More related works are summarized in Section 1.2.

We consider a general framework regardless of the type of equations for linear problems, which include hyperbolic, elliptic, and parabolic equations. Moreover, we consider two types of loss functionals. Type 1 is based on residuals of the strong form, and Type 2 is based on residuals of the weak form. The two types of loss functionals are related to some existing methods. When the feasible solutions are in the space of finite elements, the discrete Type 1 is known as least-squares collocation methods (Bochev and Gunzburger, 1998). When the feasible solutions are NNs (which we consider), Type 1 is known as physics-informed neural networks (PINNs) (Raissi et al., 2017) and Type 2 is known under the names variational PINNs (Kharazmi et al., 2019), VarNets (Khodayi-Mehr and Zavlanos, 2020), and $hp$-variational PINNs ($hp$-VPINNs) (Kharazmi et al., 2021). Type 1 loss requires smooth activation functions in the networks, while Type 2 loss does not because its formulation is based on variational forms of PDEs (variational residuals) allowing non-smooth networks.

Our main contributions are summarized as follows. First, we establish an abstract framework in analyzing the discrete loss functional whose formulation is based on the residuals of the linear problem [Eq. (1)] in strong (Type 1) and weak (Type 2) forms. Second, we derive a priori and a posteriori error estimates for both continuous and discrete loss formulations of both types: residuals in strong forms (Sections 3 and 4) and those in weak forms (Section 5). Third, under suitable assumptions, we establish strong convergence in the underlying predefined topology. See Theorem 3.2 (continuous Type 1 loss functional), Theorem 4.4 (discrete Type 1 loss functional), and Theorem 5.2 (continuous Type 2 loss functional). We also present three examples and validate the assumptions in our abstract framework in Appendix B, including elliptic, advection-reaction, and fractional diffusion equations.

Our framework can be applied to the recently developed discrete/continuous PINNs and discrete/continuous $hp$-VPINNs. Moreover, the proposed framework is more general than those in recent studies (Luo and Yang, 2020; Shin et al., 2020a) where properties of considered equations are used. We note that in Mishra and Molinaro (2022, 2023), the stability of solutions is used while no convergence is guaranteed when both the number of parameters in the NNs and sampling points go to infinity.
1.1 Assumptions

We have made the following three fundamental assumptions: (a) *(stability)* relations among graph norms defined by the linear operators and the Sobolev or Hölder norms of solutions (as in LS-FEM, e.g., Assumption 2.2 and Bochev and Gunzburger, 2016); (b) *(existence and uniqueness)* existence of a convergent sequence to solutions in such norms (Assumption 2.1); and (c) *(compatible networks for discrete formulation)* uniformity of the discretization/projection errors of continuous norms of residuals for minimizers, where the uniformity lies either in the stability concerning discrete norms (Assumption 4.1) or in the Rademacher complexity (Assumption 4.2). The first two assumptions are somewhat standard as in most numerical methods and lead to the convergence of continuous formulations in Theorem 3.1. The third is the most essential for the convergence of discrete formulations. The violation of such an assumption may lead to no convergence, i.e., no accuracy may be gained away from the training points; see Example 4.1. In Fig. 1, we summarize the relations between the fundamental assumptions and convergence.

1.2 Limitations and Remarks

Our work is the first step toward understanding and developing NN algorithms for forward and inverse problems. There are aspects and issues of these algorithms that deserve in-depth investigations, e.g., choices of energy-based or residual-based loss functionals, choices of penalty parameters for optimizing various objectives, and efficient methods for multiscale problems and nonlinear problems, especially in high dimensions. For example, the choice of optimal penalty parameters to balance all the residuals from different components to achieve better accuracy and convergence was discussed in Bramble and Schatz (1970) using high-order finite element methods for elliptic problems. Therein some penalty parameters have been introduced to balance the two terms \( \| \Delta v \|_{L^2(\Omega)} \) and \( \| v \|_{L^2(\partial \Omega)} \) (Dirichlet boundary) for all \( v \) in a finite element space to derive optimal convergence. Note that the parameter can be determined via a Bernstein-type inequality. However, such inequalities are not yet available for most NNs, especially for deep NNs. Some empirical studies have been made (e.g., in Wang et al., 2022). For multiscale problems, the constant in the lower bound of norm relations can be small and may lead to little use of the theory. Also, many intrinsic physical properties are not explicitly included in the loss functionals, such as conservation laws. These aforementioned topics are beyond the scope of the paper and should be considered case-by-case. In addition, our framework does not accommodate nonlinear problems. Some attempts have been made in Mishra and Molinaro (2022) using the stability of solutions while more efforts are required with less restrictive assumptions (see also Sirignano and Spiliopoulos, 2018). Lastly, we do not discuss the mixed formulations, which transform high-order PDEs into systems of first-order equations (see Cai et al., 2020).

[FIG. 1: Sketch of critical concepts for convergence of continuous and discrete residual minimization using neural networks. Here we assume a zero training error.]
We remark that after the first version of this work (Shin et al., 2020b) was posted on arXiv, several related and follow-up works employed the presented abstract framework and further investigated error analysis of residual minimization (RM). For example, in Gazoulis et al. (2023), the concept of gamma convergence from the variation of calculus is adopted to further reduce the theoretical requirement in the smoothness of the exact solution. In Bai et al. (2021), stability is also applied to nonlinear equations, extending the framework in Mishra and Molinaro (2022, 2023). The work of Tang et al. (2023) utilizes the error estimate for continuous RM (Theorem 3.1) to develop an adaptive sampling strategy for PINNs. Regarding the compatibility of NNs, Jiao et al. (2022) calculated the Rademacher complexity of PINNs by focusing on the two-layer rectified power unit (ReLU³) NNs, which complements the presented discrete RM formulation in Section 4.2 and provides a rate of convergence. In Doumèche et al. (2023), the compatibility was imposed via Sobolev-type regularization, similar to the one used in Shin et al. (2020a). Also, the stability was used to provide a convergence result for PINNs. Similarly, in Wu et al. (2023), the compatibility was used by means of a Lipschitz regularization and provided a convergence result via stability for elliptic interface problems.

Extensions to ill-posed problems with conditional stability (see, e.g., Dahmen et al., 2023; Kabanikhin, 2008, for definition) are possible. Conditional stability is an extension of stability in the sense that adding a regularization term will stabilize the problem if it is not well-posed/stable. For linear problems such as Poisson equations, heat equations, and wave equations, condition stability has been well established for data assimilation problems (see Burman, 2016; Dahmen et al., 2023, for examples). We briefly discuss the conditional stability in Remark 2.2, but we will not discuss the application of conditional stability in this work.

There is another NN-based approach using energy minimization. The deep ritz method (E and Yu, 2018) is a popular such approach. While this is not the focus of the present work, for completeness, we briefly review some relevant works. A prior generalization analysis was given in recent studies (Lu and Lu, 2022; Lu et al., 2021) where the Barron spectral space was employed for the compatibility. Müller and Zeinhofer (2022) derived an error estimate where the Friedrich inequality was used for the compatibility and Céa’s lemma provided the stability. A rate of convergence was studied in Duan et al. (2022) where the compatibility was handled by the Rademacher complexity and the stability was by Céa’s lemma. Dondl et al. (2022) provided abstract gamma convergence.

2. MATHEMATICAL SETUP AND PRELIMINARIES

Let \( A : X \to Y \) and \( B : X \to Z \) be linear operators, where \((X, \| \cdot \|_X), (Y, \| \cdot \|_Y), (Z, \| \cdot \|_Z)\) are Banach spaces. Let \( \Omega \) and \( \Gamma \) be two subsets of \( \mathbb{R}^d \) and consider the following linear problem

\[
\begin{align*}
A[u](x) &= f(x), & x \in \Omega \\
B[u](x) &= g(x), & x \in \Gamma,
\end{align*}
\]

where \( f \in Y \) and \( g \in Z \). For simplicity, we write \( A[u] \) as \( Au \) and similarly for \( B \). We will impose further assumptions on the operators \( A \) and \( B \) shortly.

If the problem represents a linear PDE, we usually consider that \( \Omega \) is a bounded domain (open and connected) with Lipschitz continuous boundary \( \Gamma = \partial \Omega \). The domain \( \Omega \) could be unbounded as in the exterior problems, or the domain \( \Gamma \) could be unbounded (see Appendix B.3). For computational purposes, it is often convenient to assume bounded computational domains. The choices of the spaces depend on the considered problems; see Appendix B for several examples.
Remark 2.1. For simplicity, we consider the case where the number of operators is two, and \( u \) is a scalar real-valued function. However, the framework developed in the following sections can accommodate multiple operators and vector-valued functions (systems of equations), e.g., first-order differential linear systems, which can also represent elliptic problems, e.g., in Bochev and Gunzburger (1998).

### 2.1 Solution of the Problem and Norm Relations

In this section, we present two key assumptions for our analysis. The first assumption is on the existence of a solution to the problem in Eq. (1); see Assumption 2.1. The second assumption is on the relations of graph norms associated with the linear problem in Eq. (1); see Assumption 2.2.

We first define our notion of a solution to Eq. (1), which is the underlying solution we want to approximate.

**Definition 2.1.** Let \((V, \| \cdot \|_V)\) be a Banach space and \((X, \| \cdot \|_V)\) is a dense subspace of \((V, \| \cdot \|_V)\). An element \( u^* \in V \) is said to be a solution to Eq. (1) if there exists a sequence \( \{ u^*_k \} \) in \( X \) such that

\[
\lim_{k \to \infty} \| u^*_k - u^* \|_V = 0, \quad \lim_{k \to \infty} \| Au^*_k - f \|_Y + \| Bu^*_k - g \|_Z = 0.
\]

We note that since a solution is not necessarily in \( X \), strictly speaking, \( Au^* \) is not well-defined. However, under suitable assumptions, the linear operators can be uniquely extended to \( V \). The following theorem provides a condition under which the extension exists. Hence, \( Au^* \) could be well-defined.

**Theorem 2.1** [Bounded linear transformation theorem (Reed, 2012)]. Suppose \((X, \| \cdot \|_V)\) is a dense subspace of \((V, \| \cdot \|_V)\) and let \( A \) be a bounded linear operator from \((X, \| \cdot \|_V)\) to \((Y, \| \cdot \|_Y)\). Then, there exists a unique extension \( \tilde{A} \) from \((V, \| \cdot \|_V)\) to \((Y, \| \cdot \|_Y)\) of \( A \). That is, \( \tilde{A}v = Av \) for all \( v \in X \) and \( \| A \| = \| \tilde{A} \| \), where \( \| \cdot \| \) is the operator norm.

Throughout the paper, the operators are understood up to extensions if needed.

**Assumption 2.1** (Existence). There exists a solution \( u^* \in V \) to Eq. (1) in the sense of Definition 2.1.

The following assumption plays a central role in our abstract framework.

**Assumption 2.2** (Norm relations). Assume that the operators \( A \) and \( B \) satisfy \( \| Au \|_Y, \| Bu \|_Z < \infty \), for all \( u \in V \). Assume also the following norm relations:

\[
C_1 \| u \|_V \leq \| Au \|_Y + \| Bu \|_Z, \quad \forall u \in X, \tag{2a}
\]

\[
\| Au \|_Y + \| Bu \|_Z \leq C_2 \| u \|_X, \quad \forall u \in X, \tag{2b}
\]

where the positive constants \( C_1 \) and \( C_2 \) do not depend on \( u \) but on the domain and the coefficients of the operators \( A \) and \( B \). As before, \( X \) is a dense subspace of \( V \).

This assumption on norm relations is not new and has been used for many least-squares formulations for numerical methods such as finite element methods (e.g., Bochev and Gunzburger, 2016; Bramble and Schatz, 1970). The first norm relation [Eq. (2a) in Assumption 2.2] gives the stability/regularity of the solution. The second norm relation [Eq. (2b) in Assumption 2.2] is for smooth numerical solutions in \( X \) in which we need universal approximation by NNs, instead of in \( V \); see Appendix B.1 for Case I of an elliptic problem. Also, the condition of Eq. (2a) in
Assumption 2.2 guarantees the uniqueness of the solution in $V$ as shown in the following proposition.

**Proposition 2.1 (Uniqueness).** Let the condition of Eq. (2a) in Assumption 2.2 hold. Then, the solution to Eq. (1) (Definition 2.1) is unique if it exists.

**Proof.** It suffices to consider the problem with homogeneous data $f = g = 0$. Let $u^*$ be a solution to Eq. (1) in the sense of Definition 2.1. Then, there exists a sequence $\{u_k\}$ in $X$ such that $\|u_k - u^*\|_V, \|Au_k\|_Y, \|Bu_k\| \to 0$. If

$$C_1\|u_k\|_V \leq \|Au_k\|_Y + \|Bu_k\|_Z \to 0,$$

then

$$\|u_k\|_V \to 0.$$

Therefore, $u^* = 0$, which shows the uniqueness. \hfill \Box

**Remark 2.2.** The stability (well-posedness) may be relaxed to conditional stability. If the pair $(A, B)$ is not unconditionally stable, i.e., in the sense of Eq. (2a), we may consider a regularization operator $L$ and the triplet $(A, B, L)$, where $L : X \to H$ is linear, where $H$ is a proper Banach space such that it is stable in the following sense: there exist a positive function $D(x)$ and a non-decreasing function $\rho_C : [C, \infty)$ \to $[C, \infty)$ with $\lim_{t \to 0} \rho_C(t) = 0$ for any $C > 0$, such that for $v \in X$ with $\|Lv\|_H \leq C$, it holds that

$$D(v) \leq \rho_C(\|Av\|_X + \|Bv\|_Z).$$

Here $D$ is usually a norm or a semi-norm on a Banach space that $X$ can be embedded into. When $D$ is a norm, we do not need a regularization ($L$) as the problem is well-posed. The loss function at the continuous level can be formulated as

$$\|Av - f\|_Y^2 + \|Bv - g\|_Z^2 + \epsilon^2\|Lv\|_H^2,$$

where $\epsilon$ is small. The conclusion in the following sections can be modified accordingly to obtain stability and convergence of the PINN formulations. We will limit ourselves to well-posed problems for a simple presentation. We refer to Section 3 of Dahmen et al. (2023) and the references therein for examples.

### 2.2 Loss Functionals of Residual Minimization

We present four loss functionals for the RM.

1. (Discrete RM) Given $\{x^r_i, f(x^r_i)\}_{i=1}^{M_r}$, $\{x^b_i, g(x^b_i)\}_{i=1}^{M_b}$, where $\{x^r_i\} \subset \Omega$, $\{x^b_i\} \subset \Gamma$, the discrete loss functional for RM is defined by

$$J^M(u) = \frac{1}{M_r} \sum_{i=1}^{M_r} (f(x^r_i) - A[u](x^r_i))^2 + \frac{1}{M_b} \sum_{i=1}^{M_b} (g(x^b_i) - B[u](x^b_i))^2,$$

where $M = (M_r, M_b)$. See, e.g., Raissi et al. (2017).
2. (Continuous RM) The continuous loss functional for RM is defined by
\[
\mathcal{J}(u) = \|f - Au\|_{L^2(\Omega)}^2 + \|g - Bu\|_{L^2(\partial\Omega)}^2.
\]
Let \(\Omega\) be a bounded domain in \(\mathbb{R}^d\) and \(\{\Omega_k\}_{k=1}^{K}\) be a partition of \(\Omega\). For each \(k\), let \(\{\Phi_{k,s}\}_{s \geq 1}\) be a complete orthonormal basis in \(L^2(\Omega_k)\) or \(H^1_0(\Omega_k)\). Then, by defining \(\Phi_{k,s}(x) = 0\) for all \(x \notin \Omega_k\) and \(k, s\), \(\{\Phi_{k,s}\}\) is a complete orthonormal basis of \(L^2(\Omega)\) or \(H^1_0(\Omega)\).

3. (Discrete \(hp\)-VRM) Let \(\{x_i^k, f(x_i^k)\}_{i=1}^{M_k}\) and \(\{x_i^b, g(x_i^b)\}_{i=1}^{M_b}\) be training points and \(\{\Phi_{i,j}\}_{j=1}^{N_k}\) be a set of test functions in \(L^2(\Omega_k)\) for \(1 \leq k \leq K\). Let \(N = (N_1, \cdots, N_K)\) and \(M = (M_1, \cdots, M_K, M_b)\). Then, a version of the discrete loss functional for \(hp\)-variational RM (\(hp\)-VRM) is given by
\[
\mathcal{J}^{M,N}(u) = \sum_{k=1}^{K} \sum_{s=1}^{N_k} \left( \frac{1}{M_b} \sum_{i=1}^{M_b} (g(x_i^b) - B[u](x_i^b))^2 \right) + \sum_{i=1}^{M_k} \left( \sum_{k=1}^{K} \sum_{s=1}^{N_k} \left( f(x_i^k) - A[u](x_i^k) \right) \Phi_{k,s}(x_i^k) \right)^2.
\]

By applying integration by parts (repeatedly if needed), a different but equivalent formulation of RM can be obtained where the regularity requirement for the numerical solution and the activation functions is weakened; see, e.g., Kharazmi et al. (2019, 2021).

4. (Continuous \(hp\)-VRM) The continuous loss functional for \(hp\)-VRM is given by
\[
\mathcal{J}^N(u) = \sum_{k=1}^{K} \sum_{s=1}^{N_k} \left( |(f - Au, \Phi_{k,s})_{L^2(\Omega_k)}| \right)^2 + \|g - Bu\|_{L^2(\partial\Omega)}^2.
\]

2.3 Feed-Forward Neural Networks

Throughout the paper, any NNs can be applied in our framework as long as they satisfy the universal approximation theorem required in the space of \(X\). For presentation, we assume that the feasible solutions are feed-forward NNs unless explicitly stated otherwise.

Let us first review some of known universal approximation theorems for feed-forward NNs. For a positive integer \(L\), an \(L\)-layer feed-forward NN is a function \(\mathcal{R}[\theta] : \mathbb{R}^{n_0} \rightarrow \mathbb{R}^{n_L}\) that is recursively defined by
\[
\mathcal{R}[\theta](x) = z^L(x), \quad z^l(x) = W_l \phi(z^{l-1}(x)) + b_l, \quad 2 \leq l \leq L, \quad z^1(x) = W_1 x + b_1.
\]
Here \(W_l \in \mathbb{R}^{n_l \times n_{l-1}}\) is the \(l\)th layer weight matrix and \(b_l \in \mathbb{R}^{n_l}\) is the \(l\)th layer bias vector. The activation \(\phi(x)\) is applied elementwise. The collection of network parameters is \(\theta = \{(W_1, b_1), \cdots, (W_L, b_L)\}\). The architecture of the network is represented by the vector \(\tilde{\mathbf{r}} = (n_0, \cdots, n_L)\). With the fixed architecture \(\tilde{\mathbf{r}}\), the set of all possible network parameters is denoted by \(\Theta(\tilde{\mathbf{r}})\).

\[
\Theta(\tilde{\mathbf{r}}) = \{((W_j, b_j))_{j=1}^{L} : W_j \in \mathbb{R}^{n_j \times n_{j-1}}, b_j \in \mathbb{R}^{n_j}, j = 1, 2, \ldots, L\}.
\]

\(^{1}\)It is possible to use bounded weights as the resulting network is still a universal approximator. We will not consider this for simplicity.
Let \( \{ \tilde{n}_n \}_{n \geq 1} \) be a sequence of network architectures such that \( \tilde{n}_n \leq \tilde{n}_{n+1} \) for all \( n \), where the vector inequality is understood entry-wise. We then define its corresponding sequence of NN classes by

\[
\mathcal{N}_{\tilde{n}, n} = \{ \mathcal{R}[\theta](x) : \theta \in \bigcup_{\tilde{v} \leq \tilde{n}_n} \Theta(\tilde{v}) \}.
\]

By the construction, we have \( \mathcal{N}_{\tilde{n}, n} \subset \mathcal{N}_{\tilde{n}, n+1} \). An element of \( \mathcal{N}_{\tilde{n}, n} \) is simply denoted by \( u_{\tilde{n}, n} \), where \( \mathbb{N} \) stands for NN.

Next, we make the following assumption on the sequence of network classes, which guarantees universal approximation.

**Assumption 2.3** (Uniform NN approximation of elements in \( X \)). There exists a sequence of NN classes such that \( \mathcal{N}_{\tilde{n}, n} \subset \mathcal{N}_{\tilde{n}, n+1} \) and \( X \subset \bigcup_n \mathcal{N}_{\tilde{n}, n} \) in the topology of \( (X, \| \cdot \|_X) \).

In literature, Assumption 2.3 is proved for various spaces \( X \). For example, the work of Gühring et al. (2020) shows that for any \( \epsilon \in (0, 0.5) \), \( p \in [1, \infty] \), and \( s \in [0, 1] \), there exists a deep rectified linear unit (ReLU) network architecture \( \tilde{n} \) such that for any \( f \in W_{n,p}((0,1)^d) \) with \( \|f\|_{W_{n,p}} \) being bounded for all \( f \) and \( n \geq 2 \), there exists a NN with parameters \( \theta \in \Theta(\tilde{n}) \) with \( \|\mathcal{R}[\theta] - f\|_{W_{\gamma,p}} \leq \epsilon \). Here the network architecture depends only on \( d, n, p, s, \epsilon \), and the uniform bound of \( f \). Also, the work of Mhaskar and Hahm (1997) showed a similar result for two-layer networks with smooth activation functions.

## 3. CONTINUOUS RESIDUAL MINIMIZATION

A goal of the RM is to approximate the solution to Eq. (1) by solving the optimization problem

\[
\inf_{v \in \mathcal{N}_{\tilde{n}, n} \cap X} \mathcal{J}_\tau(v),
\]

where the loss functional \( \mathcal{J}_\tau(v) \) is defined by

\[
\mathcal{J}_\tau(v) = \|f - Av\|_Y^p + \tau \|g - Bv\|_Z^p.
\]

Here \( \tau > 0, p \geq 1, \) and \( \tau \) is a fixed parameter that weighs the discrepancy of the boundary in the loss. Also, we assume that \( f \in Y \) and \( g \in Z \) and otherwise a mollifier may be applied; see, e.g., in Remark B.1.

**Remark 3.1.** In practice, it has been empirically shown that the choice of \( \tau \) significantly influences the training of NNs (Lagaris et al., 2000; Wang et al., 2021, 2022). It is observed that \( \tau \) depends on the network but may be only moderately large, in which \( \tau \) will not affect our analysis up to some constant.

**Remark 3.2.** For simplicity, we often assume the existence of the global minimizer of Eq. (5). For example, the global minimizer exists when a two-layer network is used for solving PDEs; see Luo and Yang (2020) for details. This assumption can be relaxed by introducing appropriate quasi-minimizers.

The choices of \( Y \) and \( Z \) are important to design the loss functionals; see Appendix B for examples. A guideline for choosing \( Y \) and \( Z \) is Assumption 2.2, which depends on the considered problems and the metric of accuracy (the \( V \)-norm). For PDEs, we may have \( \Gamma = \partial \Omega \) and some typical choices for \( Y \) and \( Z \) are as follows:

\[
\text{In general, it can be } \mathcal{J}_\tau(v) = \tau_r \|f - Av\|_Y^p + \tau \|g - Bv\|_Z^p, \text{ where } \tau_r, \tau > 0. \text{ In this work, we focus on } \tau_r = 1.
\]
• (Banach spaces) \( Y = L^p_\rho(\Omega) \) and \( Z = L^p_\rho(\partial\Omega) \), where \( p \geq 1, \rho : \Omega \rightarrow [0, +\infty) \), \( p \in L^1(\Omega) \), \( \rho_b : \partial\Omega \rightarrow [0, +\infty) \), and \( \rho_b \in L^1(\partial\Omega) \).

• (Banach spaces) \( Y = L^\infty(\Omega) \) and \( Z = L^\infty(\partial\Omega) \).

• (Hilbert spaces) \( Y = H^k(\Omega), k = -2, -1, 0, 1, 2, \ldots \), and \( Z = L^2_\rho(\partial\Omega) \).

### 3.1 Error Estimates

The convergence of (quasi-)minimizers of the loss functional depends on the NN classes \( \{\mathcal{N}_{\theta, n}\}_{n \geq 1} \). The following proposition shows that the universal approximation property (Assumption 2.3) and the norm relation of Eq. (2b) in Assumption 2.2 are sufficient for the convergence of the loss.

**Proposition 3.1.** Suppose Assumptions 2.1, 2.3, and Eq. (2b) of Assumption 2.2 hold. For a fixed \( \tau > 0 \), let \( u_{\tau, n}^\star \) be a quasi-minimizer of the loss of Eq. (6). Then, \( \lim_{n \to \infty} J_\tau(u_{\tau, n}^\star) = 0 \).

**Proof.** Let \( u^\star \) be a solution to Eq. (1) and \( \{v^\star_n\} \) be its corresponding sequence in \( X \) (Definition 2.1). Let \( \{\epsilon_k\} \) be a positive decreasing sequence that converges to 0. For \( k \gg 1 \), it follows from Assumption 2.3 that there exists an integer \( n_k \) and a NN \( u_{n_k} \in \mathcal{N}_{\theta, n_k} \) such that \( \|v^\star_n - u_{n_k}\|_X \leq \epsilon_k \). Observe that Eq. (2b) gives

\[
J_\tau(u_{n_k}) \leq (\|f - Av^\star_n\|_Y + C_2 \epsilon_k)^p + \tau(\|g - Bv^\star_n\|_Z + C_2 \epsilon_k)^p.
\]

Let \( \{u_{\tau, n}^\star\} \) be a sequence of quasi-minimizers of the loss functional in \( \mathcal{N}_{\theta, n} \cap X \), i.e., \( J_\tau(u_{\tau, n}^\star) \leq \inf_{v \in \mathcal{N}_{\theta, n} \cap X} J_\tau(v) + \delta_n \), where \( \delta_n \to 0 \) as \( n \to \infty \). Observe that \( J_\tau(u_{\tau, n}^\star) \leq J_\tau(u_{\tau, n_k}^\star) + \delta_{n_k} \).

By letting \( k \to \infty \), we have \( \lim_{k \to \infty} J_\tau(u_{\tau, n_k}^\star) = 0 \). For \( n_1 < n_2 \), let \( \mathcal{N}_{\theta, n_1} \subset \mathcal{N}_{\theta, n_2} \), we have \( J_\tau(u_{\tau, n_1}^\star) \leq J_\tau(u_{\tau, n_2}^\star) + \delta_{n_2} \). Hence, we can conclude that \( \lim_{n \to \infty} J_\tau(u_{\tau, n}^\star) = 0 \).

As shown in Proposition 3.1, a zero-loss can be achieved if the NN classes \( \mathcal{N}_{\theta, n} \) can capture an approximating sequence in \( X \) (in the sense of Definition 2.1), and the norm relation of Eq. (2b) holds. However, the convergence of the loss does not necessarily imply the convergence of the (quasi-)minimizers to the solution of the governing equation (Shin et al., 2020a).

Next, we present a priori and a posteriori error estimates for optimization of Eq. (5).

**Theorem 3.1 (Error estimates for continuous RM).** Let Assumptions 2.1 and 2.2 hold. Let \( u_{\tau, n}^\star \in \mathcal{N}_{\theta, n} \cap X \) be a solution to the minimization problem Eq. (5) and \( u^\star \) be the solution to Eq. (1) from Assumption 2.1. Then for \( \tau \geq 1 \), the following a posteriori estimation holds:

\[
\|u_{\tau, n}^\star - u^\star\|_V \leq C_1^{-1} 2^{(p-1)/p} \left( J_\tau(u_{\tau, n}^\star) \right)^{1/p}.
\]

(A priori estimate) Also, for any \( \epsilon > 0 \), there exists \( u^\epsilon \in X \) such that

\[
\|u_{\tau, n}^\star - u^\star\|_V \leq 2^{(p-1)/p} (1 + \tau)^{1/p} C_1^{-1} \left( C_2 \inf_{v \in \mathcal{N}_{\theta, n} \cap X} \|v - u^\star\|_X + \epsilon \right).
\]

Here the constants \( C_1 \) and \( C_2 \) are defined in the norm relations Eq. (2).

---

\( \text{\#} \text{It means that } J_\tau(u_{\tau, n}^\star) \leq \inf_{v \in \mathcal{N}_{\theta, n} \cap X} J_\tau(v) + \epsilon, \text{ where } \epsilon \geq 0 \text{ is small.} \)

\( \text{\#} \text{This implies } u_{n_k} \in \mathcal{N}_{\theta, n_k} \cap X \text{ as } \|u_{n_k}\|_X \leq \epsilon_k + \|v^\star_n\|_X < \infty. \)

\( \text{\#} \text{For any } \epsilon > 0 \text{, there exists } K \text{ such that } J_\tau(u_{\tau, n_k}^\star) \leq \epsilon/2 \text{ for all } k \geq K. \text{ Also, there exists } N \text{ such that } \delta_n \leq \epsilon/2 \text{ for all } n \geq N. \text{ By choosing } \hat{N} = \max\{n_K, N\}, \text{ we have } J_\tau(u_{\hat{N}, n}) \leq \epsilon \text{ for all } n \geq \hat{N}. \)
Proof. Since \( \tau \geq 1 \), it then follows from the condition (2a) that

\[
C_1\|u^* - w\|_V \leq 2^{(p-1)/p}(J_\tau(w))^{1/p} \leq 2^{(p-1)/p}(J_\tau(w))^{1/p}, \quad \forall w \in X \subseteq V. \tag{9}
\]

Letting \( w = u_{N,n}^\tau \) leads to the estimate Eq. (7). By Eq. (9), we have

\[
C_1\|u_{N,n}^\tau - u^*\|_V \leq 2^{(p-1)/p}(J_\tau(u_{N,n}^\tau))^{1/p} = 2^{(p-1)/p} \inf_{w \in \mathcal{N}_{\theta,n} \cap X} (J_\tau(w))^{1/p}
\]

\[
\leq 2^{(p-1)/p}(1 + \tau)^{1/p} \inf_{w \in \mathcal{N}_{\theta,n} \cap X} (\|Aw - f\|_Y + \|Bw - g\|_Z).
\tag{10}
\]

For \( \epsilon > 0 \), let \( u^*_\epsilon \in X \) such that \( \|Au^*_\epsilon - f\|_Y + \|Bu^*_\epsilon - g\|_Z < \epsilon \) from Assumption 2.1. By the triangle inequality, we have

\[
\|Aw - f\|_Y + \|Bw - g\|_Z
\]

\[
\leq (\|Aw - Au^*_\epsilon\|_Y + \|Bw - Bu^*_\epsilon\|_Z) + \|Au^*_\epsilon - f\|_Y + \|Bu^*_\epsilon - g\|_Z
\]

\[
< C_2\|w - u^*_\epsilon\|_X + \epsilon,
\tag{11}
\]

where we have used the norm relation (2b) in the last inequality. By combining it with Eq. (10), we obtain

\[
C_1\|u_{N,n}^\tau - u^*\|_V \leq 2^{(p-1)/p}(1 + \tau)^{1/p} (C_2 \inf_{w \in \mathcal{N}_{\theta,n} \cap X} \|w - u^*_\epsilon\|_X + \epsilon),
\]

which completes the proof. We note that if \( u^* \in X \), one may set \( u^*_\epsilon = u^* \) and \( \epsilon = 0 \). \qed

By combining Theorem 3.1 and Proposition 3.1, the convergence of the (quasi-)minimizers can be readily established. We formally state the result in the following.

**Theorem 3.2** (Convergence for continuous RM). Suppose Assumptions 2.1, 2.2, and 2.3 hold. For a fixed \( \tau \geq 1 \), let \( u_{N,n}^\tau \) be a quasi-minimizer of the loss functional Eq. (6). Then,

\[
\lim_{n \to \infty} \|u_{N,n}^\tau - u^*\|_V = 0.
\]

**Remark 3.3.** In practice, regularization is often used in the loss functional Eq. (6) to improve the efficiency of numerical methods. We consider the regularization of non-smooth functionals. For example, when \( Y = L^1(\Omega) \) [as in Guermond (2004)] and \( Z = L^1(\partial\Omega) \), the loss functional is not Fréchet differentiable. In such cases, the loss functional is hard to optimize using gradient-based methods.

### 4. The Effect of Discretizing the Loss Functionals

The continuous norms (integrals) in the functional Eq. (6) are discretized for simulations in finite arithmetic computers. In this section, we discuss the effect of the discretization of the functional Eq. (6). The results are based on Theorem 3.1. The core is to quantify how well the discretization approximates its corresponding continuous norm. In order to characterize the relation between the discrete norm and the continuous norm, we utilize well-designed classes of NNs, which guarantee the convergence with respect to the number of training data samples. The failure of using tailored classes may lead to no convergence even if a zero training loss is achieved. In Example 4.1, we show that even if a zero training loss is achieved, there is no convergence guarantee.

---

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Example 4.1 (Counterexample). Consider the 1D Poisson equation $-\Delta u(x) = f(x)$ on $\Omega = (0, 1)$ with the Dirichlet boundary conditions $u(x) = 0$ on $\partial \Omega = \{0, 1\}$. Suppose that $u^*$ is the unique classical solution. The discrete loss functional is given by $\mathcal{J}_M^\tau(u) = (1/Mr) \sum_{i=1}^{M_r} w_i \times |\Delta u(x_i) - f(x_i)|^2 + (1/2) (|u(0)|^2 + |u(1)|^2)$, where $M = (M_r, M_b) = (2, 2)$, $w_i$’s are some quadrature weights and $\{x_i\}_{i=1}^{M_r}$ with $x_i = i/(M_r+1)$. Let $u^{M^*}_{\mathcal{N}}$ be a minimizer in a network class. Let us consider the case where $u^{M^*}_{\mathcal{N}}(0) = u^{M^*}_{\mathcal{N}}(1) = 0$, and $\Delta u^{M^*}_{\mathcal{N}}(x) - f(x) = (2\pi (M_r + 1))^k \times \sin(2\pi (M_r + 1)x)$ for some positive integer $k \geq 2$, assuming that $f$ is sufficiently smooth. It then can be checked that the training loss is zero, while $\|\Delta u^{M^*}_{\mathcal{N}} - f\|^2_{L^2(\Omega)} = (2\pi (M_r + 1))^{2k} 0.5$. Hence, $\mathcal{J}(u^{M^*}_{\mathcal{N}}) = (2\pi (M_r + 1))^{2k} 0.5$ where $\mathcal{J}(u) = \|\Delta u - f\|^2_{L^2(\Omega)} + (1/2) (|u(0)|^2 + |u(1)|^2)$. This indicates that minimizing the discrete loss may not lead to the convergence in the continuous norm. Even no convergence in $L^2$-norm is achieved. Therefore, extra conditions are required to guarantee convergence.

Let us focus on the case where $Y = L^p(\Omega)$ and $Z = L^p(\Gamma)$. The discretized loss functional of Eq. (6) is defined as

$$\mathcal{J}_\tau^M(v) = \sum_{i=1}^{M_r} w_i^\tau (f(x_i^\tau) - Av(x_i^\tau))^P + \tau \sum_{i=1}^{M_b} w_i^b (g(x_i^b) - Bv(x_i^b))^P,$$

(12)

where $\{(x_i^\tau, w_i^\tau)\}_{i=1}^{M_r}$ is a set of training points and weights in $\Omega$, $\{(x_i^b, w_i^b)\}_{i=1}^{M_b}$ is a set of training points and weights in $\Gamma$, and $M = (M_r, M_b)$. When $p = 2$, $w_i^\tau = 1/M_r$ and $w_i^b = 1/M_b$ for all $i$, we recover the loss function used in Raissi et al. (2017). Let $Y_{M_r}$ be a set of (some special) functions $v \in Y$ such that $v$ is continuous at points $x_i^\tau$ and $\|v\|_{Y_{M_r}} := (\sum_{i=1}^{M_r} |w_i^\tau|^p (v(x_i^\tau))^p)^{1/p} < \infty$. In many cases, it can be checked that $Y_{M_r}$ is a restricted subset of $Y$. Similarly, we define $Z_{M_b}$ as a subset of $Z$. With this notation, one can simply write the discrete loss functional Eq. (12) as $\mathcal{J}_\tau^M(v) = \|f - Av\|_{Y_{M_r}}^p + \tau \|g - Bv\|_{Z_{M_b}}^p$.

4.1 Using Discrete Norm Relations

Motivated by Example 4.1, we make Assumption 4.1. The first condition in Assumption 4.1 is violated in Example 4.1, e.g., when $f = 0$.

Assumption 4.1. For any $n \in \mathbb{N}$, there exist two positive integers $M_r$ and $M_b$ such that

$$\|Av\|_{Y_{M_r}} \geq \frac{1}{2} \|Av\|_Y, \quad \forall v \in \{\mathfrak{N}_{\Theta, n} \cap X | Av \in Y_{M_r}\},$$

$$\|Bv\|_{Z_{M_b}} \geq \frac{1}{2} \|Bv\|_Z, \quad \forall v \in \{\mathfrak{N}_{\Theta, n} \cap X | Bv \in Z_{M_b}\}.$$  

(13)

Here $M_r$ and $M_b$ depend on $n$ and may increase with $n$. The constant $1/2$ can be replaced with any constant larger than 0, while the constant should not depend on $n$, $M_r$, and $M_b$. For example, one can replace $1/2$ with $1 - \epsilon$, where $\epsilon \in (0, 1)$ is independent of $n$, $M_r$, and $M_b$.

Theorem 4.1 (Error estimates of discrete RM I). Let $Y = L^2(\Omega)$, $Z = L^2(\Gamma)$, and $V = X$. Let Assumptions 2.2 and 4.1 be valid. Let $n, n_1$ be given positive integers. Let $M_r, M_b$ be chosen according to Assumption 4.1 with $n_1$. For $\tau \geq 1$, let $u^{M^*}_{\mathcal{N}}$ be a minimizer of $\mathcal{J}_\tau^M$ Eq. (12) over the network class $\mathfrak{N}_{\Theta, n} \cap X$. Assume that $\|v\|_{Y_{M_r}} \leq C_3 \|v\|_Y$ for $v \in Y_{M_r}$ and $\|v\|_{Z_{M_b}} \leq C_3 \|v\|_Z$.
for \( v \in Z_{M_b} \), where \( C_3 > 0 \) is independent of \( M_r \) and \( M_b \). Assume further that there exists \( \bar{v} \in X \) such that \( \bar{v} - u_{\tau,n}^M \in \bar{V}_{n_1} := \{ v \in \mathcal{N}_{b,n_1} \cap X : Av \in Y_{M_r}, Bu \in Z_{M_b} \} \). Then, the following error estimates hold

\[
\left\| u_{\tau,n}^M - u^* \right\|_V \leq 2\sqrt{2}C_1^{-1} \left( J^M_{11}(u_{\tau,n}^M) \right)^{1/2} + 3\sqrt{2}C_1^{-1}C_3 \varepsilon_{f,g,u_{\tau,n}^M}^{1/2}.
\]

Here \( \varepsilon_{f,g,u_{\tau,n}^M} = \inf \left( \left\| A\bar{v} - f \right\|_Y^2 + \left\| B\bar{v} - g \right\|_Z^2 \right) \), where the infimum is taken over all \( \bar{v} \in X \) satisfying \( \bar{v} - u_{\tau,n}^M \in \bar{V}_{n_1} \).

**Proof.** Since \( \bar{v} - u_{\tau,n}^M \in \bar{V}_{n_1} \), by Assumptions 2.2 and 4.1, we have

\[
C_1 \left\| \bar{v} - u_{\tau,n}^M \right\|_V \leq \left\| A(\bar{v} - u_{\tau,n}^M) \right\|_Y + \left\| B(\bar{v} - u_{\tau,n}^M) \right\|_Z
\]

\[
\leq 2 \left\| A(\bar{v} - u_{\tau,n}^M) \right\|_{Y_{M_r}} + 2 \left\| B(\bar{v} - u_{\tau,n}^M) \right\|_{Z_{M_b}}
\]

\[
\leq 2 \left\| f - Au_{\tau,n}^M \right\|_{Y_{M_r}} + 2 \left\| g - Bu_{\tau,n}^M \right\|_{Z_{M_b}} + 2\sqrt{2}(J^M_{11}(\bar{v}))^{1/2}
\]

\[
\leq 2\sqrt{2}(J^M_{11}(u_{\tau,n}^M))^{1/2} + 2\sqrt{2}(J^M_{11}(\bar{v}))^{1/2}.
\]

Then by the triangle inequality and Assumption 2.2,

\[
\left\| u^* - u_{\tau,n}^M \right\|_V \leq \left\| u^* - \bar{v} \right\|_V + \left\| \bar{v} - u_{\tau,n}^M \right\|_V
\]

\[
\leq 2\sqrt{2}C_1^{-1} \left( J^M_{11}(u_{\tau,n}^M) \right)^{1/2} + 3\sqrt{2}C_1^{-1} \left( J^M_{11}(\bar{v}) \right)^{1/2}.
\]

By the assumption, we have \( J^M_{11}(v) \leq C_3 J_{11}(v) \) and we then obtain the desired conclusion. \( \square \)

**Remark 4.1** (Existence of \( \bar{v} \) in Theorem 4.1). For Gaussian radial basis networks in Example 4.2, \( \bar{v} \) can be found from the same set of the Gaussian radial NNs for the approximation of the solution \( u \) (\( n_1 = n \)). For ReLU networks, the existence of \( \bar{v} \) results from the fact that the summation of ReLU networks is still a ReLU network.

**Example 4.2** (Gaussian radial neural networks). Consider the problem of \( Au = f \) on \( \mathbb{R}^d \) with vanishing \( u \) when \( |x| \to \infty \). Here the operator \( A = -\Delta + \text{Id} \), (Id is the identity operator) and \( Bu = 0 \) when \( |x| \to \infty \). Then Assumption 4.1 is satisfied for the following Gaussian radial basis networks \( G_{n,m}(x) \):

\[
\sum_{k=1}^{n} a_k \exp(-|x - x_k|^2) : a_k \in \mathbb{R}, \ x_k \in \mathbb{R}^d, \ \inf_{i \neq j} |x_i - x_j| > \frac{1}{m}, \ \max_{1 \leq k \leq n} |x_k| \leq cm,
\]

where \( n, m \) are user-defined integers, \( c > 1 \) is a constant, and \( a_k \) and \( x_k \) are unknown.

To establish the convergence using the discrete norm relation, we will need to use a proper \( Y_{M_r} \) and the compact set in the relation, which we find below.

Let \( I^*_N \) be the Hermite–Gaussian interpolation operator in one dimension \( (x \in \mathbb{R}) \) such that \( I^*_N v(x^{(j)}) = v(x^{(j)}) \) for all \( v = Q_N(x) \exp(-|x|^2/2) \), where \( Q_N \) is a polynomial of order
no larger than \( N \) and \( x^{(i)} \)'s are the zeros of the normalized Hermite polynomial \( h_{N+1} \). When \( x \in \mathbb{R}^d \), we still use the notation \( I_N \) to represent the \( d \)-dimension interpolation operator using the tensor product of one-dimensional interpolation. For continuous \( v \), define

\[
I_N v = \exp\left(\frac{|x|^2}{2}\right) I_N \left( \exp\left(\frac{|x|^2}{2}\right) v \right).
\]

**Theorem 4.2.** Let \( I_N \) be the interpolation operator defined in Eq. (14). For any \( v \) in the form of \( G_{n,m} \), there exist constants \( c, c_1, c_2 > 0 \) independent of \( n \) and \( m \) and \( c_2 \gg 1 \) such that

\[
\|Av - I_N Av\|_{L^2} \leq c \exp\left( -c_1 m^2 \right) \|v\|_{L^2}, \quad N = c_2 m^2.
\]

**Proof.** The proof can be found in Appendix A.

Let \( v \) be in the form of \( G_{n,m} \). By Theorem 4.2, we can find \( Y_{M_r} \) by observing that

\[
\int_{\mathbb{R}^d} (I_N Av)^2 \, dx = \int_{\mathbb{R}^d} \left( I_N \left( \exp\left(\frac{|x|^2}{2}\right) Av \right) \right)^2 \exp(-|x|^2) \, dx.
\]

By the definition of \( I_N \), we can find a quadrature rule \( \{(x^{(i)}, w_i)^{M_r}_{i=1} \} \) \((M_r = O(N^d))\), for example, such that

\[
\int_{\mathbb{R}^d} (I_N Av)^2 \, dx = \sum_{i=1}^{M_r} (Av(x^{(i)}))^2 w_i.
\]

Let \( Y = L^2(\mathbb{R}^d) \) and \( Y_{M_r} \subset Y \) be equipped with the discrete norm

\[
\|v\|_{Y_{M_r}} = \left( \sum_{i=1}^{M_r} (v(x^{(i)}))^2 w_i \right)^{1/2}.
\]

Then by the Cauchy–Schwarz inequality and Theorem 4.2, we have, for \( v \) in the form of \( G_{n,m} \),

\[
\left\| Av \right\|_Y^2 - \left\| Av \right\|_{Y_{M_r}}^2 = \left\| Av \right\|_Y^2 - \left\| I_N Av \right\|_Y^2 \\
\leq \left\| Av - I_N Av \right\|_{L^2} \left\| Av + I_N Av \right\|_{L^2} \leq C \exp\left( -c_1 m^2 \right) \left\| v \right\|_{L^2} \left\| Av \right\|_{L^2},
\]

where \( C \) is a constant depending on \( c \) from Theorem 4.2. It can be checked by energy estimates that \( \left\| v \right\|_{L^2} \leq \left\| Av \right\|_{L^2} \). Then we have \( \left\| Av \right\|_Y^2 - \left\| Av \right\|_{Y_{M_r}}^2 \leq C \exp\left( -c_1 m^2 \right) \left\| Av \right\|_{L^2}^2 \). Picking \( m \) such that \( C \exp\left( -c_1 m^2 \right) \leq 3/4 \), we obtain that \( 4 \left\| Av \right\|_{Y_{M_r}}^2 \geq \left\| Av \right\|_{Y^2}^2 \geq (4/7) \left\| Av \right\|_{Y_{M_r}}^2 \).

Then for any Gaussian NNs \( v \in W^{2,2} \) such that \( Av \in Y_{M_r} \), the first inequality with \( f = 0 \) in Assumption 4.1 is satisfied. Let \( v = \sum_{k=1}^{n} a_k \exp\left( -|x - x_k|^2 \right) \) and let \( v_f = \sum_{k=1}^{n} f_k \exp\left( -|x - x_k|^2 \right) \) be an approximation of \( f \). By the preceding discussion, we have the following discrete norm relation:

\[
\frac{2}{\sqrt{\mathcal{N}}} \|A(v - v_f)\|_{Y_{M_r}} \leq \|A(v - v_f)\|_{L^2} \leq 2 \|A(v - v_f)\|_{Y_{M_r}}.
\]

Then the error estimates of Gaussian radial basis networks for the problem \( Av = f \) and \( Bu = 0 \) when \( |x| \to \infty \) can be derived by Theorem 4.1.
In general, Assumption 4.1 is not readily verified using the preceding approach via the inverse estimate (Bernstein-type inequality). In fact, the Bernstein-type inequality for deep feed-forward NNs is unavailable for even simple ReLU networks (see a counterexample in Siegel et al., 2023) when there are no constraints on the weights and biases. In the next subsection, we will use the Rademacher complexity to capture the effect of the discretization. The Rademacher complexity for two-layer networks may suggest a lift of the curse of dimensionality as it depends logarithmically on the dimension $d$.

### 4.2 Using Rademacher Complexity

The analysis presented in this section will be based on the uniform law of large numbers for well-designed classes of NNs.

**Definition 4.1** (Rademacher complexity, Gnecco and Sanguineti, 2008; Wainwright, 2019). Given a collection $\{X_i\}_{i=1}^M$ of i.i.d. random samples, the Rademacher complexity of the function class $\mathcal{F}$ is defined by $R_M(\mathcal{F}) = \mathbb{E}_{(X_i, \epsilon_i)_{i=1}}^{\epsilon_i \sim \mathcal{D}} \left[ \sup_{f \in \mathcal{F}} \left| \frac{1}{M} \sum_{i=1}^M \epsilon_i f(X_i) \right| \right]$, where $\epsilon_i$'s are i.i.d. Rademacher random variables i.e., $\mathbb{P}(\epsilon_i = 1) = \mathbb{P}(\epsilon_i = -1) = 0.5$.

For many function classes, the upper bounds of the Rademacher complexity are known. For example, see Neyshabur et al. (2019) for a class of two-layer NNs and see E et al. (2019) for a class of Barron functions. In many cases, it can be shown that the Rademacher complexity converges to zero as the number of samples $M$ grows to infinite, such as in E et al. (2019) where the convergence rate is half.

Let $\{u_k^\star\}$ be a sequence approximating the solution, as defined in Definition 2.1. By definition, the sequences $\{Au_k^\star - f\}$ and $\{Bu_k^\star - g\}$ are uniformly bounded. In what follows, we make an additional assumption on these sequences required for the uniform law of large numbers.

**Assumption 4.2.** Let $u^\star$ be a solution to Eq. (1) in the sense of Definition 2.1 and $\{u_k^\star\}$ be its corresponding sequence in $X$. Let $G_r \geq \max \{ \|f\|_{L^\infty(\Omega)}, \sup_k \|Au_k^\star - f\|_{L^\infty(\Omega)} \}$, and $G_b \geq \max \{ \|g\|_{L^\infty(\Gamma)}, \sup_k \|Bu_k^\star - g\|_{L^\infty(\Gamma)} \}$. Assume $G_r, G_b < \infty$.

Under the Assumption 4.2, we introduce the following function classes.

**Definition 4.2.** Let $G_r, G_b$ be positive numbers defined in Assumption 4.2. Define a subclass of $\mathfrak{F}_{Q,n}$ by $\mathfrak{F}_{Q,n}^O = \{ R(\theta) \in \mathfrak{F}_{Q,n} : \theta \in \Theta_Q(\bar{\theta}_n) \}$, where $\Theta_Q(\bar{\theta}_n)$ is similarly defined as in Eq. (3) but all weights and biases are rational numbers. Introduce two function classes:

$$\mathfrak{F}_{r,n} := \left\{ Av - f \in Y : v \in \mathfrak{F}_{Q,n}^O \cap X \text{ and } \| Av - f \|_{L^\infty(\Omega)} \leq G_r \right\}$$

$$\mathfrak{F}_{b,n} := \left\{ Bv - g \in Z : v \in \mathfrak{F}_{Q,n}^O \cap X \text{ and } \| Bv - g \|_{L^\infty(\Gamma)} \leq G_b \right\}.$$

Finally, define a subclass of $\mathfrak{F}_{Q,n}^O$

$$\mathfrak{F}_{Q,n}^O := \left\{ v \in \mathfrak{F}_{Q,n}^O \cap X : Av - f \in \mathfrak{F}_{r,n}, Bv - g \in \mathfrak{F}_{b,n} \right\}. \quad (16)$$

From Assumption 4.2, the countable set $\mathfrak{F}_{Q,n}^O$ is not empty as it contains the zero function. One can also consider an uncountable function class by strengthening Assumption 4.2 with the uniform topology $C^0$. 
Next, we bound the discrepancy between the continuous norm and its discretization using the Rademacher complexity. The following lemma is obtained by applying the uniform law of large numbers on the function class defined in Definition 4.2.

**Lemma 4.1.** Suppose Assumption 4.2 holds. Let $G_r, G_b$ be positive numbers defined in Assumption 4.2. Let $\{x_1^M, x_1^M\}_{i=1}^{M_r}$ and $\{y_1^M, y_1^M\}_{i=1}^{M_b}$ be i.i.d. samples following probability densities $\rho$ over $\Omega$ and $\rho_b$ over $\Gamma$, respectively in the discrete RM loss Eq. (12). Let $Y = L^p_\rho(\Omega)$ and $Z = L^p_{\rho_b}(\Gamma)$ for $p \geq 1$. For any small $\delta_r, \delta_b > 0$,

$$\sup_{A \in \mathcal{F}_r} \left\| A - f \right\|^p_{L^p_\rho(\Omega)} - \left\| A - f \right\|^p_{L^p_\rho(\Omega)} \leq 2R_M \left( \mathcal{F}^p_{r,n} \right) + \frac{\delta_r}{2}, \text{ with prob. at least } Q_r,$$

$$\sup_{B \in \mathcal{F}_b} \left\| B - g \right\|^p_{L^p_{\rho_b}(\Gamma)} - \left\| B - g \right\|^p_{L^p_{\rho_b}(\Gamma)} \leq 2R_M \left( \mathcal{F}^p_{b,n} \right) + \frac{\delta_b}{2}, \text{ with prob. at least } Q_b,$$

where

$$Q_r = 1 - 2 \exp \left( -\frac{M_r \delta_r^2}{32G_r^2} \right), \quad Q_b = 1 - 2 \exp \left( -\frac{M_b \delta_b^2}{32G_b^2} \right).$$

Furthermore, with probability at least $Q_r, Q_b$,

$$\sup_{v \in \mathcal{F}_{r,n}} \left| J^M_r (v) - J_r (v) \right| \leq 2R_M \left( \mathcal{F}^p_{r,n} \right) + 2\tau R_M \left( \mathcal{F}^p_{b,n} \right) + \frac{\delta_r}{2} + \frac{\delta_b}{2}.$$

**Proof.** Recall from Section 4.1 that

$$\left\| A - f \right\|^p_{Y_{M_r}} = \frac{1}{M_r} \sum_{i=1}^{M_r} \left( f(x_i^r) - A(x_i^r) \right)^p, \quad \left\| B - g \right\|^p_{Z_{M_b}} = \frac{1}{M_b} \sum_{i=1}^{M_b} \left( g(x_i^b) - B(x_i^b) \right)^p.$$

We observe that

$$\left| J^M_r (v) - J_r (v) \right| \leq \left| \left\| A - f \right\|^p_{Y_{M_r}} - \left\| A - f \right\|^p_{L^p_\rho(\Omega)} \right| + \tau \left| \left\| B - g \right\|^p_{Z_{M_b}} - \left\| B - g \right\|^p_{L^p_{\rho_b}(\Gamma)} \right|.$$

For each $F \in \mathcal{F}_{r,n}$, since $\left\| F \right\|_{L^\infty(\Omega)} \leq G_r, P(\left\| F(x) \right\| \leq G_r) = 1$. Since $\mathcal{F}_{r,n}$ is countable, we have $P(\sup F \in \mathcal{F}_{r,n} | F(x) \leq G_r) = 1$ by the continuity of the probability measure. A similar argument leads to the conclusion for $\mathcal{F}_{b,n}$. Then Eqs. (17) and (18) can be obtained by invoking a uniform law via the Rademacher complexity (e.g., Theorem 4.2 of Wainwright, 2019). Combining the preceding two estimates leads to the last desired conclusion. \hfill \Box

**Example 4.3** (Rademacher complexity for two-layer networks). Let $\mathcal{F}_2 \ni n$ be the class of two-layer NNs defined by

$$\mathcal{F}_2 \ni n := \left\{ [0,1]^d \ni x \to c_0 + \sum_{i=1}^{n} c_i \phi \left( w_i^T x + b_i \right) : \max |b_i|, \| w_i \|_{\ell_1}, |c_i| \leq \omega_{\max} \right\},$$

for $\mathcal{F}_2 \ni n$. Then $G_r, G_b$ be positive numbers defined in Assumption 4.2. Let $\{x_1^M, x_1^M\}_{i=1}^{M_r}$ and $\{y_1^M, y_1^M\}_{i=1}^{M_b}$ be i.i.d. samples following probability densities $\rho$ over $\Omega$ and $\rho_b$ over $\Gamma$, respectively in the discrete RM loss Eq. (12). Let $Y = L^p_\rho(\Omega)$ and $Z = L^p_{\rho_b}(\Gamma)$ for $p \geq 1$. For any small $\delta_r, \delta_b > 0$,
where \( \phi \) is \( \gamma \)-Lipschitz and anti-symmetric, i.e., \( \phi(-x) = -\phi(x) \) (e.g., \( \phi(x) = \tanh(x) \)). For the sake of the length of the paper, we briefly give a sketch of how one can estimate \( R_{M}(\tilde{\mathcal{S}}^{p}_{b,n}) \) and \( R_{M}(\tilde{\mathcal{S}}^{p}_{b,n}) \) when \( A \) is the Laplacian \( \Delta \) on \( \Omega = [0, 1]^d \) and \( B \) is the identity operator on \( \partial \Omega \). It then can be checked that (e.g., Neyshabur et al., 2019)

\[
R_{M}(\mathcal{N}_{b,n}) \leq \frac{\omega_{\text{max}}}{\sqrt{M}} \left( 1 + 2\gamma \omega_{\text{max}}(1 + \sqrt{2\log(2d)}) \right).
\]

Observe that \( \tilde{\mathcal{S}}_{r,n} \) and \( \tilde{\mathcal{S}}_{b,n} \) are given by

\[
\tilde{\mathcal{S}}_{r,n} = \left \{ [0,1]^{d} \ni x \mapsto \sum_{i=1}^{n} c_{i} \| w_{i} \| \tilde{\phi}''(w_{i}^{T}x + b_{i}) - f(x) : \max \{ \| b_{i} \|, \| w_{i} \|, c_{i} \} \leq \omega_{\text{max}} \right \}
\]

\[
\tilde{\mathcal{S}}_{b,n} = \left \{ [0,1]^{d} \ni x \mapsto c_{0} + \sum_{i=1}^{n} c_{i} \phi(w_{i}^{T}x + b_{i}) - g(x) : \max \{ \| b_{i} \|, \| w_{i} \|, c_{i} \} \leq \omega_{\text{max}} \right \}.
\]

Since \( \| g \|_{L^{\infty}((\Omega)} < \infty \), \( R_{M}(\tilde{\mathcal{S}}_{b,n}) \) is bounded by \( R_{M}(\mathcal{N}_{b,n}) + \| g \|_{L^{\infty}((\Omega)} / \sqrt{M} \) (Chapter 4 of Wanwright, 2019). Also, since \( \| f \|_{L^{\infty}((\Omega)} < \infty \), \( R_{M}(\tilde{\mathcal{S}}_{r,n}) \) is bounded by \( R_{M}(\Delta \mathcal{N}_{b,n}) + \| f \|_{L^{\infty}((\Omega)} / \sqrt{M} \), where \( \Delta \mathcal{N}_{b,n} = \{ \Delta u : u \in \mathcal{N}_{b,n} \} \). Assuming \( \phi'' \) is \( \gamma \)-Lipschitz and anti-symmetric, \( R_{M}(\Delta \mathcal{N}_{b,n}) \) can also be estimated similarly. Lastly, since every function in \( \tilde{\mathcal{S}}_{r,n} \) (or \( \tilde{\mathcal{S}}_{b,n} \)) is bounded and \( x \mapsto x^{p} \) is Lipschitz on a bounded interval, an upper bound of the Rademacher complexity of \( \tilde{\mathcal{S}}^{p}_{r,n} \) (or \( \tilde{\mathcal{S}}^{p}_{b,n} \)) can be found.

With Lemma 4.1 and Theorem 3.1, we establish error estimates for the discrete RM.

**Theorem 4.3** (Error estimates of discrete RM II). Suppose Assumptions 2.1, 2.2, and 4.2 hold. Suppose \( \{ x_{i} \}^{M}_{i=1} \) and \( \{ x_{i} \}^{M}_{i=1} \) are i.i.d. samples following probability densities \( \rho \) over \( \Omega \) and \( \rho_{b} \) over \( \Gamma \), respectively in the discrete RM loss Eq. (12) where \( \tau \geq 1 \). Let \( Y = L_{p_{b}}^{p}(\Omega) \) and \( Z = L_{p_{b}}^{p}(\Gamma) \) for \( p \geq 1 \). Let \( u^{\tau,M}_{b,n} \) be a solution to \( \min_{u \in \tilde{\mathcal{N}}^{p}_{b,n}} \mathcal{J}^{M}(u) \), where \( M = (M_{r}, M_{b}) \). Let \( u^{*} \) be the solution to Eq. (1) in the sense of Definition 2.1. Then, for \( \delta > 0 \), with probability at least

\[
Q_{r,b} = \left( 1 - 2 \exp \left( -\frac{M_{r}\delta^{2}}{32G_{b}^{2p}} \right) \right) \left( 1 - 2 \exp \left( -\frac{M_{b}\delta^{2}}{32G_{b}^{2p}} \right) \right)
\]

we have

\[
\left\| u^{\tau,M}_{b,n} - u^{*} \right\|_{V} \leq C_{1}^{-1} \frac{2(p-1)}{p} \left[ \mathcal{J}^{M}(u^{\tau,M}_{b,n}) + 2R_{M}(\tilde{\mathcal{S}}^{p}_{b,n}) + (1 + \tau)\delta / 2 \right]^{1/p},
\]

where \( R_{M}(\tilde{\mathcal{S}}^{p}_{b,n}) := R_{M}(\mathcal{N}_{b,n}) + \tau R_{M}(\mathcal{N}_{b,n}) \). Also, for any \( \epsilon > 0 \), there exists \( u^{*}_{\epsilon} \in X \) such that with probability \( Q_{r,b} \) (at least), we have

\[
\left\| u^{\tau,M}_{b,n} - u^{*} \right\|_{V} \leq C_{1}^{-1} \frac{2(p-1)}{p} \left( 1 + \tau \inf_{w \in \mathcal{N}^{p}_{b,n}} (C_{2}\| w - u^{*}_{\epsilon} \|_{X} + \epsilon)^{p} + 4R_{M}(\tilde{\mathcal{S}}^{p}_{b,n}) + (1 + \tau)\delta \right)^{1/p}.
\]

Here \( C_{1} \) and \( C_{2} \) are the constants defined in Eq. (2).

**Proof.** From Theorem 3.1, we have \( \left\| u^{\tau,M}_{b,n} - u^{*} \right\|_{V} \leq C_{1}^{-1} \frac{2(p-1)}{p} \left[ \mathcal{J}^{\tau}(u^{\tau,M}_{b,n}) \right]^{1/p} \). Since \( u^{\tau,M}_{b,n} \in \tilde{\mathcal{N}}^{p}_{b,n} \), it follows from Lemma 4.1 that with probability \( Q_{r,b} \) (at least), we have

\[
\left\| u^{\tau,M}_{b,n} - u^{*} \right\|_{V} \leq C_{1}^{-1} \frac{2(p-1)}{p} \left[ \mathcal{J}^{\tau}(u^{\tau,M}_{b,n}) \right]^{1/p}.
\]
there exists a solution sequence 

Similarly, with probability $Q_{r,b}$ (at least), we have

For $\varepsilon > 0$, let $u^*_\varepsilon \in X$ be an approximation of $u^*$ such that $\|Au^*_\varepsilon - f\|_V + \|Bu^*_\varepsilon - g\|_Z < \varepsilon$. From Eqs. (10) and (11), we have

Combining the preceding inequality with Eq. (19), we obtain

The proof is then complete. □

Next, we characterize the conditions under which a sequence of minimizers of the discrete RM loss functionals converges to the solution strongly in $V$.

**Theorem 4.4 (Convergence of discrete RM).** Under the same conditions of Theorem 4.3, suppose $\lim_{M_\tau \to \infty} R_{M_\tau}(\tilde{\mathcal{G}}^p_{\tau,n}) = 0$, and $\lim_{M_b \to \infty} R_{M_b}(\tilde{\mathcal{G}}^p_{b,n}) = 0$ for all $n$. Suppose further that there exists a solution sequence $\{v^*_k\}$ (Definition 2.1) that belongs to $\bigcup_{n=1}^\infty \tilde{\mathcal{G}}^p_{\tau,n}$ in the topology of $(X, \| \cdot \|_X)$. Then, we have

\[
\lim_{n \to \infty} \lim_{M \to \infty} \left\| u^\tau_{n,M} - u^* \right\|_V = 0, \quad M = (M_\tau, M_b),
\]

in probability.

**Proof.** Let $\{v^*_k\}$ be the solution sequence and let $\{\epsilon_k\}$ be a positive decreasing sequence converging to 0. For $k \gg 1$, it follows from the assumption that there exists an integer $n_k$ and a NN $u^{Q}_{n_k} \in \tilde{\mathcal{G}}^Q_{\tau,n_k} \cap X$ such that $\|u^{Q}_{n_k} - v^*_k\|_X \leq \epsilon_k$. From Theorem 4.3, by choosing $\delta_\tau = 2M_\tau^{-1/2+\varepsilon}$ and $\delta_b = 2M_b^{-1/2+\varepsilon}$ for $0 < \varepsilon < 1/2$, with probability at least

\[
\left(1 - 2 \exp\left(-\frac{M^\tau_b}{8G^p_{\tau}}\right)\right) \left(1 - 2 \exp\left(-\frac{M^\tau_b}{8G^p_{\tau}}\right)\right),
\]

we have

\[
\left\| u^\tau_{n,n_k} - u^* \right\|_V \leq C_1^{-1}2^{(p-1)/p} \left[ J^M_\tau(u^\tau_{n,n_k}) + 2 \tilde{R}_M(\tilde{\mathcal{G}}^p_{\tau,n}) + M_\tau^{-1/2+\varepsilon} + \tau M_b^{-1/2+\varepsilon}\right]^{1/p}.
\]

By letting $M_\tau, M_b \to \infty$, we have $\lim_{M \to \infty} \left\| u^\tau_{n,n_k} - u^* \right\|_V \leq C_1^{-1}2^{(p-1)/p} \left[ J^M_\tau(u^Q_{n_k}) \right]^{1/p}$ with probability 1 over i.i.d. samples. Since
Remark 5.1. In practice, it is convenient to consider the following functional basis of \( J_h \) for tensor product domains. Let \( \{ \Phi_{k,i} \}_{k,i=1}^{\infty} \) be a complete orthonormal basis in a Hilbert space \( Y \). Also, let \( \{ \Phi_{k,i} \}_{k,i=1}^{\infty} \) be a complete orthonormal basis in \( Y|_{\Omega_k} \), which is defined with the same structure as in \( Y \) but over the domain \( \Omega_k \). Then, the loss functional Eq. (6) can be written as \( J_\tau(v) = \sum_{k,i=1}^{\infty} (f - Av, \Phi_{k,i})_Y^2 + \tau \|Bu - g\|_Z^2 \), and its corresponding truncation is given by

\[
J_\tau h,N(v) = \sum_{k=1}^{K_h} \sum_{i=1}^{N_k} (f - Av, \Phi_{k,i})_Y^2 + \tau \|Bu - g\|_Z^2,
\]

where \( N = (N_1, \ldots, N_{K_h}) \). For simplicity, we write \( K_h \) as \( K \). If \( N_k = N \) for all \( k \), we write \( J_\tau h,N \) as \( J_\tau h,N \). We can perform integration by parts on \( (f - Av, \Phi_{k,i})_Y \). The goal of \( hp \)-VRM is to find a solution to the minimization problem \( \inf_{v \in S} J_\tau h,N(v) \), where the feasible space \( S \) is to be determined shortly.

When \( f - Av \) is merely in \( L^p(\Omega) \) \((p \in [1, \infty))\), we cannot use the RM formulation. In contrast, we can still use the \( hp \)-VRM formulation by performing integration by parts. In other words, the \( hp \)-VRM formulation with the piecewise constant basis is a weak formulation of RM.

Remark 5.1. In practice, it is convenient to consider the following functional \( J_\tau h,N(v) = \sum_{k=1}^{K_h} \sum_{i=1}^{N_k} \alpha_{k,i} (f - Av, \Phi_{k,i})_Y^2 + \tau \|Bu - g\|_Z^2 \), where \( 0 < M_0 \leq \alpha_{k,i} \leq M \) as \( M_0 J_\tau h,N(v) \). We have the freedom to choose \( \alpha_{k,i} \) and \( \Phi_{k,i} \). To simplify the analysis, we always assume that for each \( k \), \( \{ \Phi_{k,i} \}_{i=1}^{\infty} \) is a complete orthonormal basis of \( Y|_{\Omega_k} \) and \( \alpha_{k,i} = 1 \).

Remark 5.2. We can also treat the boundary residual in a similar way. In practice, the boundary might be irregular. It is then practical to use piecewise constants as the basis, instead of piecewise polynomials.

To illustrate the \( hp \)-VRM formulation, we consider two special cases when \( Y = L^2(\Omega) \) and \( Y|_{\Omega_k} = L^2(\Omega_k) \). The first one is the basis of orthonormal polynomials over smooth regular domains. This formulation with Jacobi-type polynomials as the basis is used in Kharazmi et al. (2019) for tensor product domains.

The second one is the basis of piecewise constants \( (i.e., N = 1) \) over possibly very complicated domains, leading to a weak formulation of RM. The first term in the functional \( J_\tau h,N(v) \)
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It means that

\[ \sum_{k=1}^{K} \| (f - Av, \Phi_{k,i})_{L^2(\Omega_k)} \|^2 = \sum_{k=1}^{K} (1/|\Omega_k|)(f_{\Omega_k} f - Av dx)^2. \]

Specifically, we employ \( \{ \Phi_{k,i}(x) = |\Omega_k|^{-1/2} \Phi_{k,i}(x) \}_{k=1}^{K} \), which is an orthonormal basis in \( L^2(\Omega) \). Here \( |\Omega_k| \) represents the Lebesgue measure (volume) of the domain \( \Omega_k \).

Let \( f, v \), and the coefficients of \( A \) be smooth enough so that \( f - Av \) is continuous (or in \( L^\infty \)).

Then, by the mean value theorem of definite integrals, there exists a point \( x_k^* \in \Omega_k \) such that the preceding term becomes

\[ \sum_{k=1}^{K} (1/|\Omega_k|)(f(x_k^*) - A[v](x_k^*))^2, \]

which is the first term in the discrete RM formulation Eq. (12). If \( f - Av \) is not in \( L^\infty \), we may apply integration by parts in the following formula:

\[ \sum_{k=1}^{K} (1/|\Omega_k|)(f_{\Omega_k} f - Av dx)^2 + \tau \sum_{i=1}^{M}(1/|\Gamma_i|)(f_{\Gamma_i}(Bu - g) dx)^2. \]

Here \( \Gamma_i \)'s form a partition of \( \Gamma \).

Remark 5.3. With integration by parts, the formulation can accommodate bases for overlapping domains; e.g., piecewise linear polynomials in Khodayi-Mehr and Zavlanos (2020), which form a complete basis in \( H^1 \).

5.2 Error Estimates

In this section, we present error estimates for continuous \( hp \)-VRM but do not present detailed analysis for the discrete \( hp \)-VRM, as it is straightforward to combine the analysis of discrete RM and continuous \( hp \)-VRM.

The key idea is to identify a class of functions and a set of orthogonal basis that satisfy a certain norm relation between the projection operator and the full operator. We then apply Theorem 3.1 to derive an error estimate for the \( hp \)-VRM.

For a set \( \{ \Phi_{k,i} \}_{i=1}^{N_k} \) of orthogonal basis for \( Y |_{\Omega_k} \), \( k = 1, \cdots, K \), let us define the associated projection operator \( P_{h,N} \) by

\[ P_{h,N} v = \sum_{k=1}^{K} P_k v, \quad \text{where} \quad P_k v = \sum_{i=1}^{N_k} (v, \Phi_{k,i})_{Y|_{\Omega_k}} \Phi_{k,i}, \quad \forall v \in Y, \quad (21) \]

with \( N = (N_1, \cdots, N_K) \).

Following the idea in Section 4.1, we may assume that there exists a compact set \( Y_c \) of \( Y \) such that for all \( v \in \mathcal{N}_{\theta,n} \cap X \cap Y_c \) such that \( 2\| P_{h,N} v \|_Y \geq \| P_{h,N} v \|_Y \). As in Section 4.1, such inequality relies on Bernstein-type inequality for networks but is unavailable for deep feed-forward networks. Instead, we follow a similar approach used in Section 4.2.

Definition 5.1 (Definition of \( \hat{V}_K \)). Let Assumptions 2.1 and 2.3 hold. Let \( \{ u_{n}^* \} \) be an approximation sequence in \( X \) from Definition 2.1. For a positive decreasing sequence \( \{ \epsilon_n \} \) that converges to 0, let \( u_{m_n} \in \mathcal{N}_{\theta,m_n} \) be a NN satisfying \( \| u_{m_n} - u_{n}^* \|_X \leq \epsilon_n \) (this is guaranteed by Assumption 2.3). Let \( \Omega = \bigcup_{k=1}^{K} \Omega_k \). For each \( k \), let \( G_k \) be a compact set in \( Y |_{\Omega_k} \) containing the sequence \( \{ (A u_{m_n} - f) |_{\Omega_k} \} \). We then define a class of functions in \( X \) as follows:

\[ \hat{V}_K := \{ v \in X : (Av - f) |_{\Omega_k} \in G_k, \forall k = 1, \cdots, K \}. \]

Next, we show that the function class \( \hat{V}_K \) is sufficiently large enough to reach a zero training loss.

Proposition 5.1 (Loss convergence). Suppose Assumptions 2.1 and 2.3 and Eq. (2b) of Assumption 2.2 hold. For any \( N = (N_1, \cdots, N_K) \) and \( \tau \geq 1 \), let \( J_{\tau}^{h,N} \) be the loss functional Eq. (20) and \( u_{\hat{V}_k}^{h,N} \) be its quasi-minimizer\(^*\). Then, \( \lim_{n \to \infty} J_{\tau}^{h,N} (u_{\hat{V}_k}^{h,N}) = 0. \)

\(^*\)It means that \( J_{\tau}^{h,N} (u_{\hat{V}_k}^{h,N}) \leq \inf_{v \in \mathcal{N}_{\theta,n} \cap \hat{V}_k} J_{\tau}^{h,N} (v) + \epsilon, \) where \( \epsilon \geq 0 \) is small.
Proof. Let \( \{u_k^\varepsilon\} \) and \( \{u_{nk}\} \) be the sequences from Definition 5.1. Let \( u_{n,1}^{h,N} \in \mathcal{N}_{0,n} \cap \tilde{V}_K \) be a quasi-minimizer of the loss functional, i.e., \( J_{\tau}^{h,N}(u_{n,k}^{\varepsilon}) \leq \inf_{v \in \mathcal{N}_{0,n} \cap \tilde{V}_K} J_{\tau}^{h,N}(v) + \delta_n \), where \( \lim_{n \to \infty} \delta_n = 0 \). Since \( u_{nk} \in \mathcal{N}_{0,n} \cap \tilde{V}_K \), we have

\[
J_{\tau}^{h,N}(u_{n,k}^{\varepsilon}) \leq J_{\tau}^{h,N}(u_{nk}) + \delta_n \leq J_{\tau}(u_{nk}) + \delta_n.
\]

Since \( \lim_{k \to \infty} J_{\tau}(u_{nk}) = 0 \) [by Eq. (2b) of Assumption 2.2], we have \( \lim_{k \to \infty} J_{\tau}^{h,N}(u_{n,k}^{\varepsilon}) = 0 \). Since \( J_{\tau}^{h,N}(u_{n,k}^{\varepsilon}) \leq J_{\tau}^{h,N}(u_{nk}) + \delta_n \) for all \( s_1 < s_2 \), the proof is completed. \( \square \)

The training loss being zero, however, does not necessarily imply the convergence of quasi-minimizers to the solution to Eq. (1). In the next lemma, we show that if the \( hp \)-VRM loss is carefully constructed, the loss functional of Eq. (20) is a good approximation to the loss functional of Eq. (6).

Lemma 5.1. Let Assumptions 2.1 and 2.3 hold. Let \( \tilde{V}_K \subset X \) be a class of functions defined in Definition 5.1. Let \( \Omega = \bigcup_{k=1}^K \Omega_k \). For any \( \varepsilon > 0 \), there exists a set of orthogonal basis \( \{ \Phi_{k,i} \}_{i=1}^{N_{e,k}} \) in \( Y|_{\Omega_k} \) for \( k = 1, \ldots, K \) that defines \( J_{\tau}^{h,N,e} \) with \( N_e = (N_{e,1}, \ldots, N_{e,K}) \), which satisfies \( J_{\tau}^{h,N,e}(v) \geq J_{\tau}(v) - \varepsilon, \forall v \in \tilde{V}_K \).

Proof. Let \( f_k = f|_{\Omega_k} \) and let \( G_k \) be the compact set in \( Y|_{\Omega_k} \) from Definition 5.1. Then, for any \( \varepsilon > 0 \), there exists a finite-dimensional subspace \( \tilde{K}^{e,K} \) of \( Y|_{\Omega_k} \) such that for any \( u \in G_k \), there exists \( u_\varepsilon \in \tilde{K}^{e,K} \) satisfying \( \|u - u_\varepsilon\|_{Y|_{\Omega_k}} \leq \sqrt{\varepsilon/K} \). Let \( \tilde{K}^{e,K} \) be spanned by \( \{ \Phi_{k,i} \}_{i=1}^{N_{e,k}} \) and let \( P_{h,N_e} \) be defined through this basis. Observe that for any \( v \in \tilde{V}_K \), since \( Av|_{\Omega_k} - f_k \in G_k \), there exists \( \tilde{g}_k \in \tilde{K}^{e,K} \) such that \( \|Av|_{\Omega_k} - f_k - \tilde{g}_k\|_{Y|_{\Omega_k}} \leq \sqrt{\varepsilon/K} \). Hence, \( \|I-P_{h,N_e}(Av - f_k)\|_2^2 = \sum_{k=1}^K \|I-P_{h,N_e}(Av|_{\Omega_k} - f_k)\|_2^2 \leq \varepsilon, \forall v \in \tilde{V}_K \). Thus, we have \( J_{\tau}^{h,N,e}(v) = J_{\tau}(v) - \|I-P_{h,N_e}(Av - f_k)\|_2^2 \geq J_{\tau}(v) - \varepsilon \), and the proof is completed. \( \square \)

To establish error estimates and convergence, we now consider the \( hp \)-VRM formulation under \( \mathcal{N}_{0,n} \cap \tilde{V}_K \) with the loss functional defined through the specific basis from Lemma 5.1. That is,

\[
\min_{v \in \mathcal{N}_{0,n} \cap \tilde{V}_K} J_{\tau}^{h,N,e}(v).
\]

The feasible function class \( \tilde{V}_K \) depends only on the number of partitions of the domain \( \Omega \) and an approximation sequence \( \{u_{nk}\}_{k \geq 1} \) from Definition 5.1. Also, \( \tilde{V}_K \) is non-empty as it includes \( \{u_{nk}\}_{k \geq 1} \).

Theorem 5.1 (Error estimates for \( hp \)-VRM). Under the same assumptions in Lemma 5.1, suppose Assumption 2.2 holds. Let \( \tilde{V}_K \subset X \) be a function class defined in Definition 5.1. For any \( \varepsilon > 0 \) and \( \tau \geq 1 \), let \( \{ \Phi_{k,i} \}_{i=1}^{N_{e,k}} \) be a set of orthonormal basis with respect to \( Y|_{\Omega_k} \) for \( k = 1, \ldots, K \) from Lemma 5.1. Let \( u_{n,1}^{\varepsilon,N_e} \in \mathcal{N}_{0,n} \cap \tilde{V}_K \) be a quasi-minimizer of Eq. (22), and \( u^* \) be the solution to Eq. (1) in the sense of Definition 2.1. Then, the following a posteriori estimation holds:

\[
\|u_{n,1}^{\varepsilon,N_e} - u^*\|_V \leq \sqrt{2C_{e}^{-1}} \left( J_{\tau}^{h,N,e}(u_{n,1}^{\varepsilon,N_e}) + \delta_n + \varepsilon \right)^{1/2},
\]

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where $C_1$ is the constant defined in the norm relation Eq. (2) and $\delta_n$ is a vanishing sequence stemming from the choice of quasi-minimizers.

**Proof.** Let $u^*$ be the solution to Eq. (1). For $\epsilon > 0$, let $u^*_n$ be a quasi-minimizer of the loss $J_{\epsilon}^{h,N_k}$ defined through Lemma 5.1 over $\Omega_{0,n} \cap \mathcal{V}_K$. That is, $J_{\epsilon}^{h,N_k} (u^*_n) \leq \inf_{w \in \Omega_{0,n} \cap \mathcal{V}_K} J_{\epsilon}^{h,N_k} (w) + \delta_n$, where $\delta_n \to 0$ as $n \to \infty$. By Lemma 5.1, since $J_{\epsilon} (v) \leq J_{\epsilon}^{h,N_k} (v) + \epsilon$ for all $v \in \mathcal{V}_K$, we obtain

$$J_{\epsilon} (u^*_n) = J_{\epsilon}^{h,N_k} (u^*_n) + \|((I - P_h)A u^*_n - f)\|^2_{Y} \leq \inf_{w \in \Omega_{0,n} \cap \mathcal{V}_K} J_{\epsilon}^{h,N_k} (w) + \delta_n + \epsilon.$$  

It then follows from Theorem 3.1 that

$$C_1^2 \|u^*_n - u^*\|^2_{V} \leq 2J_{\epsilon} (u^*_n) \leq 2 \left( \inf_{w \in \Omega_{0,n} \cap \mathcal{V}_K} J_{\epsilon}^{h,N_k} (w) + \delta_n + \epsilon \right).$$

Letting $w = u^*_n$ completes the proof. \(\square\)

**Theorem 5.2 (Convergence of $hp$-VRM).** Under the same conditions and assumptions of Theorem 5.1, for $\epsilon > 0$, let $u^*_n$ be a quasi-minimizer of Eq. (22) defined through Lemma 5.1. Then, $\lim_{\epsilon \to 0} \lim_{n \to \infty} \|u^*_n - u^*\|^2_{V} = 0$, where $u^*$ is the solution to Eq. (1) from Assumption 2.1.

**Proof.** It follows from Theorem 5.1 and Proposition 5.1 that $\lim_{n \to \infty} \|u^*_n - u^*\|^2_{V} \leq \sqrt{2}C_1^{-1} \epsilon^{1/2}$. By letting $\epsilon \to 0$, the proof is completed. \(\square\)

**Remark 5.4 (Weaker formulation).** Let $\{\Phi_{k,i}\}$ be an orthonormal basis in $H^1_0 (\Omega)$. Then the functional in the $hp$-VRM formulation Eq. (20) becomes

$$J_{\epsilon} (v) = \|f - Av\|^2_{H^{-1}} + \tau \|Bu - g\|^2_{Z}, \quad \tau \geq 0, \quad (23)$$

when $h \to 0$ and $N \to \infty$. If $\nabla \Phi_{k,i}$ form a complete basis in $L^2$ (which is the case for piecewise linear polynomials), then performing integration by parts will lead to problems as in the case of $L^2$ orthonormal bases. For example, when $Av = - \Delta v$, we then have

$$J_{\epsilon} (v) = \|F - \nabla v\|^2_{L^2} + \tau \|Bu - g\|^2_{Z}, \quad \tau \geq 0. \quad (24)$$

Here $f = \text{div} F$ and $F \in [H_0^1 (\Omega)]^2$ and we assume $\nabla \Phi_{k,i}$ form a complete orthogonal basis. In fact, $\sum_{k,i=1}^\infty (f - \Delta v, \Phi_{k,i}) = \sum_{k,i=1}^\infty (F - \nabla v, \nabla \Phi_{k,i}) = \|\nabla v - F\|^2_{L^2}$.

**6. CONCLUSION AND DISCUSSION**

We proposed an abstract framework for analyzing the convergence of RM for linear PDEs using NNs. When Bernstein-type inequalities are available for NNs, we use the discrete norm relations to obtain the convergence; see Theorem 4.1 and Example 4.2. When Bernstein-type inequalities are unavailable, we use the Rademacher complexity to obtain the convergence. We also present some examples in Appendix B on verification of our assumptions. Both approaches introduced tailored classes of NNs that enjoy some desired properties.
The framework developed in this paper may serve as guidance in designing loss functionals of the RM. First, we need the stability of the equations under user-defined metrics. Second, we need to balance the number of training points and the networks’ size as in Example 4.2. However, the conditions for convergence are not readily verifiable for deep NNs. Besides the limitations mentioned in Section 1, the verification of Bernstein-type inequalities and the Rademacher complexity is limited to two-layer networks. Also, the verification may be complicated depending on the operators and equations under consideration. These aspects are being investigated in the community, and more efforts are required.

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**APPENDIX A. PROOF OF THEOREM 4.3**

The proof is similar to the proof of Proposition 4.5 in Mhaskar (2005). The key step is to establish the following lemma.

**Lemma A.1.** Let $g(x) = \exp \left( -|x-w|^2 \right)$, where $x, w \in \mathbb{R}^d$. Let $I_n$ be the interpolation operator defined in Eq. (14). Then there exist constants $c_1, c > 0$ such that

$$
\left\| D^j g - I_n D^j g \right\|_{L^2} \leq c_1 n^c \frac{\sqrt{2d}|w|^{n+1}}{\sqrt{n!}} \exp \left( d|w|^2 \right),
$$

for any multiindex $j \in \mathbb{N}^d$.

The observation here is that $g(x)$ is closely related to Hermite polynomials. Let $h_k(x_1)$ be the orthonormal Hermite polynomials on the real line with respect to the weight $\exp \left( -|x_1|^2 \right)$: $\int_{\mathbb{R}} h_k(x_1) h_j(x_1) \exp \left( -|x_1|^2 \right) dx_1 = \delta_{k,j}$. Then by the generating function of the Hermite polynomials, we have $\exp (2x_1 t - t^2) = \pi^{1/4} \sum_{k=0}^{\infty} (h_k(x_1)/\sqrt{k!})(\sqrt{2}t)^k$. For the multiindex $\mathbf{k}$, $h_{\mathbf{k}} = \Pi_{j=1}^d h_{k_j}(x_j)$. Then with the standard multivariate notation, we have

$$
g(x,w) = \exp \left( -|x-w|^2 \right) = \pi^{d/4} \sum_{|\mathbf{k}| \geq 0} \frac{h_{\mathbf{k}}(x) \exp \left( -|x|^2 \right)}{\sqrt{\mathbf{k}!}} \left( \sqrt{2}w \right)^{\mathbf{k}}.
$$

For integer $n \geq 1$, let

$$
P_n(x,w) := \pi^{d/4} \sum_{0 \leq |\mathbf{k}| \leq n} \frac{h_{\mathbf{k}}(x) \exp \left( -|x|^2 \right)}{\sqrt{\mathbf{k}!}} \left( \sqrt{2}w \right)^{\mathbf{k}}
$$

$$
P_n^\perp(x,w) = g(x,w) - P_n(x,w).
$$

Then by Lemma 4.6 of Mhaskar (2005), there exist constants $c_1, c > 0$ such that

$$
\left\| \exp \left( -|\mathbf{v} - w|^2 \right) - P_n(\mathbf{v},w) \right\|_{W^{r,2}} \leq c_1 n^c \frac{\sqrt{2d}|w|^{n+1}}{\sqrt{n!}} \exp \left( d|w|^2 \right)
$$

for any integer $r, n \geq 1$. 

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Proof. By the fact that $I_N^k \left( \exp \left( |x|^2 / 2 \right) P_n(x, w) \right) = \exp \left( |x|^2 / 2 \right) P_n(x, w) \ (N \geq n)$ and the triangle inequality,

$$\| D^j g - \exp \left( - \frac{|c|^2}{2} \right) I_N^k \left( \exp \left( \frac{|c|^2}{2} \right) \right) D^j g \|_{L^2}$$

$$\leq \| \exp \left( \frac{|c|^2}{2} \right) D^j g - I_N^k \left( \exp \left( \frac{|c|^2}{2} \right) \right) D^j g \|_{L^2}$$

$$\leq \| \exp \left( \frac{|c|^2}{2} \right) D^j (g - P_n(o, w)) \|_{L^2} \ + \ \| I_N^k \left( D^1 (g - P_n(o, w)) \exp \left( \frac{|c|^2}{2} \right) \right) \|_{L^2} =: I + II.$$

We first estimate the term $I$. A careful check of the proof of Lemma 4.6 in Mhaskar (2005) leads to

$$I = \left\| \exp \left( \frac{|c|^2}{2} \right) D^j P_n^\perp(o, w) \right\|_{L^2} \leq c N^c \left( \sqrt{2 \delta |w|} \right)^{n+1} \exp \left( 2 |w|^2 \right) \left( \frac{1}{\sqrt{n!}} \right).$$

(A.3)

We now estimate the term $II$. By the stability of the interpolation operator $I_N^k$ [multidimensional analog of Lemma 3.1 in Guo et al. (2003)],

$$\| I_N^k \left( D^j P_n^\perp(o, w) \exp \left( \frac{|c|^2}{2} \right) \right) \|_{L^2} \leq c \sum_{|i| \leq 1} \| D^j \left( D^i P_n^\perp(o, w) \exp \left( \frac{|c|^2}{2} \right) \right) \|_{L^2}.$$  

Recall that in Theorem 2.2 of Guo et al. (2003), it is shown that for any $v = Q_N \exp(-|x|^2/2)$, $x \in \mathbb{R}$, then for $m \geq 0$, $\| \partial_x^n v \|_{L^2} \leq (2N + 1)^{m/2} \|v\|_{L^2}$. Since we are using a tensor product of interpolation, a multidimensional inverse estimate also holds $\| D^i \left( h_k \exp(-|c|^2/2) \right) \|_{L^2} \leq C(|k| + 1)$ for $|i| \leq 1$. Then, by Eq. (A.1) and the inverse estimate,

$$\| I_N^k \left( D^j P_n^\perp(o, w) \exp \left( \frac{|c|^2}{2} \right) \right) \|_{L^2} \leq c \sum_{|i| \leq 1} \| D^j \left( D^i P_n^\perp(o, w) \exp \left( \frac{|c|^2}{2} \right) \right) \|_{L^2}$$

$$\leq c \sum_{|i| \leq 1} \sum_{|k| \geq n+1} \| D^j \left( h_k + j \right) \exp \left( - \frac{|c|^2}{2} \right) \|_{L^2} \ (\sqrt{2} |j| \frac{\sqrt{2} (k+j)!}{k!} \left( \sqrt{2} w \right)^{k})$$

$$\leq c \sum_{|i| \leq 1} \sum_{|k| \geq n+1} (|k| + 1) \left( \sqrt{2} |j| \frac{\sqrt{2} (k+j)!}{k!} \left( \sqrt{2} w \right)^{k}.\right.$$

In the second inequality, we use the fact (by Rodrigues' formula) that

$$D^j \left( h_k \exp(-|x|^2) \right) = (- \sqrt{2} j \frac{\sqrt{2} (k+j)!}{k!} h_{k+j} \exp(-|x|^2). \right.$$

Then by the same argument in the proof of Lemma 4.6 in Mhaskar (2005), there exist $c_1, c > 0$ such that

$$II = \| I_N^k \left( D^j P_n^\perp(o, w) \exp \left( \frac{|c|^2}{2} \right) \right) \|_{L^2} \leq c_1 N^{c \left( \sqrt{2 d |w|} \right)^{n+1} \exp \left( 2 |w|^2 \right) / \sqrt{n!}}.$$  

(A.4)
Then the desired conclusion follows from Eqs. (A.3) and (A.4).

The proof of Theorem 4.2 is verbatim the same as that of Proposition 4.5 in Mhaskar (2005), except using Lemma A.1 in place of the estimate (A.2).

**APPENDIX B. ILLUSTRATION EXAMPLES AND VERIFICATION OF ASSUMPTIONS**

In this section, we consider linear elliptic, advection equations, and an integro-differential equation and demonstrate the key assumptions in Section 3 are satisfied.

**APPENDIX B.1 Elliptic Problems**

Let \( A \) be a linear differential operator of the form

\[
A = - \sum_{i,j=1}^{d} a_{i,j}(x) \partial_{x_{i}} \partial_{x_{j}} + \sum_{i=1}^{d} b_{i}(x) \partial_{x_{i}} + c(x), \quad \partial_{x_{i}} := \frac{\partial}{\partial x_{i}},
\]

and \( B \) be the identity operator, i.e., \( B = \text{Id} \), which leads to a Dirichlet boundary condition on \( \partial \Omega \). Also, we make the following assumptions.

**Assumption B.1.** The coefficients \( a_{i,j} \) satisfy the uniformly elliptic condition and the coefficients are in \( C^{2} \), i.e., twice continuously differentiable. Also, the only solution with zero input data is the zero solution.

**Lemma B.1** (Theorem 2.1 in Bramble and Schatz, 1970). In addition to Assumption B.1, assume that \( A \) is with \( C^{\infty} \) coefficients, defined on \( C^{\infty} \) bounded domain \( \Omega \) on \( \mathbb{R}^{d} \). For any real number \( l \), \( \| u \|_{H^{l}(\Omega)} \leq C(\| Au \|_{H^{l-2}(\Omega)} + \| u \|_{H^{l-1/2}(\partial \Omega)}) \), for all \( u \in C^{\infty}(\bar{\Omega}) \) and \( C \) is independent of \( u \).

From this lemma, we can deduce from the density argument that for all \( l \leq 1/2 \),

\[
\| u \|_{H^{l}(\Omega)} \leq C \left( \| Au \|_{H^{-1/2}(\Omega)} + \| u \|_{L^{2}(\partial \Omega)} \right) \leq C \left( \| Au \|_{L^{2}(\Omega)} + \| Bu \|_{L^{2}(\partial \Omega)} \right), \tag{B.2}
\]

holds for any \( u \in H^{2}(\Omega) \). Thus, Eq. (2a) of Assumption 2.2 is verified with \( V = H^{1}(\Omega) \) for any \( l \leq 1/2 \), \( Y = L^{2}(\Omega) \), and \( Z = L^{2}(\partial \Omega) \). It follows from the trace inequality (e.g., Theorem 1.6.6 of Brenner and Scott, 2007) and \( u \in H^{2}(\Omega) \) that Eq. (2b) of Assumption 2.2 is verified with \( X = H^{2}(\Omega) \subset V \).

The verification of Assumption 2.3 is straightforward as feed-forward neural networks are universal approximators in Sobolev–Hilbert spaces, see, e.g., Mhaskar (1996). Therefore, Theorem 3.1 provides the error estimates in \( X = H^{2}(\Omega) \) under the conditions in Lemma B.1.

**Remark B.1** (Non-smooth data, Bramble and Schatz, 1970). If \( f \in H^{s}(\Omega), \ -2 \leq s \leq 0 \), a non-smooth data, we may use a mollifier \( \Phi_{h} \) such that for some \( C > 0 \) independent of \( h \) and \( f \), the following holds: \( \| \Phi_{h}f - f \| \leq Ch^{s}\| f \|_{H^{-s}}, \) and \( \| \Phi_{h}f - f \|_{-2} \leq Ch^{2+s}\| f \|_{H^{-s}} \).

**APPENDIX B.2 Advection-Reaction Problems**

Let \( \Omega \subset \mathbb{R}^{d} \) be an open bounded domain, with Lipschitz boundary \( \partial \Omega \) oriented by a unit outward normal vector \( n \). We consider an advection-reaction problem. Let \( b \) be a smooth vector field in \( \mathbb{R}^{d} \) such that \( b \in L^{\infty}(\Omega)^{d} \) and \( \nabla \cdot b \in L^{\infty}(\Omega) \). Let the inflow boundary be \( \partial \Omega_{-} = \{ x \} \in \partial \Omega | b \cdot n < 0 \). For \( c \in L^{\infty}(\Omega) \), let \( A \) be the differential operator defined by
and $B$ be the identity operator on the inflow boundary $\partial \Omega^+$. This formulation also covers time-dependent advection-reactions; see Remark B.1.

For $p \in [1, \infty]$, we define the graph space $G^p_b(\Omega) = \{v \in L^p(\Omega) | b \cdot \nabla v \in L^p(\Omega)\}$, which is endowed with the norm $\|v\|_{G^p_b} = \left(\|v\|_{L^p}^p + \|b \cdot \nabla v\|_{L^p}^2\right)^{1/2}$. We also introduce the following space

$$L^p_{[b,n]}(\partial \Omega) = \left\{ v \text{ is measurable on } \partial \Omega \mid \int_{\partial \Omega} |b \cdot n| |v|^p \, dx < \infty \right\}.$$ By the trace inequality (Lemma B.2) and Poincaré’s inequality (Theorem B.1), it can be checked that the following condition holds

$$C_1 \|v\|_X \leq \|Av\|_Y + \|Bv\|_Z \leq C_2 \|v\|_X,$$ where $X = G^p_b(\Omega)$, $Y = L^p(\Omega)$, $p \in (1, \infty)$, $Z = L^p_{[b,n]}(\partial \Omega)$, and $p \in (1, \infty)$. This verifies Assumption 2.2.

**Lemma B.2** (Trace inequality, Lemma 2.1 of Cantin, 2017). Let $\partial \Omega^+= \{x \in \partial \Omega | b \cdot n > 0\}$. Assume that the inflow and outflow boundaries are well-separated: $\partial \Omega^+ \cap \partial \Omega^- = \emptyset$. Let $p \in (1, \infty)$ and $g \in L^p_{[b,n]}(\partial \Omega)$, there exists $v_g \in G^p_b(\Omega)$ such that $v_g = g$ on $\partial \Omega^+ \cup \partial \Omega^-$. In other words, the trace of $v_g \in G^p_b(\Omega)$ exists in $L^p_{[b,n]}(\partial \Omega)$ and $\|g\|_{L^p_{[b,n]}(\partial \Omega)} \leq C\|v_g\|_{G^p_b}\$.

**Theorem B.1** (Poincare inequality, Cantin, 2017). Let $p \in (1, \infty)$. Assume that there exists an Lipschitz continuous function $\eta(x)$ and a positive constant $\mu_1$ such that

$$c(x) - \frac{1}{p} \nabla \cdot b(x) - \frac{1}{p} b(x) \cdot \nabla \eta(x) \geq \mu_1 > 0, \text{ a.e. } x \in \Omega.$$ Then for $v \in \{v \in G^p_b(\Omega) | v(x) = 0, x \in \partial \Omega^-\}$, $\|v\|_{L^p} \leq C\|cv + b \cdot \nabla v\|_{L^p}$.

The condition (B.5) in Theorem B.1 can be satisfied in the cases of Friedrich’s positivity assumption or $\Omega$-filling advection, with which the norm equivalence (B.4) also holds with $p = 1$ (see, e.g., Bochev and Gunzburger, 2016; Guermond, 2004).

- (Friedrich’s positivity assumption) There exists a constant $\mu_0 > 0$ such that $\mu(x) - (1/p) \nabla \cdot b \geq \mu_0$, a.e. $x \in \Omega$.

- ($\Omega$-filling advection) If $c = 0$ and $\nabla \cdot b = 0$, assume that there exists $z_\pm \in G^{p\infty}_b(\Omega)$ with $\|z_\pm\|_{L^\infty} > 0$ such that $-b \cdot \nabla z_\pm = p$ in $\Omega$ and $z_\pm = 0$ on $\partial \Omega^\pm$.

**Remark B.2** (Time-dependent advection-reaction equations). The problem $\partial_t u + b \cdot \nabla u + cu = f$ with initial and boundary values can be recast into the form of Eq. (B.3). In fact, we may introduce the following notations $\hat{x} = (x_1, x_2, \ldots, x_{n+1}, t)$ and $Q = \Omega \times (0, T), \partial Q = \partial \Omega \times (0, T) \cup (\Omega \times \{T\} \cup \{0\})$. Also, we define the normal vector

$$\hat{n} = \begin{cases} (1,0) & \text{on } \partial \Omega \times (0, T) \\ (0,1) & \text{on } \Omega \times \{T\} \\ (0,-1) & \text{on } \Omega \times \{0\}. \end{cases}$$ Let $\tilde{b}(\hat{x}) = (b(x,t), 1)$ and $\partial Q^- = \{\hat{x} \in \partial Q | \tilde{b} \cdot \hat{n} < 0\} = (\partial \Omega^- \times (0, T)) \cup (\Omega \times \{0\})$, and $\nabla \equiv (\nabla, \partial_t)$. Then the problem can be written as $\tilde{b} \cdot \nabla u + cu = f$ with $u$ given on $\partial Q^-$. This reformulation has been used in many works, e.g., in Pousin and Azerad (1996).
APPENDIX B.3 Integro-Differential Equations

Let $\Omega$ be a bounded Lipschitz domain satisfying the exterior ball condition or a $C^2$ bounded domain. Consider the following operator $A = (-\Delta)^{\alpha/2} + b \cdot \nabla + c$, $x \in \Omega \subset \mathbb{R}^d$, $1 < \alpha < 2$, and $B = \text{Id}$ on $\mathbb{R}^d \setminus \Omega$ and the image of $B$ has a compact support and the fractional Laplacian is defined as a singular integral operator on $\mathbb{R}^d$ (see, e.g., Lischke et al., 2020)

$$(-\Delta)^{\alpha/2} u(x) = c_{d, \alpha} \int_{\mathbb{R}^d} \frac{u(x) - u(y)}{|x - y|^{d+\alpha}} \, dy, \quad c_{d, \alpha} = \frac{2^{\alpha} \Gamma\left(\frac{\alpha + d}{2}\right)}{\pi^{d/2} \Gamma\left(\frac{-\alpha}{2}\right)}.$$

(B.6)

Assume that there exists a constant $c_0 > 0$ such that $2c - \nabla \cdot b \in L^\infty(\Omega)$ and $2c - \nabla \cdot b \geq 2c_0 > 0$. By the Lax–Milgram Lemma, we can readily obtain the existence and uniqueness of a solution and there exists a constant $C_1 > 0$ that

$$C_1 \|u\|_{H^{\alpha/2}(\mathbb{R}^d)} \leq \|Au\|_{H^{-\alpha/2}(\Omega)} + \|Bu\|_{H^{\alpha/2}(\mathbb{R}^d \setminus \Omega)}.$$

(B.7)

The fractional Laplacian can be written as

$$c_{d, \alpha} \int_{\mathbb{R}^d} \frac{2u(x) - u(x + y) - u(x - y)}{2|y|^{d+\alpha}} \, dy.$$

Then we obtain that when $b$ and $c$ are in $L^\infty$, there exists a constant $C_2 > 0$ such that for $u \in C^2_c(\mathbb{R}^d)$, $\|Au\|_{H^{-\alpha/2}(\Omega)} + \|Bu\|_{H^{\alpha/2}(\mathbb{R}^d \setminus \Omega)} \leq C_2 \|u\|_{C^2(\mathbb{R}^d)}$. Here $C^2_c(\mathbb{R}^d)$ is a subspace of $C^2(\mathbb{R}^d)$ and elements in $C^2_c(\mathbb{R}^d)$ are compactly supported.

Assumption 2.2 is verified with $V = H^{\alpha/2}(\mathbb{R}^d)$, $Y = L^2(\Omega)$, $Z = H^{\alpha/2}(\mathbb{R}^d \setminus \Omega)$, $X = C^2_c(\mathbb{R}^d)$.

Remark B.3. When $Y = L^\infty(\Omega)$, norm relations in Hölder spaces can be obtained using regularity results for the fractional Poisson equation e.g., in Grubb (2015) and Ros-Oton and Serra (2014).