ON THE CONVERGENCE AND GENERALIZATION OF PHYSICS INFORMED NEURAL NETWORKS[*]

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Abstract. Physics informed neural networks (PINNs) are deep learning based techniques for solving partial differential equations (PDEs). Guided by data and physical laws, PINNs find a neural network that approximates the solution to a system of PDEs. Such a neural network is obtained by minimizing a loss function in which any prior knowledge of PDEs and data are encoded. Despite its remarkable empirical success, there is little theoretical justification for PINNs. In this paper, we establish a mathematical foundation of the PINNs methodology.

As the number of data grows, PINNs generate a sequence of minimizers which correspond to a sequence of neural networks. We want to answer the question: Does the sequence of minimizers converge to the solution to the PDE? This question is also related to the generalization of PINNs. We consider two classes of PDEs: elliptic and parabolic. By adapting the Schuader approach, we show that the sequence of minimizers strongly converges to the PDE solution in L^2. Furthermore, we show that if each minimizer satisfies the initial/boundary conditions, the convergence mode can be improved to H^1. Computational examples are provided to illustrate our theoretical findings. To the best of our knowledge, this is the first theoretical work that shows the consistency of the PINNs methodology.

Key words. Physics Informed Neural Networks, Convergence and Generalization, Hölder Regularization, Elliptic and Parabolic PDEs, Schuader approach

AMS subject classifications. 65M12, 41A46, 35J25, 35K20

1. Introduction. Machine learning techniques using deep neural networks have been successfully applied in various fields [15] such as computer vision, natural language processing. Such techniques have also been applied in solving partial differential equations (PDEs) [22, 13, 5, 14, 2, 25], and it has become a new sub-field under the name of Scientific Machine Learning (SciML) [1, 17]. The term Physics-Informed Neural Networks (PINNs) was introduced [22] and it has become one of the most popular deep learning methodologies in SciML. PINNs employ a neural network as a solution surrogate and seek to find the best network guided by data and physical laws expressed as PDEs.

A series of works have shown the effectiveness of PINNs: fractional PDEs [20, 26], stochastic differential equations [28, 11], biomedical problems [23], and fluid mechanics [18]. Despite such remarkable success in these and related areas, PINNs lack theoretical justification. In this paper, we establish a mathematical foundation of the PINNs methodology.

Given a set of m-training data, PINNs require one to choose a function class $\mathcal{H}_m$ and a loss function. The loss functions used in PINNs penalize neural networks that fail to satisfy both governing equations (PDEs) and initial/boundary conditions on the training data. The goal is then to find a minimizer h_m of the loss in $\mathcal{H}_m$. However, even in an extreme case where $\mathcal{H}_m$ contains the exact solution u^* to PDEs and a global minimizer is found, since there could be multiple (often infinitely many) global minimizers, there is no guarantee that a minimizer one found and the solution u^* coincide. We want to answer the question: Does the sequence of minimizers converge to the solution to PDEs? This question is also related to the generalization of PINNs.

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The total errors of PINNs can be decomposed into three components: approximation error, optimization errors, and generalization error. We illustrate the decomposition of the total errors in Figure 1. The approximation error is relatively well understood. [21] showed that a single layer neural network with a sufficiently large width can uniformly approximate a function and its partial derivative. It also has been shown that neural networks are capable of approximating the solutions for some classes of PDEs: Quasilinear parabolic PDEs [25], the Black-Scholes PDEs [10], and the Hamilton-Jacobi PDEs [?, 4]. The optimization error is, however, poorly understood as the objective function is highly nonconvex. Optimization often involves many engineering tricks and tedious trial and error type fine-tuning of parameters. Gradient-based optimization methods are commonly used for the training. Numerous variants of the stochastic gradient descent method have been proposed [24]. Among many, `Adam` [12] and `L-BFGS` [16] are popularly employed for the PINNs methodology. In machine learning, the generalization error is referred to as a measure of the accuracy of the prediction on unseen data [19]. In PDE problems, the generalization error is defined to be the distance between a global minimizer of the loss and the (projected) solution to the PDE, where the distance has be to defined appropriately to reflect its regularity.
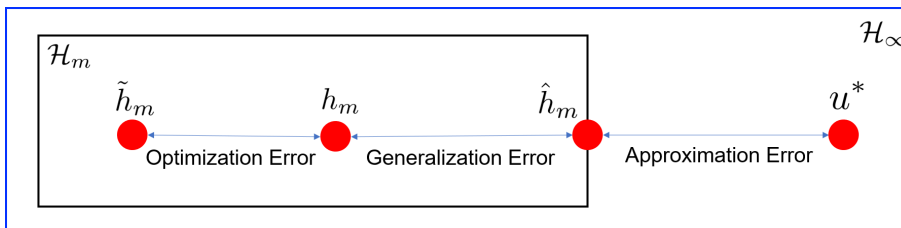

FIG. 1. *Illustration of the total errors by the PINNs methodology. The number of training data is m. $\mathcal{H}_m$ is the chosen function class at m training data. $\mathcal{H}_\infty$ is the function class that contains all $\mathcal{H}_m$ and the solution u^* to the PDE. h_m is a minimizer of the loss with m data. $\hat{h}_m$ is a function in $\mathcal{H}_m$ that is the closest to u^*. $\tilde{h}_m$ is an approximation that one obtains in practice, e.g., the result obtained after 1M epochs of a gradient-based optimization.*

Contributions. In this work, we study the generalization error and its convergence with respect to the number of training data. By adopting probabilistic space filling arguments [7, 3], we derive an upper bound of the expected unregularized PINN loss [22] (Theorem 3.2). The upper bound reveals a specific regularized empirical loss. We then consider the problem of minimizing the regularized loss with respect to the number of training samples. By focusing on two classes of PDEs – linear elliptic and linear parabolic – we show that the sequence of minimizers of the regularized loss converges to the solution to the PDE uniformly. This also implies the L^2-convergence. In addition, we show that if minimizers satisfy the initial/boundary conditions, the mode of convergence is improved to H^1. To ensure the existence, regularity and uniqueness of the solution, we adopt the Schauder approach. To the best of our knowledge, this is the first theoretical work that proves the consistency of the PINNs methodology in the sample limit. Computational examples are provided to demonstrate our theoretical findings.

The rest of the paper is organized as follows. Upon briefly introducing mathematical setup in section 2, we present the convergence and generalization analysis in section 3. There, we derive an upper bound of the expected PINN loss in terms of a regularized empirical loss. With the derived regularized loss, we discuss the conver-

gence and generalization. Computational examples are provided in section 4. Finally, we conclude the paper in section 5.

2. Mathematical Setup and Preliminaries. Let U be a bounded domain (open and connected) in $\mathbb{R}^d$. We consider partial differential equations (PDEs) of the form

$$(2.1) \qquad \mathcal{L}[u](\mathbf{x}) = f(\mathbf{x}) \quad \forall \mathbf{x} \in U, \qquad \mathcal{B}_k[u](\mathbf{x}) = g_k(\mathbf{x}) \quad \forall \mathbf{x} \in \Gamma_k \subset \partial U,$$

for $k = 1, \cdots, N_B$, where $\mathcal{L}[\cdot]$ is a differential operator and $\mathcal{B}_k[\cdot]$ could be Dirichlet, Neumann, Robin, or periodic boundary conditions. This paper considers PDEs that admit a unique classical solution $u(\mathbf{x})$ with $\mathbf{x} = (x_1, \cdots, x_d)$. The classical solution should satisfy the governing equation everywhere on U and $\cup_{k=1}^{N_B}\Gamma_k$. We remark that for time-dependent problems, we consider time t as a special component of $\mathbf{x}$, and U contains the temporal domain. The initial condition can be simply treated as a special type of Dirichlet boundary condition on the spatio-temporal domain.

The goal is to approximate the solution to the PDE (2.1) from a set of training data. The training data consist of two types of data sets: residual and initial/boundary data. A residual datum is a pair of input and output $(\mathbf{x}_f, f(\mathbf{x}_f))$, where $\mathbf{x}_f \in U$ and an initial/boundary datum is a pair of input and output $(\mathbf{x}_{b,k}, g_k(\mathbf{x}_{b,k}))$, where $\mathbf{x}_{b,k} \in \Gamma_k$. The set of m_f residual input data points and the set of $m_{b,k}$ initial/boundary input data points from Γ_k are denoted by $\mathcal{T}_f^{m_f} = \{\mathbf{x}_f^i\}_{i=1}^{m_f}$ and $\mathcal{T}_{b,k}^{m_{b,k}} = \{\mathbf{x}_{b,k}^i\}_{i=1}^{m_{b,k}}$, respectively. Let us denote the vector of the number of training samples by $\boldsymbol{m} = (m_f, m_{b,1}, \cdots, m_{b,N_B})$. Note that we slightly abuse notation as in [22]: $\mathbf{x}_f$ refers to a point in U. Similarly, $\mathbf{x}_{b,k}$ refers to a point in Γ_k. m_f and $m_{b,k}$ represent the number of training data points in U and Γ_k, respectively.

Given a function class $\mathcal{H}_{\boldsymbol{m}}$ such as neural networks that may depend on the number of training samples $\boldsymbol{m}$, we seek to find a function h^* in $\mathcal{H}_{\boldsymbol{m}}$ that minimizes an objective (loss) function. To define an appropriate objective function, let us consider a loss integrand, which is the standard choice in physics informed neural networks (PINNs) [22]:

$$(2.2)$$
$$\mathbf{L}(\mathbf{x}_f, \vec{\mathbf{x}}_b; h, \boldsymbol{\lambda}, \boldsymbol{\lambda}^R) = \left(\lambda_f \|\mathcal{L}[h](\mathbf{x}_f) - f(\mathbf{x}_f)\|^2 + \lambda_f^R R_f(h)\right) \mathbb{I}_U(\mathbf{x}_f)$$
$$+ \sum_{k=1}^{N_B} \left(\lambda_{b,k} \|\mathcal{B}_k[h](\mathbf{x}_{b,k}) - g_k(\mathbf{x}_{b,k})\|^2 + \lambda_{b,k}^R R_{b,k}(h)\right) \mathbb{I}_{\Gamma_k}(\mathbf{x}_{b,k}),$$

where $\| \cdot \|$ is the Euclidean norm, $\mathbb{I}_A(\mathbf{x})$ is the indicator function on the set A, $\vec{\mathbf{x}}_b = (\mathbf{x}_{b,1}, \cdots, \mathbf{x}_{b,N_B})$, $\boldsymbol{\lambda} = (\lambda_f, \lambda_{b,1}, \cdots, \lambda_{b,N_B})$, $\boldsymbol{\lambda}^R = (\lambda_f^R, \lambda_{b,1}^R, \cdots, \lambda_{b,N_B}^R)$, and $R_f(\cdot), R_{b,k}(\cdot)$ are regularization functionals. Here $\lambda_f, \lambda_f^R, \lambda_{b,k}, \lambda_{b,k}^R \in \mathbb{R}_+ \cup \{0\}$.

Suppose $\mathcal{T}_f^{m_f}$ and $\mathcal{T}_{b,k}^{m_{b,k}}$ are independently and identically distributed (iid) samples from probability distributions μ_f and $\mu_{b,k}$, respectively. One can then define the empirical probability distribution on $\mathcal{T}_f^{m_f}$ by $\mu_f^{m_f} = \frac{1}{m_f} \sum_{i=1}^{m_f} \delta_{\mathbf{x}_f^i}$. Similarly, $\mu_{b,k}^{m_{b,k}}$ is defined for $k = 1, \cdots, N_B$. The empirical loss and the expected loss are obtained by taking the expectations on the loss integrand (2.2) with respect to $\mu^{\boldsymbol{m}} = \mu_f^{m_f} \times \prod_{k=1}^{N_B} \mu_{b,k}^{m_{b,k}}$ and $\mu = \mu_f \times \prod_{k=1}^{N_B} \mu_{b,k}$, respectively:

$$(2.3) \qquad \begin{aligned} \text{Loss}_{\boldsymbol{m}}(h; \boldsymbol{\lambda}, \boldsymbol{\lambda}^R) &= \mathbb{E}_{\mu^{\boldsymbol{m}}}[\mathbf{L}(\mathbf{x}_f, \vec{\mathbf{x}}_b; h, \boldsymbol{\lambda}, \boldsymbol{\lambda}^R)], \\ \text{Loss}(h; \boldsymbol{\lambda}, \boldsymbol{\lambda}^R) &= \mathbb{E}_{\mu}[\mathbf{L}(\mathbf{x}_f, \vec{\mathbf{x}}_b; h, \boldsymbol{\lambda}, \boldsymbol{\lambda}^R)]. \end{aligned}$$

In order for the expected loss to be well-defined, it is assumed that $\mathcal{L}[h]$ and f are in $L^2(U; \mu_f)$, and $\mathcal{B}_k[h]$ and g_k are in $L^2(\Gamma_k; \mu_{b,k})$ for all $h \in \mathcal{H}_{\boldsymbol{m}}$. If the expected loss function were available, its minimizer would be the solution to the PDE (2.1) or close to it. However, since it is unavailable in practice, the empirical loss function is employed. This leads to the following minimization problem:

$$(2.4) \qquad \min_{h \in \mathcal{H}_{\boldsymbol{m}}} \mathrm{Loss}_{\boldsymbol{m}}(h; \boldsymbol{\lambda}, \boldsymbol{\lambda}^R).$$

We then hope a minimizer of the empirical loss to be close to the solution to the PDE (2.1).

We remark that in general, global minimizers to the problem of (2.4) need not exist. However, for $\epsilon > 0$, there always exists a ϵ-suboptimal global solution $h_{\boldsymbol{m}}^\epsilon \in \mathcal{H}_{\boldsymbol{m}}$ [?] satisfying $\mathrm{Loss}_{\boldsymbol{m}}(h_{\boldsymbol{m}}^\epsilon) \leq \inf_{h \in \mathcal{H}_{\boldsymbol{m}}} \mathrm{Loss}_{\boldsymbol{m}}(h) + \epsilon$. All the results of the present paper remain valid if one replace global minimizers to ϵ-suboptimal global minimizers for sufficiently small ϵ. Henceforth, for the sake of readability, we assume the existence of at least one global minimizer of the minimization problem (2.4).

When $\boldsymbol{\lambda}^R = 0$, we refer to the (either empirical or expected) loss as the (empirical or expected) PINN loss [22]. We denote the empirical and the expected PINN losses by $\mathrm{Loss}_{\boldsymbol{m}}^{\mathrm{PINN}}(h; \boldsymbol{\lambda})$ and $\mathrm{Loss}^{\mathrm{PINN}}(h; \boldsymbol{\lambda})$, respectively. Specifically,

$$\mathrm{Loss}_{\boldsymbol{m}}^{\mathrm{PINN}}(h; \boldsymbol{\lambda}) = \frac{\lambda_f}{m_f} \sum_{j=1}^{m_f} \|\mathcal{L}[h](\mathbf{x}_f^j) - f(\mathbf{x}_f^j)\|^2$$

$$(2.5) \qquad\qquad + \sum_{k=1}^{N_B} \frac{\lambda_{b,k}}{m_{b,k}} \sum_{i=1}^{m_{b,k}} \|\mathcal{B}_k[h](\mathbf{x}_{b,k}^i) - g_k(\mathbf{x}_{b,k}^i)\|^2,$$

$$\mathrm{Loss}^{\mathrm{PINN}}(h; \boldsymbol{\lambda}) = \lambda_f \|\mathcal{L}[h] - f\|_{L^2(U;\mu)}^2 + \sum_{k=1}^{N_B} \lambda_{b,k} \|\mathcal{B}_k[h] - g_k\|_{L^2(\Gamma_k;\mu_{b,k})}^2.$$

Also, note that for $\boldsymbol{\lambda} \leq \boldsymbol{\lambda}'$ and $\boldsymbol{\lambda}^R \leq \boldsymbol{\lambda}'^R$ (element-wise inequality), we have $\mathrm{Loss}_{\boldsymbol{m}}(h; \boldsymbol{\lambda}, \boldsymbol{\lambda}^R) \leq \mathrm{Loss}_{\boldsymbol{m}}(h; \boldsymbol{\lambda}', \boldsymbol{\lambda}'^R)$.

2.1. Function Spaces and Regular Boundary. Throughout this paper, we adopt the notation from [9]. Let U be a bounded domain in $\mathbb{R}^d$. Let $\mathbf{x} = (x_1, \cdots, x_d)$ be a point in $\mathbb{R}^d$. Given a multi-index $\mathbf{k} = (k_1, \cdots, k_d)$ where $k_j \in \mathbb{N} \cup \{\infty\}$, let $C^{\mathbf{k}}(U)$ be the set of functions having partial derivatives with respect to x_j of order $\leq k_j$ in U for all $1 \leq j \leq d$. Also, let $C^{\mathbf{k}}(\bar{U})$ be the set of functions in $C^k(U)$ whose partial derivatives with respect to x_j of order $\leq k_j$ have continuous extensions to $\bar{U}$ (the closure of U).

We call a function u uniformly Hölder continuous with exponent α in U if the quantity

$$(2.6) \qquad [u]_{\alpha;U} = \sup_{x,y \in U, x \neq y} \frac{\|u(x) - u(y)\|}{\|x - y\|^\alpha} < \infty, \qquad 0 < \alpha \leq 1,$$

is finite. Also, we call a function u locally Hölder continuous with exponent α in U if u is uniformly Hölder continuous with exponent α on compact subsets of U. $[u]_{\alpha;U}$ is called the Hölder constant (coefficient) of u on U.

DEFINITION 2.1. *Given a multi-index $\boldsymbol{k} = (k_1, \cdots, k_d)$ where $k_j \in \mathbb{N} \cup \{\infty\}$, the Hölder spaces $C^{\boldsymbol{k},\alpha}(\bar{U})$ $(C^{\boldsymbol{k},\alpha}(U))$ are the subspaces of $C^{\boldsymbol{k}}(\bar{U})$ $(C^{\boldsymbol{k}}(U))$ consisting of functions whose k_j-th order partial derivatives with respect to x_j are uniformly Hölder continuous (locally Hölder continuous) with exponent α in U for all $1 \leq j \leq d$.*

For simplicity, we often write $C^{\mathbf{k},0} = C^{\mathbf{k}}$ and $C^{0,\alpha} = C^{\alpha}$ for $0 < \alpha < 1$.

Given a multi-index $\mathbf{k} = (k_1, \cdots, k_d)$, we define

$$D^{\mathbf{k}}u = \frac{\partial^{|\mathbf{k}|}u}{\partial x_1^{k_1} \cdots \partial x_d^{k_d}},$$

where $|\mathbf{k}| = \sum_{i=1}^{d} k_i$. Let $\mathbf{k} = (k_1, \cdots, k_d)$ and $\mathbf{k}' = (k_1', \cdots, k_d')$. If $k_j' \leq k_j$ for all j, we write $\mathbf{k}' \leq \mathbf{k}$. Let us define

$$[u]_{j,0;U}^{\mathbf{k}} = \sup_{|\mathbf{k}'|=j, \mathbf{k}' \leq \mathbf{k}} \sup_{U} |D^{\mathbf{k}'}u|, \qquad j = 0, 1, \cdots, |\mathbf{k}|,$$

$$[u]_{j,\alpha;U}^{\mathbf{k}} = \sup_{|\mathbf{k}'|=j, \mathbf{k}' \leq \mathbf{k}} [D^{\mathbf{k}'}u]_{\alpha;U} = \sup_{|\mathbf{k}'|=j, \mathbf{k}' \leq \mathbf{k}} \left[\sup_{x,y \in U, x \neq y} \frac{\|D^{\mathbf{k}'}u(x) - D^{\mathbf{k}'}u(y)\|}{\|x - y\|^{\alpha}} \right].$$

Then, the related norms are defined on $C^{\mathbf{k}}(\bar{U})$ and $C^{\mathbf{k},\alpha}(\bar{U})$, respectively, by

$$\|u\|_{C^{\mathbf{k}}(\bar{U})} = \sum_{j=0}^{|\mathbf{k}|} [u]_{j,0;U}^{\mathbf{k}},$$

$$\|u\|_{C^{\mathbf{k},\alpha}(\bar{U})} = \|u\|_{C^{\mathbf{k}}(\bar{U})} + [D^{\mathbf{k}}u]_{\alpha;U}, \qquad 0 < \alpha \leq 1.$$

With these norms, $C^{\mathbf{k}}(\bar{U})$ and $C^{\mathbf{k},\alpha}(\bar{U})$ are Banach spaces. If all k_j's are equal to k, with slight abuse of notation, we simply write $C^{\mathbf{k},\alpha}$ as $C^{k,\alpha}$. Also, we denote $\frac{\partial u}{\partial x_j}$ as $D_j u$ and $\frac{\partial^2 u}{\partial x_i \partial x_j}$ as $D_{ij}u$.

DEFINITION 2.2. *A bounded domain U in $\mathbb{R}^d$ and its boundary are said to be of class $C^{k,\alpha}$ where $0 \leq \alpha \leq 1$, if at each point $x_0 \in \partial U$ there is a ball $B = B(x_0)$ and a one-to-one mapping ψ of B onto $D \subset \mathbb{R}^d$ such that (i) $\psi(B \cap U) \subset \mathbb{R}_+^d$, (ii) $\psi(B \cap \partial U) \subset \partial \mathbb{R}_+^d$, (iii) $\psi \in C^{k,\alpha}(B), \psi^{-1} \in C^{k,\alpha}(D)$.*

A domain of class $C^{0,1}$ is Lipschitz.

2.2. Neural Networks. Among many choices of function classes $\mathcal{H}_{\boldsymbol{m}}$, we consider a class of neural networks. Let $h^L : \mathbb{R}^d \to \mathbb{R}^{d_{\text{out}}}$ be a feed-forward neural network having L layers and n_ℓ neurons in the ℓ-th layer. The weights and biases in the l-th layer are represented by a weight matrix $\mathbf{W}^l \in \mathbb{R}^{n_l \times n_{l-1}}$ and a bias vector $\mathbf{b}^l \in \mathbb{R}^{n_l}$, respectively. Let $\boldsymbol{\theta}_L := \{\boldsymbol{W}^j, \boldsymbol{b}^j\}_{1 \leq j \leq L}$. For notational completeness, let $n_0 = d$ and $n_L = d_{\text{out}}$. For a fixed integer L, let $\vec{\boldsymbol{n}} = (n_0, n_2, \cdots, n_L) \in \mathbb{N}^{L+1}$ where $\mathbb{N} = \{1, 2, 3, \cdots\}$. Then, $\vec{\boldsymbol{n}}$ describes a network architecture. Given an activation function $\sigma(\cdot)$ which is applied element-wise, the feed-forward neural network is defined by

$$h^\ell(\mathbf{x}) = \boldsymbol{W}^\ell \sigma(h^{\ell-1}(\mathbf{x})) + \boldsymbol{b}^\ell \in \mathbb{R}^{N_\ell}, \qquad \text{for} \quad 2 \leq \ell \leq L$$

and $h^1(\mathbf{x}) = \boldsymbol{W}^1 \mathbf{x} + \boldsymbol{b}^1$. The input is $\mathbf{x} \in \mathbb{R}^{n_0}$, and the output of the ℓ-th layer is $h^\ell(\mathbf{x}) \in \mathbb{R}^{n_\ell}$. Popular choices of activation functions include the sigmoid $(1/(1+e^{-x}))$, the hyperbolic tangent $(\tanh(x))$, and the rectified linear unit $(\max\{x, 0\})$. Note that h^L is called a $(L-1)$-hidden layer neural network or a L-layer neural network.

Since a network $h^L(\mathbf{x})$ depends on the network parameters $\boldsymbol{\theta}_L$ and the architecture $\vec{\boldsymbol{n}}$, we often denote $h^L(\mathbf{x})$ by $h^L(\mathbf{x}; \vec{\boldsymbol{n}}, \boldsymbol{\theta}_L)$. If $\vec{\boldsymbol{n}}$ is clear in the context, we simple write $h^L(\mathbf{x}; \boldsymbol{\theta}_L)$. Given a network architecture, we define a neural network function class

$$(2.7) \qquad \mathcal{H}_{\vec{\boldsymbol{n}}}^{\text{NN}} = \left\{ h^L(\cdot; \vec{\boldsymbol{n}}, \boldsymbol{\theta}_L) : \mathbb{R}^d \mapsto \mathbb{R}^{d_{\text{out}}} | \boldsymbol{\theta}_L = \{(\boldsymbol{W}^j, \boldsymbol{b}^j)\}_{j=1}^L \right\}.$$

Since $h^L(\mathbf{x}; \boldsymbol{\theta}_L)$ is parameterized by $\boldsymbol{\theta}_L$, the problem of (2.4) with $\mathcal{H}_{\vec{n}}^{\mathrm{NN}}$ is equivalent to

$$\min_{\boldsymbol{\theta}_L} \mathrm{Loss}_{\boldsymbol{m}}(\boldsymbol{\theta}_L; \boldsymbol{\lambda}, \boldsymbol{\lambda}^R), \quad \text{where} \quad \mathrm{Loss}_{\boldsymbol{m}}(\boldsymbol{\theta}_L; \boldsymbol{\lambda}, \boldsymbol{\lambda}^R) = \mathrm{Loss}_{\boldsymbol{m}}(h(\mathbf{x}; \boldsymbol{\theta}_L); \boldsymbol{\lambda}, \boldsymbol{\lambda}^R).$$

Throughout this paper, the activation function is assumed to be smooth at least upto required by the PDE (2.1).

LEMMA 2.3. *Let U be a bounded domain and $\mathcal{H}_{\vec{n}}^{NN}$ be a class of neural networks whose architecture is $\vec{n} = (n_0, \cdots, n_L)$ whose activation function $\sigma(x) \in C^{k'}(\mathbb{R})$ satisfies that for each $s \in \{0, \cdots, k\}$ where $k < k'$, $\frac{d^s \sigma(x)}{dx^s}$ is bounded and Lipschitz continuous. For a function $u \in C^k(\bar{U})$, let $\{h_j\}_{j=1}^{\infty}$ be a sequence of networks in $\mathcal{H}_{\vec{n}}^{NN}$ such that the associated weights and biases are uniformly bounded and $h_j \to u$ in $C^0(\bar{U})$. Then, $h_j \to u$ in $C^k(\bar{U})$.*

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

It can be checked that the tanh activation function satisfies the conditions of Lemma 2.3 as follows: Note that $\tanh(x)$ is bounded by 1 and is 1-Lipschitz continuous. The k-th derivative of $\tanh(x)$ is expressed as a polynomial of $\tanh(x)$ with a finite degree, which shows both the boundedness and Lipschitz continuity.

3. Convergence and Generalization Analysis. If the expected loss function were available, a function that minimizes it would be sought. However, since the expected loss is not available in practice, the empirical loss function is employed. We first derive an upper bound of the expected PINN loss (2.5). The bound involves a specific regularized empirical loss.

The derivation is based on the probabilistic space filling arguments [3, 7]. In this regard, we make the following assumptions on the training data distributions.

ASSUMPTION 3.1. *Let U be a bounded domain in $\mathbb{R}^d$ that is at least of $C^{0,1}$ and $\Gamma = \cup_{k=1}^{N_B} \Gamma_k$ be a closed subset of ∂U. Let μ_f and $\mu_{b,k}$ be probability distributions defined on U and Γ_k, respectively. Let ρ_f be the probability density of μ_f with respect to d-dimensional Lebesgue measure on U. Similarly, $\rho_{b,k}$ is the probability density of $\mu_{b,k}$ with respect to $(d-1)$-dimensional Lebesgue measure on Γ_k.*

1. *ρ_f and $\rho_{b,k}$ are supported on U and Γ_k, respectively. Also, $\inf_U \rho_f > 0$ and $\inf_{\Gamma_k} \rho_{b,k} > 0$.*
2. *Let $H_\epsilon(\boldsymbol{x})$ be a cube of side length ϵ centered at $\boldsymbol{x}$ in $\mathbb{R}^d$. Then,*

$$\|\boldsymbol{y} - \boldsymbol{y}'\| \le \sqrt{d-1}\epsilon, \quad \forall \boldsymbol{y}, \boldsymbol{y}' \in H_\epsilon(\boldsymbol{x}_{b,k}) \cap \Gamma_k, \quad \forall \boldsymbol{x}_{b,k} \in \Gamma_k.$$

3. *Let $B_\epsilon(\boldsymbol{x})$ be a closed ball of radius ϵ centered at $\boldsymbol{x}$ in $\mathbb{R}^d$. There exist positive constants $C_f, c_f, C_{b,k}, c_{b,k}$ such that $\forall \boldsymbol{x}_f \in U$ and $\forall \boldsymbol{x}_{b,k} \in \Gamma_k$,*

$$c_f \epsilon^d \le \mu_f(H_\epsilon(\boldsymbol{x}_f) \cap U), \quad \mu_f(B_\epsilon(\boldsymbol{x}_f) \cap U) \le C_f \epsilon^d,$$
$$c_{b,k} \epsilon^{d-1} \le \mu_{b,k}(H_\epsilon(\boldsymbol{x}_{b,k}) \cap \Gamma_k), \quad \mu_{b,k}(B_\epsilon(\boldsymbol{x}_{b,k}) \cap \Gamma_k) \le C_{b,k} \epsilon^{d-1}.$$

Here C_f, c_f depend only on (U, μ_f) and $C_{b,k}, c_{b,k}$ depend only on $(\Gamma_k, \mu_{b,k})$.
4. *When $d = 1$, we assume that all boundary points are available. Thus, no random sample is needed on the boundary.*

We remark that Assumption 3.1 guarantees that random samples drawn from probability distributions can fill up both the interior of the domain U and the boundary ∂U. These are mild assumptions and can be satisfied in many practical cases.

For example, let $U = (0,1)^d$. Then the uniform probability distributions on both U and ∂U satisfy Assumption 3.1.

Also, note that since the domain is of $C^{0,1}$-smoothness, the d-dimensional Lebesgue measure of ∂U is zero. To properly sample training data from ∂U, the boundary sampling distributions $\mu_{b,k}$ have to be introduced.

We now state our result that bounds the expected PINN loss in terms of a regularized empirical loss. Let us recall that $\boldsymbol{m}$ is the vector of the number of training data points, i.e., $\boldsymbol{m} = (m_f, m_{b,1}, \cdots, m_{b,N_B})$. The constants $c_f, C_f, c_{b,k}, C_{b,k}$ are introduced in Assumption 3.1. For a function u, $[u]_{\alpha;U}$ is the Hölder constant of u with exponent α in U (2.6).

THEOREM 3.2. *Suppose Assumption 3.1 holds. Let m_f and $m_{b,k}$ be the number of iid samples from μ_f and $\mu_{b,k}$, respectively. For some $0 < \alpha \leq 1$, let h, f, g_k satisfy*

$$\left[\mathcal{L}[h]\right]_{\alpha;U}^2 \leq R_f(h) < \infty, \quad \left[\mathcal{B}_k[h]\right]_{\alpha;\Gamma_k}^2 \leq R_{b,k}(h) < \infty, \quad \left[f\right]_{\alpha;U}, \left[g_k\right]_{\alpha;\Gamma_k} < \infty.$$

Let $\boldsymbol{\lambda} = (\lambda_f, \lambda_{b,1}, \ldots, \lambda_{b,N_B})$ be a fixed vector. Let $\hat{\boldsymbol{\lambda}}_{\boldsymbol{m}}^R = (\hat{\lambda}_{f,\boldsymbol{m}}^R, \hat{\lambda}_{b,1,\boldsymbol{m}}^R, \cdots, \hat{\lambda}_{b,N_B,\boldsymbol{m}}^R)$.

For $d \geq 2$, with probability at least, $(1 - \sqrt{m_f}(1 - 1/\sqrt{m_f})^{m_f}) \prod_{k=1}^{N_B}(1 - \sqrt{m_{b,k}}(1 - 1/\sqrt{m_{b,k}})^{m_{b,k}})$, we have

$$Loss^{PINN}(h; \boldsymbol{\lambda}) \leq C_{\boldsymbol{m}} \cdot Loss_{\boldsymbol{m}}(h; \boldsymbol{\lambda}, \hat{\boldsymbol{\lambda}}_{\boldsymbol{m}}^R) + C'(m_f^{-\frac{\alpha}{d}} + N_B \max_k m_{b,k}^{-\frac{\alpha}{d-1}}),$$

where $\kappa_f = \frac{C_f}{c_f}$, $\kappa_{b,k} = \frac{C_{b,k}}{c_{b,k}}$, $C_{\boldsymbol{m}} = 3 \max\{\kappa_f \sqrt{d}^d m_f^{\frac{1}{2}}, \max_k\{\kappa_{b,k} \sqrt{d-1}^{d-1} m_{b,k}^{\frac{1}{2}}\}\}$, C' is a universal constant that depends only on $\boldsymbol{\lambda}$, d, c_f, $c_{b,k}$, α, f, g_k, and

$$(3.1) \quad \hat{\lambda}_{f,\boldsymbol{m}}^R = \frac{3\lambda_f \sqrt{d}^{2\alpha} c_f^{-\frac{2\alpha}{d}}}{C_{\boldsymbol{m}}} \cdot m_f^{-\frac{\alpha}{d}}, \quad \hat{\lambda}_{b,k,\boldsymbol{m}}^R = \frac{3\lambda_{b,k} \sqrt{d-1}^{2\alpha} c_{b,k}^{-\frac{2\alpha}{d-1}}}{C_{\boldsymbol{m}}} \cdot m_{b,k}^{-\frac{\alpha}{d-1}},$$

for $1 \leq k \leq N_B$.

For $d = 1$, with probability at least, $1 - \sqrt{m_f}(1 - 1/\sqrt{m_f})^{m_f}$, we have

$$Loss^{PINN}(h; \boldsymbol{\lambda}) \leq C_{\boldsymbol{m}} \cdot Loss_{\boldsymbol{m}}(h; \boldsymbol{\lambda}, \hat{\boldsymbol{\lambda}}_{\boldsymbol{m}}^R) + C'm_f^{-\alpha},$$

where $C_{\boldsymbol{m}} = 3\kappa_f m_f^{\frac{1}{2}}$, $\hat{\lambda}_{f,\boldsymbol{m}}^R = \frac{\lambda_f c_f^{-2\alpha}}{\kappa_f} \cdot m_f^{-\alpha-\frac{1}{2}}$, $\hat{\lambda}_{b,k,\boldsymbol{m}}^R = 0$ for all k, and C' is a universal constant that depends only on λ_f, c_f, α, f.

Proof. The proof can be found in Appendix B. $\square$

Let $\boldsymbol{\lambda}$ be a vector independent of $\boldsymbol{m}$ and $\boldsymbol{\lambda}_{\boldsymbol{m}}^R = [\lambda_{f,\boldsymbol{m}}^R, \lambda_{b,1,\boldsymbol{m}}^R, \cdots, \lambda_{b,N_B,\boldsymbol{m}}^R]$ be a vector satisfying

$$(3.2) \quad \boldsymbol{\lambda}_{\boldsymbol{m}}^R \geq \hat{\boldsymbol{\lambda}}_{\boldsymbol{m}}^R, \quad \|\boldsymbol{\lambda}_{\boldsymbol{m}}^R\|_\infty = \mathcal{O}(\|\hat{\boldsymbol{\lambda}}_{\boldsymbol{m}}^R\|_\infty),$$

where $\hat{\boldsymbol{\lambda}}_{\boldsymbol{m}}^R$ is defined in (3.1). For a vector v, $\|v\|_\infty$ is the maximum norm, i.e., $\|v\|_\infty = \max_i |v_i|$.

By letting $R_f(h) = \left[\mathcal{L}[h]\right]_{\alpha;U}^2$ and $R_{b,k}(h) = \left[\mathcal{B}_k[h]\right]_{\alpha;\Gamma_k}^2$, let us define the Hölder regularized empirical loss:

$$(3.3) \quad \begin{aligned} &\text{Loss}_{\boldsymbol{m}}(h; \boldsymbol{\lambda}, \boldsymbol{\lambda}_{\boldsymbol{m}}^R) \\ &= \begin{cases} \text{Loss}_{\boldsymbol{m}}^{\text{PINN}}(h; \boldsymbol{\lambda}) + \lambda_{f,\boldsymbol{m}}^R \left[\mathcal{L}[h]\right]_{\alpha;U}^2 + \sum_{k=1}^{N_B} \lambda_{b,k,\boldsymbol{m}}^R \left[\mathcal{B}_k[h]\right]_{\alpha;U}^2, & \text{if } d \geq 2 \\ \text{Loss}_{\boldsymbol{m}}^{\text{PINN}}(h; \boldsymbol{\lambda}) + \lambda_{f,\boldsymbol{m}}^R \left[\mathcal{L}[h]\right]_{\alpha;U}^2, & \text{if } d = 1 \end{cases} \end{aligned}$$

where $\boldsymbol{\lambda}_{\boldsymbol{m}}^R$ are vectors satisfying (3.2). We note that the Hölder regularized loss (3.3) is greater than or equal to the empirical loss shown in Theorem 3.2 (assuming $R_f(h) = \left[\mathcal{L}[h]\right]_{\alpha;U}^2$ and $R_{b,k}(h) = \left[\mathcal{B}_k[h]\right]_{\alpha;\Gamma_k}^2$). Since $\left[\mathcal{L}[h]\right]_{\alpha;U}^2$ and $\left[\mathcal{B}_k[h]\right]_{\alpha;U}^2$ do not depend on the training data and $\hat{\lambda}_{f,\boldsymbol{m}}^R, \hat{\lambda}_{b,k,\boldsymbol{m}}^R \to 0$ as $m_f, m_{b,k} \to \infty$, this suggests that the more data we have, the less regularization is needed.

Theorem 3.2 indicates that minimizing the Hölder regularized loss (3.3) over h results in minimizing an upper bound of the expected PINN loss (2.5). This suggests that the Hölder regularized loss could be used as a loss function in a way to have a small expected PINN loss. In general, however, the Hölder-regularization functionals (the Hölder constants) are impractical to be evaluated numerically. Also, minimizing an upper bound does not necessarily imply minimizing the expected PINN loss.

If the domain is convex and the Hölder exponent is $\alpha = 1$ (i.e., Lipschitz constant), it follows from Rademacher's Theorem [6] that the Lipschitz constant of $\mathcal{L}[h]$ is the supremum of the sup norm of $\nabla \mathcal{L}[h]$ over U. Thus, one can use the maximum of the sup norm of the derivative over the set of training data points to estimate the Lipschitz constant. The resulting Lipschitz regularized (LIPR) loss is given by

$$\text{Loss}_{\boldsymbol{m}}^{\text{LIPR}}(h; \boldsymbol{\lambda}) = \text{Loss}_{\boldsymbol{m}}^{\text{PINN}}(h; \boldsymbol{\lambda}) + \lambda_f^R \max_{1 \leq i \leq m_f} \|\nabla \mathcal{L}[h](\mathbf{x}_f^i)\|_\infty^2$$

(3.4)
$$+ \sum_{k=1}^{N_B} \lambda_{b,k}^R \max_{1 \leq j \leq m_{b,k}} \|\nabla \mathcal{B}_k[h](\mathbf{x}_{b,k}^j)\|_\infty^2,$$

where $\text{Loss}_{\boldsymbol{m}}^{\text{PINN}}(h; \boldsymbol{\lambda})$ is defined in (2.5) and $\lambda_f^R, \lambda_{b,k}^R$ are weights of the regularization penalty terms.

3.1. Expected PINN Loss. We now concern with the problem of minimizing the Hölder regularized loss (3.3). In particular, we want to quantify how well a minimizer of the regularized empirical loss performs on the expected PINN loss (2.5).

We make the following assumptions to properly define function classes for the minimization problems (2.4).

ASSUMPTION 3.3. *Let $\boldsymbol{k} = (k_1, \cdots, k_d)$ be the highest order of the derivative shown in the PDE (2.1). For some $0 < \alpha \leq 1$, let $f(\boldsymbol{x}) \in C^{0,\alpha}(U)$ and $g_k \in C^{0,\alpha}(\Gamma_k)$.*
1. *For each $\boldsymbol{m}$, let $\mathcal{H}_{\boldsymbol{m}}$ be a function class in $C^{\boldsymbol{k},\alpha}(U) \cap C^{0,\alpha}(\bar{U})$ such that for any $h \in \mathcal{H}_{\boldsymbol{m}}$, $\mathcal{L}[h] \in C^{0,\alpha}(U)$ and $\mathcal{B}_k[h] \in C^{0,\alpha}(\Gamma_k)$.*
2. *For each $\boldsymbol{m}$, $\mathcal{H}_{\boldsymbol{m}}$ contains a function $u_{\boldsymbol{m}}^*$ satisfying $\text{Loss}_{\boldsymbol{m}}^{PINN}(u_{\boldsymbol{m}}^*; \boldsymbol{\lambda}) = 0$.*
3. *For $h \in \mathcal{H}_{\boldsymbol{m}}$, $\left[\mathcal{L}[h]\right]_{\alpha;U}$ and $\left[\mathcal{B}_k[h]\right]_{\alpha;\Gamma_k}$ are finite. Also,*

$$\sup_{\boldsymbol{m}} \left[\mathcal{L}[u_{\boldsymbol{m}}^*]\right]_{\alpha;U} < \infty, \quad \sup_{\boldsymbol{m}} \left[\mathcal{B}_k[u_{\boldsymbol{m}}^*]\right]_{\alpha;\Gamma_k} < \infty.$$

All the assumptions are essential for the proof. Our proof relies on the compactness argument and Assumption 3.3 guarantees the uniform equicontinuity of subsequences. The second assumption holds automatically if $\mathcal{H}_{\boldsymbol{m}}$ contains the solution to the PDE for all $\boldsymbol{m}$. For example, [?, 4] showed that the solution to some Hamilton-Jacobi PDEs can be exactly represented by neural networks. It could be relaxed, however, we do not discuss it here for the readability (See Appendix C).

For the rest of this paper, we use the following notation. When the number of the initial/boundary training data points $m_{b,k}$ is completely determined by the number of residual points m_f (e.g. $m_f^{d-1} = \mathcal{O}(m_{b,k}^d)$), the vector of the number of training data $\boldsymbol{m}$ depends only on m_f. In this case, we simply write $\mathcal{H}_{\boldsymbol{m}}, \boldsymbol{\lambda}_{\boldsymbol{m}}^R, \text{Loss}_{\boldsymbol{m}}$ as $\mathcal{H}_{m_f}, \boldsymbol{\lambda}_{m_f}^R, \text{Loss}_{m_f}$, respectively.

We now show that minimizers of the Hölder regularized loss (3.3) indeed produce a small expected PINN loss.

THEOREM 3.4. *Suppose Assumptions 3.1 and 3.3 hold. Let m_f and $m_{b,k}$ be the number of iid samples from μ_f and $\mu_{b,k}$, respectively, and $m_f = \mathcal{O}(m_{b,k}^{\frac{d}{d-1}})$ for all k. Let $\boldsymbol{\lambda}_{m_f}^R$ be a vector satisfying (3.2). Let $h_{m_f} \in \mathcal{H}_{m_f}$ be a minimizer of the Hölder regularized loss $Loss_{m_f}(\cdot; \boldsymbol{\lambda}, \boldsymbol{\lambda}_{m_f}^R)$ (3.3). Then the following holds.*

- *With probability at least $(1 - \sqrt{m_f}(1 - c_f/\sqrt{m_f})^{m_f}) \prod_{k=1}^{N_B}(1 - \sqrt{m_{b,k}}(1 - c_{b,k}/\sqrt{m_{b,k}})^{m_{b,k}})$ over iid samples,*

$$Loss^{PINN}(h_{m_f}; \boldsymbol{\lambda}) = \mathcal{O}(m_f^{-\frac{\alpha}{d}}).$$

- *With probability 1 over iid samples,*

$$(3.5) \qquad \lim_{m_f \to \infty} \mathcal{L}[h_{m_f}] = f \text{ in } C^0(U), \qquad \lim_{m_f \to \infty} \mathcal{B}_k[h_{m_f}] = g_k \text{ in } C^0(\Gamma_k),$$

for $k = 1, \cdots, N_B$.

Proof. The proof can be found in Appendix C. □

Theorem 3.4 shows that the expected PINN loss (2.5) at minimizers of the Hölder regularized losses (3.3) converges to zero with the rate at least of $\mathcal{O}(m_f^{-\frac{\alpha}{d}})$. This rate can be interpreted as the worst rate of convergence. Furthermore, the uniform convergences of $\mathcal{L}[h_{m_f}] \to f$ and $\mathcal{B}_k[h_{m_f}] \to g_k$ as $m_f \to \infty$ are achieved. These results are meaningful, however, it is insufficient to claim the convergence of h_{m_f} to the solution to the PDE (2.1). In the next subsections, we consider two classes of PDEs and discuss the convergence of minimizers.

Remark that the uniform convergences of (3.5) do not necessarily imply the convergence of h_m to the solution u^*. For example, let $f_n(x) = n\cos(x/n)$ on $U = [-1, 1]$. It can be checked that for any $k \geq 1$, the k-th derivative of f_n converges to 0 uniformly. However, $f_n(x)$ does not even converge.

3.2. Linear Elliptic PDEs. In this subsection, we combine all the boundary conditions into one and write

$$g(\mathbf{x}) = \sum_{k=1}^{N_B} g_k(\mathbf{x})\mathbb{I}_{\Gamma_k}(\mathbf{x}), \quad \mathbf{x} \in \Gamma = \cup_{k=1}^{N_B}\Gamma_k = \partial U.$$

We consider the second-order linear elliptic PDEs with the Dirichlet boundary condition:

$$(3.6) \qquad \begin{cases} \mathcal{L}[u] = f & \text{in } U, \\ u = g & \text{in } \partial U, \end{cases}$$

where $f : U \to \mathbb{R}$, $g : \partial U \mapsto \mathbb{R}$, and

$$\mathcal{L}[u] = \sum_{i,j=1}^{d} D_i\left(a^{ij}(\mathbf{x})D_j u + b^i(x)u\right) + \sum_{i=1}^{d} c^i(\mathbf{x})D_i u + d(\mathbf{x})u.$$

The coefficients are defined on U. To guarantee the existence, regularity and uniqueness of the classical solution to (3.6), we adopt the Schauder approach (Chapter 6 of [9]). For the proof, the following assumptions are made.

ASSUMPTION 3.5. *Let $\lambda(\boldsymbol{x})$ be the minimum eigenvalues of $[a^{ij}(\boldsymbol{x})]$ and $\alpha \in (0,1)$.*
1. *(Strictly elliptic) For some constant λ_0, $\lambda(\boldsymbol{x}) \geq \lambda_0 > 0$ in U.*
2. *The coefficients of the operator $\mathcal{L}$ are in $C^\alpha(U)$.*
3. *There are constants $\Lambda, v \geq 0$ such that for all $x \in U$*

$$\sum_{i,j} |a^{ij}(\boldsymbol{x})|^2 \leq \Lambda, \qquad \lambda_0^{-2}(\|\boldsymbol{b}(\boldsymbol{x})\|^2 + \|\boldsymbol{c}(\boldsymbol{x})\|^2) + \lambda_0^{-1}|d(\boldsymbol{x})| \leq v^2,$$

   where $\boldsymbol{b}(\boldsymbol{x}) = [b^1(\boldsymbol{x}), \cdots, b^d(\boldsymbol{x})]^T$ and $\boldsymbol{c}(\boldsymbol{x}) = [c^1(\boldsymbol{x}), \cdots, c^d(\boldsymbol{x})]^T$.
4. *a^{ij} and b^i are in $C^{1,\alpha}(U)$. Also g is continuous on ∂U.*
5. *U satisfies the exterior sphere condition at every boundary point.*

Since a^{ij} and b^i are differentiable, one can rewrite the differential operator as

$$\mathcal{L}[u] = \sum_{i,j=1}^d a^{ij}(\mathbf{x})D_{ij}u + \sum_{i=1}^d \tilde{b}^i(\mathbf{x})D_i u + \tilde{c}(\mathbf{x})u.$$

where

$$\tilde{b}^i(\mathbf{x}) = \sum_{j=1}^d D_j a^{ij}(\mathbf{x}) + b^i(\mathbf{x}) + c^i(\mathbf{x}), \qquad \tilde{c}(\mathbf{x}) = \sum_{i=1}^d D_i b^i(\mathbf{x}) + d(\mathbf{x}).$$

We now present our main convergence result for the linear elliptic PDEs.

THEOREM 3.6. *Suppose Assumptions 3.1, 3.3 and 3.5 hold and $\tilde{c}(\boldsymbol{x}) \leq 0$. Let m_f and $m_{b,k}$ be the number of iid samples from μ_f and $\mu_{b,k}$, respectively, and $m_f = \mathcal{O}(m_{b,k}^{\frac{d}{d-1}})$ for all k. Let $\boldsymbol{\lambda}_{m_f}^R$ be a vector satisfying (3.2). Let $h_{m_f} \in \mathcal{H}_{m_f}$ be a minimizer of the Hölder regularized loss $\mathrm{Loss}_{m_f}(\cdot; \boldsymbol{\lambda}, \boldsymbol{\lambda}_{m_f}^R)$ (3.3). Then the following holds.*
1. *For each PDE data set $\{f, g\}$, there exists a unique classical solution u^* to the PDE (3.6).*
2. *With probability 1 over iid samples,*

$$\lim_{m_f \to \infty} h_{m_f} = u^*, \qquad in \ C^0(U).$$

Proof. The proof can be found in Appendix D. □

Theorem 3.6 affirmatively shows that minimizers of the Hölder regularized empirical losses (3.3) converge to the unique classical solution to the PDE (3.6). This verifies that the PINNs approach is a correct methodology that finds the PDE solution in the sample limit.

The mode of convergence in Theorem 3.6 is the uniform convergence C^0, which implies the L^2-convergence. Next, we show that if each minimizer exactly satisfies the boundary conditions, the mode of convergence can be improved to H^1.

THEOREM 3.7. *Under the same conditions of Theorem 3.6, suppose each minimizer of (2.4) satisfies the boundary conditions. Then, with probability 1 over iid samples, the sequence of minimizers stated in Theorem 3.6 converges to the solution u^* to the PDE (3.6) in $H^1(U)$.*

Proof. The proof can be found in Appendix E. □

In the literature, there are several ways to enforce neural networks to satisfy the boundary conditions. The work of [13] considered the function classes that exactly satisfy the boundary conditions. The idea was then extended and generalized in [14, 2] to deal with irregular domains. This approach consists of two steps. First, extra structures are added on neural networks. The resulting surrogate is a sum of two networks where one is the boundary network that is designed for fitting boundary data and the other is for fitting residual data. Importantly, the boundary network is pre-trained (or trained first) to fit the boundary data. The rest of learning is done on the function that (approximately) satisfy the boundary conditions.

PINNs [22, 14] do require neither extra structures on the solution surrogate nor pre-training with the boundary data. However, it has been empirically reported [14, 2, 27] that properly chosen boundary weights ($\lambda_{b,k}$) could accelerate the overall training and result in a better performance.

On the top of these existing works, Theorem 3.8 theoretically sheds light on the importance of learning the boundary conditions. The result also indicates that how one can improve the training in term of the convergence mode. By putting large weights on the boundary penalty terms, neural networks are expected to learn the boundary data first and fast. In section 4, we demonstrate the effects of the boundary weights in the training. It was also mentioned in [14] that the boundary weight takes a large positive value to accurately satisfy the boundary conditions.

Finally, we show that when a function class of neural networks with a fixed architecture contains the solution to the PDE (3.6), one can further improve the mode of convergence.

COROLLARY 3.8. *Under the same conditions of Lemma 2.3 and Theorem 3.6, suppose a neural network function class $\mathcal{H}_{\vec{n}}^{NN}$ (2.7) satisfies Assumption 3.3 by letting $\mathcal{H}_{m_f} = \mathcal{H}_{\vec{n}}^{NN}$ for all m_f. Let u^* be the solution to the PDE (3.6) and $u^* \in \mathcal{H}_{\vec{n}}^{NN}$. Then, with probability 1 over iid samples, the sequence of minimizers stated in Theorem 3.6 converges to u^* in $C^k(U)$, where k is stated in Lemma 2.3.*

Proof. By Theorem 3.6, we have $\|h_{m_f} - u^*\|_{C^0(U)} \to 0$ as $m_f \to \infty$. Since $u^* \in \mathcal{H}_{\vec{n}}^{NN}$, $u^* \in C^k(\bar{U})$ as well. It then follows from Lemma 2.3 that $\|h_{m_f} - u^*\|_{C^k(U)} \to 0$ as $m_f \to \infty$. □

3.3. Linear Parabolic PDEs. In this section, we consider the second-order linear parabolic equations. Let U be a bounded domain in $\mathbb{R}^d$ and let $U_T = U \times (0, T]$ for some fixed time $T > 0$. Let us denote the parabolic boundary as $\Gamma_T = \overline{U}_T - U_T$. Also, let $D = U \times (0, T)$. $(\mathbf{x}, t) = (x_1, \cdots, x_d, t)$ is a point in $\mathbb{R}^{d+1}$.

Let us consider the initial/boundary-value problem:

$$\text{(3.7)} \quad \begin{cases} -u_t + \mathcal{L}[u] = f, & \text{in } U_T \\ u = \varphi, & \text{in } \partial U \times [0, T] \\ u = g, & \text{in } \bar{U} \times \{t = 0\}, \end{cases}$$

where $f : U_T \mapsto \mathbb{R}$, $g : \bar{U} \mapsto \mathbb{R}$, $\varphi : \partial U \times [0, T] \mapsto \mathbb{R}$, and

$$\mathcal{L}[u] = \sum_{i,j=1}^d D_i \left(a^{ij}(\mathbf{x}, t) D_j u + b^i(\mathbf{x}, t) u \right) + \sum_{i=1}^d c^i(\mathbf{x}, t) D_i u + d(\mathbf{x}, t) u.$$

In order to ensure the existence, regularity and uniqueness of the PDE (3.7), the following assumptions are made. Again, we follow the Schauder approach [8].

ASSUMPTION 3.9. *Let $\lambda(\boldsymbol{x}, t)$ be the minimum eigenvalues of $[a^{ij}(\boldsymbol{x}, t)]$.*
1. *For some constant λ_0, $\lambda(\boldsymbol{x}, t) \geq \lambda_0 > 0$ for all $(\boldsymbol{x}, t) \in D$.*
2. *There are constants $\Lambda, v \geq 0$ such that for all $(\boldsymbol{x}, t) \in D$*

$$\sum_{i,j} |a^{ij}(\boldsymbol{x}, t)|^2 \leq \Lambda, \qquad \lambda_0^{-2}(\|\boldsymbol{b}(\boldsymbol{x}, t)\|^2 + \|\boldsymbol{c}(\boldsymbol{x}, t)\|^2) + \lambda_0^{-1}|d(\boldsymbol{x}, t)| \leq v^2,$$

   where $\boldsymbol{b}(\boldsymbol{x}, t) = [b^1(\boldsymbol{x}, t), \cdots, b^d(\boldsymbol{x}, t)]^T$ and $\boldsymbol{c}(\boldsymbol{x}, t) = [c^1(\boldsymbol{x}, t), \cdots, c^d(\boldsymbol{x}, t)]^T$.
3. *The coefficients of $\mathcal{L}$ in (3.7) are in $C^\alpha(D)$ and a^{ij} and b^i are in $C^{1,\alpha}(D)$.*
4. *There exists $\theta > 0$ such that $\theta^2 a^{11}(\boldsymbol{x}, t) + \theta \tilde{b}^1(\boldsymbol{x}, t) \geq 1$ in D.*
5. *f is Hölder continuous (exponent α) in D. Also g is continuous on $\bar{U} \times \{t = 0\}$ and φ is continuous on $\partial \bar{U} \times [0, T]$.*

Since a^{ij} and b^i are differentiable, one can rewrite the differential operator as

$$\mathcal{L}[u] = \sum_{i,j=1}^d a^{ij}(\mathbf{x}, t)D_{ij}u + \sum_{i=1}^d \tilde{b}^i(\mathbf{x}, t)D_i u + \tilde{c}(\mathbf{x}, t)u.$$

where

$$\tilde{b}^i(\mathbf{x}, t) = \sum_{j=1}^d D_j a^{ij}(\mathbf{x}, t) + b^i(\mathbf{x}, t) + c^i(\mathbf{x}, t), \qquad \tilde{c}(\mathbf{x}, t) = \sum_{i=1}^d D_i b^i(\mathbf{x}, t) + d(\mathbf{x}, t).$$

By adopting the notation of Theorem 3.6, we now present the convergence theorem for the linear parabolic PDEs.

THEOREM 3.10. *Suppose Assumptions 3.1, 3.3 and 3.9 hold and $\tilde{c}(\boldsymbol{x}, t) \leq 0$. Let m_f and $m_{b,k}$ be the number of iid samples from μ_f and $\mu_{b,k}$, respectively, and $m_f = \mathcal{O}(m_{b,k}^{\frac{d+1}{d}})$ for all k. Let $\boldsymbol{\lambda}_{m_f}^R$ be a vector satisfying (3.2). Let $h_{m_f} \in \mathcal{H}_{m_f}$ be a minimizer of the Hölder regularized loss $Loss_{m_f}(\cdot; \boldsymbol{\lambda}, \boldsymbol{\lambda}_{m_f}^R)$ (3.3). Then the following holds:*
1. *For each PDE data set $\{f, g, \varphi\}$, there exists a unique classical solution u^* to the PDE (3.7).*
2. *With probability 1 over iid samples,*

$$\lim_{m_f \to \infty} h_{m_f} = u^*, \qquad in \ C^0(U_T).$$

Proof. The proof can be found in Appendix F. □

Theorem 3.10 shows that PINNs can find the solutions to the linear parabolic type PDEs in the sample limit. Again, this theoretically justifies the PINNs methodology. The mode of convergence is the uniform, which also implies the $L^2(0, T; L^2(U))$-convergence.

Similarly, the convergence mode can be improved if each minimizer satisfies both the initial and the boundary conditions.

THEOREM 3.11. *Under the same conditions of Theorem 3.10, suppose the sequence of minimizers of (2.4) satisfies both the boundary and the initial conditions. Then, with probability 1 over iid samples, the sequence of minimizers stated in Theorem 3.10 strongly converges to the solution u^* to (3.7) in $L^2(0, T; H^1(U))$.*

Proof. The proof can be found in Appendix G. □

Again, Theorem 3.11 shows the importance of learning the initial and boundary conditions. The result indicates that one would put more weights on not only the boundary penalties but also the initial penalty in the empirical loss (2.2). In this manner, the neural network approximation is expected to learn the initial and boundary conditions first and fast during the training.

Similarly to Corollary 3.8, when a function class of neural networks with a fixed architecture contains the solution to the PDE (3.7), one could further improve the mode of convergence.

COROLLARY 3.12. *Under the same conditions of Lemma 2.3 and Theorem 3.10, suppose a neural network function class $\mathcal{H}_{\vec{n}}^{NN}$ (2.7) satisfies Assumption 3.3 by letting $\mathcal{H}_{m_f} = \mathcal{H}_{\vec{n}}^{NN}$ for all m_f. Let u^* be the solution to the PDE (3.7) and $u^* \in \mathcal{H}_{\vec{n}}^{NN}$. Then, with probability 1 over iid samples, the sequence of minimizers stated in Theorem 3.10 converges to u^* in $C^k(U_T)$, where k is stated in Lemma 2.3.*

Proof. Since the proof is similar to the proof of Corollary 3.8, we omitted it. □

3.4. Generalization Error. As we briefly discussed in the introduction, the generalization error is the distance between a global minimizer of the empirical loss and the projected solution in the current function class. The distance has to be carefully determined to appropriately reflect the releated regularities. From Theorem 3.6 and 3.10, we employ the topology of uniform convergence. With the uniform norm, we can characterize the generalization error.

Let m be the number of training data, $\mathcal{H}_m$ be a function class and u^* be the solution to the PDE. Let h_m be a global minimizer of the Hölder regularized empirical loss (3.3). Note that for the sake of readability, we assume that a global minimizer of (3.3) exists. Again, all the results remain true if ϵ-suboptimal global solutions to (3.3) are used for sufficiently small ϵ.

Let us consider the problem of $\min_{h \in \mathcal{H}_m} \|h - u^*\|_{C^0}$. In general, global minimizers need not exist. However, if there is one, say, $\hat{h}_m$, it induces the generalization error defined by $\|h_m - \hat{h}_m\|_{C^0}$. If there is no global minimizer, we consider a ϵ-suboptimal global solution [?]. For any small $\epsilon > 0$, $\hat{h}_m^\epsilon \in \mathcal{H}_m$ is a ϵ-suboptimal global solution to $\min_{h \in \mathcal{H}_m} \|h - u^*\|_{C^0}$ if it satisfies

$$(3.8) \qquad \|\hat{h}_m^\epsilon - u^*\|_{C^0} \le \inf_{h \in \mathcal{H}_m} \|h - u^*\|_{C^0} + \epsilon.$$

The generalization error with respect to $\hat{h}_m^\epsilon$ is then defined to be $\|h_m - \hat{h}_m^\epsilon\|_{C^0}$.

If the expected PINN loss were available and the function class is large enough to contain a global minimizer that produces the zero expected loss, the following proposition shows that any global minimizer is a classical solution to the PDE.

PROPOSITION 3.13. *For a function class $\mathcal{H}$, suppose there exists $h \in \mathcal{H}$ such that $Loss^{PINN}(h; \boldsymbol{\lambda}) = 0$. Also, suppose $\mathcal{L}[h]$ and f are continuous on $\bar{U}$ and $\mathcal{B}_k[h]$ and g_k are continuous on $\bar{\Gamma}_k$. Then, h is a classical solution to the PDE (2.1).*

Proof. Since $Loss^{PINN}(h; \boldsymbol{\lambda}) = 0$, we have $\mathcal{L}[h] = f$ in $L^2(U)$ and $\mathcal{B}_k[h] = g_k$ in $L^2(\Gamma_k)$. Since $\mathcal{L}[h] - f$ and $\mathcal{B}_k[h] - g_k$ are both continuous, we conclude that $\mathcal{L}[h] = f$ in $\bar{U}$ and $\mathcal{B}_k[h] = g_k$ in $\bar{\Gamma}_k$. Hence, h is a classical solution to the PDE (2.1). □

With the same function class and the conditions of Proposition 3.13, if the empirical loss were used, the generalization error is solely induced by the discrepancy between the empirical and the expected losses. If this is the case, Theorem 3.6 and 3.10 show that the generalization error goes to zero as the number of training data

goes to ∞. Next, we show that a similar result holds without the assumption on the function class having u^*.

THEOREM 3.14. *For the elliptic PDEs* (3.6)*, suppose the conditions of Theorem* 3.6 *hold. For the parabolic PDEs* (3.7)*, suppose the conditions of Theorem* 3.10 *hold. Let* $\{\epsilon_{m_f}\}$ *be a sequence of positive numbers such that* $\limsup_{m_f \to \infty} \epsilon_{m_f} = 0$. *Then, the generalization error with respect to* $\hat{h}_{m_f}^{\epsilon_{m_f}}$ (3.8) *by the Hölder regularized loss* (3.3) *converges to 0 as* $m_f \to \infty$.

Proof. Let u^* be the solution to the PDE (2.1). For each m_f, let us consider the generalization error with respect to $\hat{h}_{m_f}^{\epsilon_{m_f}}$, where $\limsup_{m_f} \epsilon_{m_f} = 0$. We observe that

$$
\begin{aligned}
\|h_{m_f} - \hat{h}_{m_f}^{\epsilon_{m_f}}\|_{C^0} &\le \|h_{m_f} - u^*\|_{C^0} + \|\hat{h}_{m_f}^{\epsilon_{m_f}} - u^*\|_{C^0} \\
&\le \|h_{m_f} - u^*\|_{C^0} + \inf_{h \in \mathcal{H}_{m_f}} \|h - u^*\|_{C^0} + \epsilon_m \\
&\le 2\|h_{m_f} - u^*\|_{C^0} + \epsilon_{m_f}.
\end{aligned}
$$

It follows from Theorem 3.6 and 3.10 that $\|h_{m_f} - u^*\|_{C^0} \to 0$. Thus, the proof is completed. $\square$

4. Computational Examples. In this section, we provide computational examples to demonstrate our theoretical findings. Mainly, we illustrate (i) the L^2 and H^1 convergence of the trained neural networks as the number of training data grows, and (ii) the faster learning processes when the initial/boundary penalty terms have large weights in the loss. We confine ourselves to one or two-dimensional problems.

As an effort to find a neural network that minimizes the loss, we employ a combination of two optimization methods; `Adam` [12] and `L-BFGS` [16]. We consecutively apply these in the order of `Adam` and `L-BFGS`. `Adam` is employed with its default hyperparameter setting. This combination has been used in other works (e.g. [17]).

4.1. Poisson's equation. Let us consider the one-dimensional Poisson's equation:

$$
-u_{xx}(x) = f(x) \quad \text{in } U = (-1, 1), \qquad u(-1) = g, u(1) = h.
$$

The force term is simply obtained by substituting exact solution in the equation. To reduce an extra randomness, the training data are set to the equidistant points on $[-1, 1]$. The prediction errors are computed based on the fixed grid of either 10,000 or 50,000 equidistant points on $[-1, 1]$. The discrete L^2 and H^1 predictive errors are reported. We show the training results by the original PINN loss (2.5) and the Lipschitz regularized loss (3.4). We refer to the results by the original PINN loss as 'PINN' and to the results by the LIPschitz Regularized loss as 'LIPR'. Specifically, the results by 'PINN' and the results by 'LIPR' are obtained by minimizing

(4.1)
$$
\begin{aligned}
\text{Loss}_{m_f}^{\text{PINN}}(h) &= \frac{1}{m_f} \sum_{j=1}^{m_f} \|\mathcal{L}[h](\mathbf{x}_f^j) - f(\mathbf{x}_f^j)\|^2 + \frac{\lambda_b}{2}(|h(-1)|^2 + |h(1)|^2), \\
\text{Loss}_{m_f}^{\text{LIPR}}(h) &= \text{Loss}_{m_f}^{\text{PINN}}(h) + \lambda_R \max_i |\nabla \mathcal{L}[h](\mathbf{x}_f^i)|^2,
\end{aligned}
$$

respectively. Here m_f is the number of residual training data points.

4.1.1. Error Convergence. We first consider the case where the exact solution is given by $u^*(x) = \tanh(x)$. For this task, we employ the 2-hidden layer residual neural network u_{NN} having 50 neurons at each layer with the tanh-activation function. That is,

$$u_{\mathrm{NN}}(x) = W^3 \tanh(W^2(\mathbf{1}x + \tanh(W^1 x + b^1)) + b^2) + b^3,$$

where $W^j \in \mathbb{R}^{n_j \times n_{j-1}}$, $b^j \in \mathbb{R}^{n_j}$, $\mathbf{1} \in \mathbb{R}^{n_1}$ whose entries are all 1, and $\vec{n} = (n_0 = 1, n_1 = 50, n_2 = 50, n_3 = 1)$. We remark that in this case, the solution can be exactly represented by a neural network. In Figure 2, the predictive errors are plotted with respect to the number of training data points from 100 to 10,000. We set $\lambda_b = 1$ and $\lambda_R = m_f^{-1.5}$ as suggested by Theorem 3.2. The maximum number of epochs of `Adam` is set to 25,000 and the full-batch is used. As expected by Corollary 3.8, the results by 'LIPR' exhibit both L^2- and H^1-convergence of the errors. We see that the rate of convergence approximately follows $\mathcal{O}(m_f^{-1})$, which matches the rate of convergence of the expected PINN loss (Theorem 3.4). For reference, we plot a dotted-line showing the $\mathcal{O}(m_f^{-1})$ rate of convergence with respect to the number of training data. The results by 'PINN' do not show any convergence with respect to the number of training data. However, without any regularization terms, the 'PINN' somehow finds an accurate approximation to u^* at all the number of data points we considered. We observe that the predictive errors by 'PINN' stay at the level of 10^{-6} at all time.
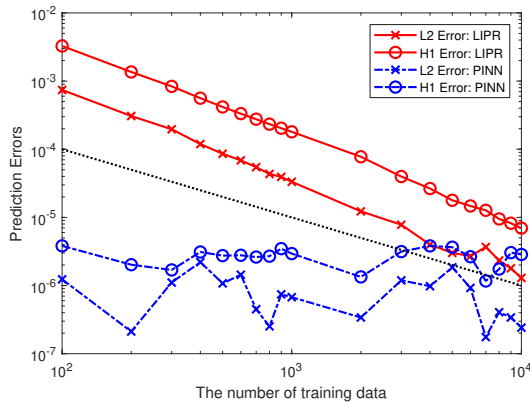

FIG. 2. *The L^2 and H^1 convergence for the 1D Poisson equation whose exact solution is $u^*(x) = \tanh(x)$ with respect to the number of training data points. The residual neural networks of depth 2 and width 50 are employed. The 'PINN' results are shown as dash-dot lines and the 'LIPR' results are shown as solid lines. The dotted line is a reference line indicating the $\mathcal{O}(m_f^{-1})$-rate of convergence.*

Next, we consider the case where the exact solution is given by $u^*(x) = (1 - x^2)\sin(6\pi x)$. For the training, we choose the function class that satisfies the boundary conditions automatically by adopting the following construction:

$$(4.2) \qquad \hat{u}_{\mathrm{NN}}(x) = (1 - x^2)u_{\mathrm{NN}}(x).$$

Again, u_{NN} is the 2-hidden layer residual neural network having 50 neurons at each layer with the tanh-activation function. Since the boundary conditions are automatically satisfied, the choice of λ_b does not affect the training results. We set $\lambda_R = m_f^{-1.5}$, the maximum number of epochs of `Adam` to either 5,000 or 25,000

and use the mini-batch of size 100. Figure 3 shows the L^2- and H^1-predictive errors with respect to the number of training data points from 100 to 5,000. As expected by Theorem 3.6 and 3.7, we see both the L^2- and H^1-convergence of the errors by 'LIPR'. Furthermore, we observe that the convergence rate approximately follows m_f^{-1}. As a reference, the $\mathcal{O}(m_f^{-1})$ rate of convergence is plotted as a dotted line. We see that the slopes of the predictive errors by 'LIPR' are well matched to the slope of the dotted line. The predictive errors by 'PINN', however, fluctuate and do not exhibit any convergence behavior. However, we see that the training by 'PINN' results in much smaller predictive errors at all training data points. In this case, the predictive errors by 'PINN' saturate at the level of 10^{-4}. This again indicates that PINNs find an approximation that also generalizes well without having explicit regularization terms.

Although our experiments may not find global minimums, our results clearly demonstrate both the L^2- and H^1-convergence of the errors by the Lipschitz regulared empirical loss (3.4).
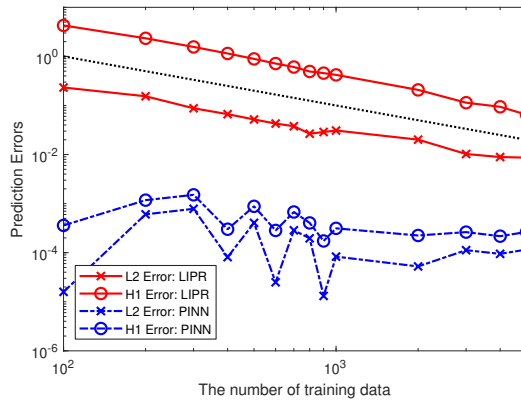

FIG. 3. *The L^2 and H^1 convergence for the 1D Poisson equation whose exact solution is $u^*(x) = (1 - x^2)\sin(6\pi x)$ with respect to the number of training data points. The neural networks (4.2) that automatically satisfy the boundary conditions are employed. The 'PINN' results are shown as dash-dot lines and the 'LIPR' results are shown as solid lines. The dotted line is a reference line indicating the $\mathcal{O}(m_f^{-1})$-rate of convergence.*

4.1.2. Boundary Weights: Acceleration of the PINNs training. By Theorem 3.7, if minimizers satisfy the boundary conditions, the H^1-mode of convergence can be achieved. Motivated by this result, we investigate the effect of the weights λ_b in the PINN loss (4.1). We consider the case where the exact solution is given by $u^*(x) = (1 - x^2)\sin(4\pi x)$. For the training, we apply `Adam` [12] and use 100 equi-distant points on $[-1, 1]$ as the training residual data. The predictive errors are computed on $10,000$ equi-distant points on $[-1, 1]$. We employ the 2-hidden layer residual neural network u_{NN} having 50 neurons at each layer with the tanh-activation function.

In Figure 4, the training results by three different choices of λ_b are shown with respect to the number of epochs. The training losses are plotted as dash-dot lines, the prediction L_2-errors are plotted as solid lines, and the prediction H_1-errors are plotted as dashed lines. To see how accurately the neural networks meet the boundary

conditions, we also report the boundary distance defined by

$$\text{Boundary Distance} = \sqrt{\frac{|u_{\text{NN}}(-1) - u^*(-1)|^2 + |u_{\text{NN}}(1) - u^*(1)|^2}{2}},$$

as dotted lines. The results by three choices of λ_b are shown: $\lambda_b = 1$ (left), $\lambda_b = 25$ (middle) and $\lambda_b = 50$ (right). We see that with $\lambda_b = 50$, the boundary distance reaches at the level of 10^{-4} at around after 1,000 epochs while other choices require more number of epochs. This indicates that by putting more weights on the boundary terms, the neural network learns the boundary conditions fast. Also, we see that the behaviors of the L^2- and H^1-errors are similar to those of the boundary distance in all cases of λ_b. Furthermore, we observe that the decay of the predictive errors are followed by the decay of the boundary distance in this case.
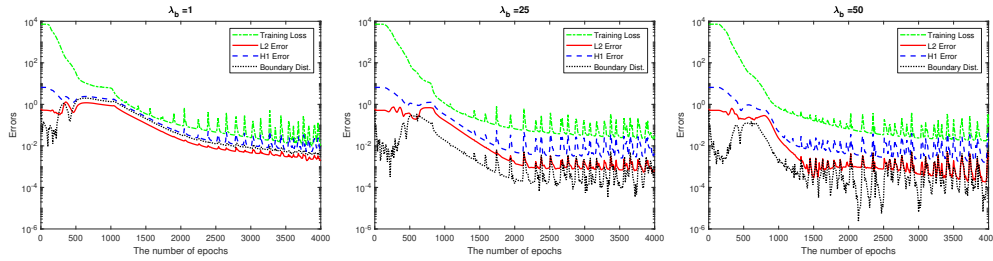

FIG. 4. *The training results for the 1D Poisson equation whose exact solution is $u^*(x) = (1-x^2)\sin(4\pi x)$. The training losses are shown as dash-dot lines. The predictive L^2- and H^1-errors are shown as solid and dash lines, respectively. The boundary distances are shown as dotted-lines. Three boundary weights are considered: (Left) $\lambda_b = 1$, (Middle) $\lambda_b = 25$, (Right) $\lambda_b = 50$. All results are shown with respect to the number of epochs of* Adam.

4.2. Heat Equation. Let us consider the 1D heat equation:

$$-u_t + \nu u_{xx} = f \quad \text{in } (x,t) \in U_T = (-1,1) \times (0,T],$$

with the Dirichlet initial/boundary condition. There are two boundary domains (Γ_1, Γ_2) and one initial domain (Γ_3): $\Gamma_1 = \{-1\} \times [0,T]$, $\Gamma_2 = \{1\} \times [0,T]$, and $\Gamma_3 = (-1,1) \times \{0\}$. We consider the case where the exact solution is given by $u^*(x,t) = \sin(\pi x)e^{-t}$ and $T = 1$. Let $m_{b,j}$ be the number of training points on Γ_j and m_f be the number of residual points on U_T. The training points are randomly uniformly drawn from its corresponding domains. We set $m_{b,2} = m_{b,1}$, $m_{b,3} = 2m_{b,1}$ and $m_f = 2m_{b,1}m_{b,2}$. This satisfies the condition of $m_f = \mathcal{O}(m_{b,k}^2)$ for all k, which is stated in Theorem 3.10. Again, we report two training results: the original PINN loss (2.5) ('PINN') and the Lipschitz regularized loss (3.4) ('LIPR'). For the 'PINN' loss, we set all the weights to 1. For the 'LIPR' weights, we set $\boldsymbol{\lambda} = \mathbf{1}$, $\lambda_f^R = \frac{2}{m_f}$, $\lambda_{b,1}^R = \frac{1}{m_{b,1}\sqrt{m_f}}$, $\lambda_{b,2}^R = \frac{1}{m_{b,2}\sqrt{m_f}}$, and $\lambda_{b,3}^R = \frac{1}{m_{b,3}\sqrt{m_f}}$. The standard feed-forward tanh-neural networks of depth 2 and width 50 are employed for the experiments. We set the maximum number of epoch of Adam to be 10,000 and use the mini-batch training.

In Figure 5, we show the predictive L^2- and H^1-errors with respect to the increasing the number of residual training data points m_f. The number of residual training data increases according to $m_f = 2m_{b,1}^2$ for $m_{b,1} = 10, 20, \cdots, 100$. The predictive errors are computed on the tensor-grid constructed by using 400 and 200

equidistant points on $[-1, 1]$ and $[0, 1]$, respectively. We report the average of three independent simulations. We see that the results by 'LIPR' exhibit both the L^2- and H^1-convergence. We also observe that the rate of the L^2-convergence by 'LIPR' approximately follows $\mathcal{O}(m_f^{-1})$. For a reference, we plot a line showing the $\mathcal{O}(m_f^{-1})$-rate of convergence as dotted line starting at $(200, 0.1)$. It can be seen that the slope of the L^2-errors by 'LIPR' is well matched to those of the dotted line. We see that the rate of the H^1-convergence by 'LIPR' lies between $\mathcal{O}(m_f^{-1})$ and $\mathcal{O}(m_f^{-\frac{1}{2}})$. Again, we plot a line showing the $\mathcal{O}(m_f^{-\frac{1}{2}})$-rate of convergence as dotted line starting at $(200, 0.2)$. It follows from Theorem 3.4 that in this case, the expected PINN loss decays at the rate at least $\mathcal{O}(m_f^{-\frac{1}{2}})$. We observe that this rate continues to hold for the predictive errors as demonstrated in Figure 5. Although the results by 'PINN' do not show clear convergence of the errors, the training results produce small predictive errors in all cases compared to those by 'LIPR'. This again indicates that the empirical PINN loss is capable of producing a good approximation to the solution without having explicit regularization.
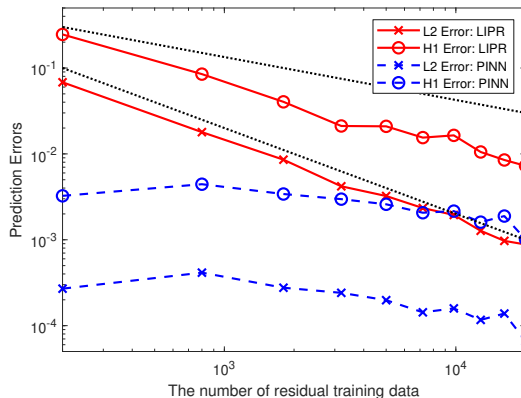

FIG. 5. *The L^2- and H^1-convergence of the errors with respect to the number of training data point for the 1D Heat equation whose exact solution is $u^*(x) = \sin(\pi x)e^{-t}$. The feed-forward neural networks of depth 2 and width 50 are employed. The 'PINN' results are shown as dash-dot lines and the 'LIPR' results are shown as solid lines. The dotted lines are reference lines indicating the $\mathcal{O}(m_f^{-\frac{1}{2}})$- and $\mathcal{O}(m_f^{-1})$-rate of convergence.*

5. Conclusion. In this work, we establish a mathematical foundation of physics informed neural networks (PINNs). Upon deriving an upper bound of the expected PINN loss, we obtain a Hölder regularized empirical loss. Under some assumptions, we show that the expected PINN loss at minimizers of the Hölder regularized loss converges to zero with the rate at least $\mathcal{O}(m^{-\frac{\alpha}{d}})$, where m is the number of residual training data points and α is the Hölder exponent. By considering two classes of PDEs –linear elliptic and parabolic– we show that with probability 1 over iid training samples, a sequence of minimizers of the Hölder regularized loss converges to the solution to the PDE uniformly. This also implies the L^2-convergence. Furthermore, we show that if each minimizer exactly satisfies the boundary conditions, the mode of convergence can be improved to H^1. Computational examples are provided to demonstrate our theoretical findings. To the best of our knowledge, this is the first theoretical work that shows the consistency of the PINNs methodology from the

sample limit perspective.

Appendix A. Proof of Lemma 2.3.

Proof. For each h_j, let $\boldsymbol{\theta}^j$ be its associated weights and biases. Since $\{\boldsymbol{\theta}^j\}$ is uniformly bounded, there exists a convergent subsequence, say, $\{\boldsymbol{\theta}^{j_i}\}$. Let $\{h_{j_i}\}$ be its corresponding neural network sequence. Let $\boldsymbol{\theta}^*$ be the limit of $\{\boldsymbol{\theta}^{j_i}\}$ and $h^* \in \mathcal{H}_{\vec{\boldsymbol{n}}}^{NN}$ be the corresponding limit network. Note that since $\{\boldsymbol{\theta}_j\}$ is uniformly bounded, U is bounded, and $\sigma^{(s)}$ is bounded for all $s \in \{0, \cdots, k\}$, $D^{\boldsymbol{s}} h_{j_i}$ is bounded continuous in $\bar{U}$ for all $\boldsymbol{s}$ with $0 \le |\boldsymbol{s}| \le k$.

CLAIM A.1. *Let $\{h^L(\boldsymbol{x}; \boldsymbol{\theta}^{j_i})\}$ be a sequence of L-layer neural networks having the same architecture $\vec{\boldsymbol{n}}$ whose activation function σ is of $C^k(\mathbb{R})$ and $\frac{d^s \sigma(x)}{dx^s}$ is bounded and Lipschitz continuous for $s = 0, \cdots, k$. Let $\boldsymbol{s} = (s_1, \cdots, s_d)$ be a multi-index with $|\boldsymbol{s}| = \sum_{i=1}^d s_i$. Then, for each $\boldsymbol{s}$ with $0 \le |\boldsymbol{s}| \le k$, the sequence $\{D^s h^L(\boldsymbol{x}; \boldsymbol{\theta}^{j_i})\}$ is uniformly convergent to $D^s h^L(\boldsymbol{x}; \boldsymbol{\theta}^*)$ on $\bar{U}$.*

Proof of Claim A.1. Let $\vec{\boldsymbol{n}} = (n_0, \cdots, n_L)$ be the network architecture. Let us recall that given $\vec{\boldsymbol{n}}$,

$$h^l(\mathbf{x}) = \boldsymbol{W}^l \sigma(h^{l-1}(\mathbf{x})) + \boldsymbol{b}^l, \qquad 1 < l \le L,$$

and $h^1(\mathbf{x}) = \boldsymbol{W}^1 \mathbf{x} + \boldsymbol{b}^1$, where $\boldsymbol{W}^l \in \mathbb{R}^{n_l \times n_{l-1}}$ and $\boldsymbol{b}^l \in \mathbb{R}^{n_l}$. For each l, let h_k^l be the k-th output of h^l, where $1 \le k \le n_l$. Let $\boldsymbol{\theta}_l = \{\boldsymbol{W}^j, \boldsymbol{b}^j\}_{j=1}^l$. With a slight abuse of notation, we regard $\boldsymbol{\theta}_l$ as a column vector. Also, let $\boldsymbol{\theta}_l' = \{\boldsymbol{W}'^j, \boldsymbol{b}'^j\}_{j=1}^l$.

We want to prove the following statement for all $l = 1, \cdots, L$:

$$D^{\boldsymbol{s}} h^l(\mathbf{x}; \boldsymbol{\theta}^{j_i}) \text{ converges to } D^{\boldsymbol{s}} h^l(\mathbf{x}; \boldsymbol{\theta}^*) \text{ in } C^0(U), \forall \boldsymbol{s} \text{ with } 0 \le |\boldsymbol{s}| \le k.$$

We prove it by applying induction on l.

When $l = 1$, it is clear that for $r = 1, \cdots, n_1$, we have

$$
\begin{aligned}
|h_r^1(\mathbf{x}; \boldsymbol{\theta}_1) - h_r^1(\mathbf{x}; \boldsymbol{\theta}_1')|^2 &\le 2 \left(|\boldsymbol{b}_r^1 - \boldsymbol{b}_r'^1|^2 + \|\boldsymbol{W}_r^1 - \boldsymbol{W}_r'^1\|^2 \|x\|^2 \right) \\
&\le C \|\boldsymbol{\theta}_1 - \boldsymbol{\theta}_1'\|^2,
\end{aligned}
$$

where $C = 2 \max\{1, \sup_U \|x\|^2\}$, and for $\boldsymbol{s} = (s_1, \cdots, s_d)$ with $1 \le |\boldsymbol{s}| \le k$,

$$|D^{\boldsymbol{s}} h_r^1(\mathbf{x}; \boldsymbol{\theta}) - D^{\boldsymbol{s}} h_r^1(\mathbf{x}; \boldsymbol{\theta}')| = \begin{cases} 0 & \text{if } \max s_i > 1, \\ |\boldsymbol{W}_{ri}^1 - \boldsymbol{W}_{ri}'^1| & \text{if } s_i = 1. \end{cases}$$

Hence, for $\boldsymbol{s} = (s_1, \cdots, s_d)$ with $0 \le |\boldsymbol{s}| \le k$, $D^{\boldsymbol{s}} h^1(\mathbf{x}; \boldsymbol{\theta}_1^{j_i})$ converges to $D^{\boldsymbol{s}} h^1(\mathbf{x}; \boldsymbol{\theta}_1^*)$ in $C^0(U)$.

Suppose the statement is true for $l-1$ where $l \ge 2$ and we want to show the case for l. For $\boldsymbol{s}$ with $0 \le |\boldsymbol{s}| \le k$, it then can be checked that for $1 \le r \le n_l$,

$$D^{\boldsymbol{s}} h_r^l(\mathbf{x}; \boldsymbol{\theta}_l) = \frac{\partial^{|\boldsymbol{s}|} h_r^l(\mathbf{x}; \boldsymbol{\theta}_l)}{\partial x_1^{s_1} \cdots \partial x_d^{s_d}} = \sum_{i=1}^{n_l} \boldsymbol{W}_{ri}^l \sum_{t=0}^{|\boldsymbol{s}|} Q_{i,t}^{l-1}(\boldsymbol{\theta}_{l-1}, |\boldsymbol{s}|, \mathbf{x}) \sigma^{(t)}(h_i^{l-1}(\mathbf{x}; \boldsymbol{\theta}_{l-1})),$$

where $\sigma^{(t)}$ is the t-th derivative of σ and $\{Q_{i,t}^l(\boldsymbol{\theta}_l, |\boldsymbol{s}|, \boldsymbol{x})\}_{t=1}^{|\boldsymbol{s}|}$ is recursively defined as

follows: Let $\bar{x}_j = x_i$ if $\sum_{l=1}^{i-1} s_l < j \leq \sum_{l=1}^{i} s_l$. Then, for $s \geq 2$,

$$Q_{i,t}^{l-1}(\boldsymbol{\theta}_{l-1}, s, \boldsymbol{x})$$

$$= \begin{cases} Q_{i,s-1}^{l-1}(\boldsymbol{\theta}_{l-1}, s-1, \boldsymbol{x}) \frac{\partial h_i^{l-1}(\mathbf{x};\boldsymbol{\theta}_{l-1})}{\partial \bar{x}_s} & \text{if } t = s, \\ \frac{\partial}{\partial \bar{x}_s} Q_{i,t}^{l-1}(\boldsymbol{\theta}_{l-1}, s-1, \boldsymbol{x}) + Q_{i,t-1}^{l-1}(\boldsymbol{\theta}_{l-1}, s-1, \boldsymbol{x}) \frac{\partial h_i^{l-1}(\mathbf{x};\boldsymbol{\theta}_{l-1})}{\partial \bar{x}_s} & \text{if } 1 < t < s, \\ \frac{\partial}{\partial \bar{x}_s} Q_{i,1}^{l-1}(\boldsymbol{\theta}_{l-1}, s-1, \boldsymbol{x}) & \text{if } t = 1, \\ 0 & \text{if } t = 0, \end{cases}$$

with $Q_{i,1}^{l-1}(\boldsymbol{\theta}_{l-1}, 1, \boldsymbol{x}) = \frac{\partial h_i^{l-1}(\mathbf{x};\boldsymbol{\theta}_1)}{\partial \bar{x}_1}$, $Q_{i,0}^{l-1}(\boldsymbol{\theta}_{l-1}, 1, \boldsymbol{x}) = 0$, and $Q_{i,0}^{l-1}(\boldsymbol{\theta}_{l-1}, 0, \boldsymbol{x}) = 1$. Thus,

$$|D^{\boldsymbol{s}} h_r^l(\mathbf{x};\boldsymbol{\theta}_{l-1}) - D^{\boldsymbol{s}} h_r^l(\mathbf{x};\boldsymbol{\theta}'_{l-1})|$$

$$\leq \sum_{i=1}^{n_l} \sum_{t=0}^{|\boldsymbol{s}|} |\boldsymbol{W}_{ri}^l Q_{i,t}^{l-1}(\boldsymbol{\theta}_{l-1}, |\boldsymbol{s}|, \mathbf{x}) - \boldsymbol{W}_{ri}'^l Q_{i,t}^{l-1}(\boldsymbol{\theta}'_{l-1}, |\boldsymbol{s}|, \mathbf{x})||\sigma^{(t)}(h_i^{l-1}(\mathbf{x};\boldsymbol{\theta}_{l-1}))|$$

$$+ \sum_{i=1}^{n_l} \sum_{t=0}^{|\boldsymbol{s}|} |\boldsymbol{W}_{ri}'^l Q_{i,t}^{l-1}(\boldsymbol{\theta}'_{l-1}, |\boldsymbol{s}|, \mathbf{x})||\sigma^{(t)}(h_i^{l-1}(\mathbf{x};\boldsymbol{\theta}_{l-1})) - \sigma^{(t)}(h_i^{l-1}(\mathbf{x};\boldsymbol{\theta}'_{l-1}))|.$$

Since $\sigma^{(s)}$ is Lipchitz continuous and bounded for all $0 \leq s \leq k$, there exists two constants M and L such that

$$|\sigma^{(t)}(h_i^{l-1}(\mathbf{x};\boldsymbol{\theta}_{l-1})) - \sigma^{(t)}(h_i^{l-1}(\mathbf{x};\boldsymbol{\theta}'_{l-1}))| \leq L|h_i^{l-1}(\mathbf{x};\boldsymbol{\theta}_{l-1}) - h_i^{l-1}(\mathbf{x};\boldsymbol{\theta}'_{l-1})|,$$
$$|\sigma^{(t)}(h_i^{l-1}(\mathbf{x};\boldsymbol{\theta}_{l-1}))| \leq M.$$

Let $G^l(\mathbf{x};\boldsymbol{\theta}_l) = \boldsymbol{W}_{ri}^l Q_{i,t}^{l-1}(\boldsymbol{\theta}_{l-1}, |\boldsymbol{s}|, \mathbf{x})$. By the induction hypothesis, $D^{\boldsymbol{s}} h^{l-1}(\mathbf{x};\boldsymbol{\theta}_{l-1}^{j_i})$ converges to $D^{\boldsymbol{s}} h^{l-1}(\mathbf{x};\boldsymbol{\theta}_{l-1}^*)$ in $C^0(U)$ for any $\boldsymbol{s}$ with $0 \leq |\boldsymbol{s}| \leq k$. Recall that the product of two uniformly convergent sequences of bounded continuous functions is also uniformly convergent to the product of limits. Thus, $G^l(\mathbf{x};\boldsymbol{\theta}_l^{j_i})$ uniformly converges to $G^l(\mathbf{x};\boldsymbol{\theta}_l^*)$ in U. Therefore, by combining all the above, we conclude that $D^{\boldsymbol{s}} h^l(\mathbf{x};\boldsymbol{\theta}_l^{j_i})$ converges to $D^{\boldsymbol{s}} h^l(\mathbf{x};\boldsymbol{\theta}_l^*)$ in $C^0(U)$. By induction, the proof is completed. □

By Claim A.1, we conclude that $\lim_{i\to\infty} \|h_{j_i} - h^*\|_{C^k(U)} = 0$. Since $\lim_{j\to\infty} \|h_j - u\|_{C^0(U)} = 0$, we have $h^* = u$. Hence, $\lim_{i\to\infty} \|h_{j_i} - u\|_{C^k(U)} = 0$. Since the subsequence was chosen arbitrarily, the proof is completed. □

Appendix B. Proof of Theorem 3.2. The proof consists of two lemmas.

LEMMA B.1. Let $\mathcal{T}_f = \{\boldsymbol{x}_f^i\}_{i=1}^{m_f}$ and $\mathcal{T}_{b,k} = \{\boldsymbol{x}_{b,k}^i\}_{i=1}^{m_{b,k}}$ for $k = 1, \cdots, N_B$. Suppose m_f and $m_{b,k}$ are large enough to satisfy the following: for any $\boldsymbol{x}_f \in U$ and $\boldsymbol{x}_{b,k} \in \Gamma_k$, $k = 1, \cdots, N_B$, there exists $\boldsymbol{x}'_f \in \mathcal{T}_f$ and $\boldsymbol{x}'_{b,k} \in \mathcal{T}_{b,k}$ such that

$$\|\boldsymbol{x}_f - \boldsymbol{x}'_f\| \leq \epsilon_f, \qquad \|\boldsymbol{x}_{b,k} - \boldsymbol{x}'_{b,k}\| \leq \epsilon_{b,k}, \quad \forall k.$$

Then, we have

$$Loss^{PINN}(h;\boldsymbol{\lambda})$$

(B.1)
$$\leq C_{\boldsymbol{m}} \cdot \left[Loss_{\boldsymbol{m}}^{PINN}(h;\boldsymbol{\lambda}) + \frac{3\lambda_f \epsilon_f^{2\alpha}}{C_{\boldsymbol{m}}} \left[\mathcal{L}[h]\right]_{\alpha;U}^2 + \sum_{k=1}^{N_B} \frac{3\lambda_{b,k}\epsilon_{b,k}^{2\alpha}}{C_{\boldsymbol{m}}} \left[\mathcal{B}_k[h]\right]_{\alpha;\Gamma_k}^2 \right]$$

$$+ 3\lambda_f \epsilon_f^{2\alpha} \left[f\right]_{\alpha;U}^2 + 3 \sum_{k=1}^{N_B} \lambda_{b,k}\epsilon_{b,k}^{2\alpha} \left[g_k\right]_{\alpha;\Gamma_k}^2,$$

where C_f and $C_{b,k}$ are from Assumption 3.1 and

$$C_{\boldsymbol{m}} = 3 \max \left\{ C_f m_f \epsilon_f^d, \max_k \{C_{b,k} m_{b,k} \epsilon_{b,k}^{d-1}\} \right\}.$$

Proof. Let us first recall that for any three vectors x, y, z, we have

$$\|x + y + z\|^2 \leq 3(\|x\|^2 + \|y\|^2 + \|z\|^2).$$

For $x_f, x_f' \in U$, we have

$$\|\mathcal{L}[h](\mathbf{x}_f) - f(\mathbf{x}_f)\|^2$$
$$\leq 3 \left(\|\mathcal{L}[h](\mathbf{x}_f) - \mathcal{L}[h](\mathbf{x}_f')\|^2 + \|\mathcal{L}[h](\mathbf{x}_f') - f(\mathbf{x}_f')\|^2 + \|f(\mathbf{x}_f') - f(\mathbf{x}_f)\|^2 \right).$$

Similarly, for each k and $x_{b,k}, x_{b,k}' \in \Gamma_k$, we have

$$\|\mathcal{B}_k[h](\mathbf{x}_{b,k}) - g_k(\mathbf{x}_{b,k})\|^2 \leq 3\|\mathcal{B}_k[h](\mathbf{x}_{b,k}) - \mathcal{B}_k[h](\mathbf{x}_{b,k}')\|^2$$
$$+ 3\|\mathcal{B}_k[h](\mathbf{x}_{b,k}') - g_k(\mathbf{x}_{b,k}')\|^2 + 3\|g_k(\mathbf{x}_{b,k}') - g_k(\mathbf{x}_{b,k})\|^2.$$

By assumption, $\forall \mathbf{x}_f \in U$ and $\forall \mathbf{x}_{b,k} \in \Gamma_k$, there exists $\mathbf{x}_f' \in \mathcal{T}_f^{m_f}$ and $\mathbf{x}_{b,k}' \in \mathcal{T}_b^{m_{b,k}}$ such that $\|\mathbf{x}_f - \mathbf{x}_f'\| \leq \epsilon_f$ and $\|\mathbf{x}_{b,k} - \mathbf{x}_{b,k}'\| \leq \epsilon_{b,k}$. Thus, we have

$$\mathbf{L}(\mathbf{x}_f, \vec{\mathbf{x}}_b; h, \boldsymbol{\lambda}, \mathbf{0})$$

$$= \lambda_f \|\mathcal{L}[h](\mathbf{x}_f) - f(\mathbf{x}_f)\|^2 + \sum_{k=1}^{N_B} \lambda_{b,k} \|\mathcal{B}_k[h](\mathbf{x}_{b,k}) - g_k(\mathbf{x}_{b,k})\|^2$$

$$\leq 3\lambda_f \|\mathcal{L}[h](\mathbf{x}_f) - \mathcal{L}[h](\mathbf{x}_f')\|^2 + 3\lambda_f \|f(\mathbf{x}_f') - f(\mathbf{x}_f)\|^2 + 3\lambda_f \|\mathcal{L}[h](\mathbf{x}_f') - f(\mathbf{x}_f')\|^2$$

$$+ 3\sum_{k=1}^{N_B} \lambda_{b,k} \|\mathcal{B}_k[h](\mathbf{x}_{b,k}) - \mathcal{B}_k[h](\mathbf{x}_{b,k}')\|^2 + 3\sum_{k=1}^{N_B} \lambda_{b,k} \|g_k(\mathbf{x}_{b,k}') - g_k(\mathbf{x}_{b,k})\|^2$$

$$+ 3\sum_{k=1}^{N_B} \lambda_{b,k} \|\mathcal{B}_k[h](\mathbf{x}_{b,k}') - g_k(\mathbf{x}_{b,k}')\|^2$$

$$\leq 3\mathbf{L}(\mathbf{x}_f', \vec{\mathbf{x}}_b'; h, \boldsymbol{\lambda}, \mathbf{0}) + 3\lambda_f \epsilon_f^{2\alpha} \left[\mathcal{L}[h]\right]_{\alpha;U}^2 + 3\sum_{k=1}^{N_B} \lambda_{b,k} \epsilon_{b,k}^{2\alpha} \left[\mathcal{B}_k[h]\right]_{\alpha;\Gamma_k}^2$$

$$+ 3\lambda_f \epsilon_f^{2\alpha} [f]_{\alpha;U}^2 + 3\sum_{k=1}^{N_B} \lambda_{b,k} \epsilon_{b,k}^{2\alpha} [g_k]_{\alpha;\Gamma_k}^2.$$

For $\mathbf{x}_f^i \in \mathcal{T}_f^{m_f}$, let $A_{\mathbf{x}_f^i}$ be the Voronoi cell assciated with $\mathbf{x}_f^i$, i.e.,

$$A_{\mathbf{x}_f^i} = \{\mathbf{x} \in U | \|\mathbf{x} - \mathbf{x}_f^i\| = \min_{\mathbf{x}' \in \mathcal{T}_f^{m_f}} \|\mathbf{x} - \mathbf{x}'\|\},$$

and let $\gamma_f^i = \mu_f(A_{\mathbf{x}_i})$. Similarly, for $\mathbf{x}_{b,k}^i \in \mathcal{T}_{b,k}^{m_{b,k}}$, let

$$A_{\mathbf{x}_{b,k}^i} = \{\mathbf{x} \in \Gamma | \|\mathbf{x} - \mathbf{x}_{b,k}^i\| = \min_{\mathbf{x}' \in \mathcal{T}_{b,k}^{m_{b,k}}} \|\mathbf{x} - \mathbf{x}'\|\}.$$

and let $\gamma_{b,k}^i = \mu_{b,k}(A_{\mathbf{x}_{b,k}^i})$. Note that $\sum_{i=1}^{m_f} \gamma_f^i = 1$ and $\sum_{i=1}^{m_{b,k}} \gamma_{b,k}^i = 1$. By taking the expectation with respect to $(\mathbf{x}_f, \vec{\mathbf{x}}_b) \sim \mu = \mu_f \times \prod_{k=1}^{N_B} \mu_{b,k}$, we have

$$\mathbb{E}_\mu[\mathbf{L}(\mathbf{x}_f, \vec{\mathbf{x}}_b; h, \boldsymbol{\lambda}, \mathbf{0})]$$
$$\leq 3 \sum_{k=1}^{N_B} \sum_{j=1}^{m_{b,k}} \sum_{i=1}^{m_f} \gamma_f^i \gamma_{b,k}^j \mathbf{L}(\mathbf{x}_f^i, \vec{\mathbf{x}}_{b,k}^j; h, \boldsymbol{\lambda}, \mathbf{0}) + 3\lambda_f \epsilon_f^{2\alpha} [\mathcal{L}[h]]_{\alpha;U}^2$$
$$+ 3\sum_{k=1}^{N_B} \lambda_{b,k} \epsilon_{b,k}^{2\alpha} [\mathcal{B}_k[h]]_{\alpha;\Gamma_k}^2 + 3\lambda_f \epsilon_f^{2\alpha} [f]_{\alpha;U}^2 + 3\sum_{k=1}^{N_B} \lambda_{b,k} \epsilon_{b,k}^{2\alpha} [g_k]_{\alpha;\Gamma_k}^2.$$

By letting $\gamma_f^{m_f,*} = \max_i \gamma_f^i$ and $\gamma_{b,k}^{m_{b,k},*} = \max_i \gamma_{b,k}^i$, we obtain

$$\mathbb{E}_\mu[\mathbf{L}(\mathbf{x}_f, \vec{\mathbf{x}}_b; h, \boldsymbol{\lambda}, \mathbf{0})]$$
$$\leq 3m_f \gamma_f^{m_f,*} \cdot \frac{\lambda_f}{m_f} \sum_{i=1}^{m_f} \|\mathcal{L}[h](\mathbf{x}_f^i) - f(\mathbf{x}_f^i)\|^2$$
$$+ 3\sum_{k=1}^{N_B} m_{b,k} \gamma_{b,k}^{m_{b,k},*} \cdot \frac{\lambda_{b,k}}{m_{b,k}} \sum_{j=1}^{m_{b,k}} \|\mathcal{B}[h](\mathbf{x}_{b,k}^j) - g(\mathbf{x}_{b,k}^j)\|^2 + 3\lambda_f \epsilon_f^{2\alpha} [\mathcal{L}[h]]_{\alpha;U}^2$$
$$+ 3\sum_{k=1}^{N_B} \lambda_{b,k} \epsilon_{b,k}^{2\alpha} [\mathcal{B}_k[h]]_{\alpha;\Gamma_k}^2 + 3\lambda_f \epsilon_f^{2\alpha} [f]_{\alpha;U}^2 + 3\sum_{k=1}^{N_B} \lambda_{b,k} \epsilon_{b,k}^{2\alpha} [g_k]_{\alpha;\Gamma_k}^2.$$

Note that $m_f \gamma_f^{m_f,*}, m_{b,k} \gamma_{b,k}^{m_{b,k},*} \geq 1$. Let $B_\epsilon(\mathbf{x})$ be a closed ball centered at $\mathbf{x}$ with radius ϵ. Let $P_f^* = \max_{\mathbf{x} \in U} \mu_f(B_{\epsilon_f}(\mathbf{x}))$ and $P_{b,k}^* = \max_{\mathbf{x} \in \Gamma_k} \mu_{b,k}(B_{\epsilon_{b,k}}(\mathbf{x}))$. Since for any $\mathbf{x}_f \in U$ and $\mathbf{x}_{b,k} \in \Gamma_k$, $k = 1, \cdots, N_B$, there exists $\mathbf{x}_f' \in \mathcal{T}_f$ and $\mathbf{x}_{b,k}' \in \mathcal{T}_{b,k}$ such that

$$\|\mathbf{x}_f - \mathbf{x}_f'\| \leq \epsilon_f, \qquad \|\mathbf{x}_{b,k} - \mathbf{x}_{b,k}'\| \leq \epsilon_{b,k}, \quad \forall k,$$

for each i, there are closed balls B_{ϵ_f} and $B_{\epsilon_{b,k}}$ that include $A_{\mathbf{x}_f^i}$ and $A_{\mathbf{x}_{b,k}^i}$, respectively. Thus, we have $\gamma_f^{m_f,*} \leq P_f^*, \gamma_{b,k}^{m_{b,k},*} \leq P_{b,k}^*$. Moreover, it follows from Assumption 3.1 that

(B.2) $$\gamma_f^{m_f,*} \leq P_f^* \leq C_f \epsilon_f^d, \qquad \gamma_{b,k}^{m_{b,k},*} \leq P_{b,k}^* \leq C_{b,k} \epsilon_{b,k}^{d-1}.$$

Therefore, we obtain

$$\mathbb{E}_\mu[\mathbf{L}(\mathbf{x}_f, \vec{\mathbf{x}}_b; h, \boldsymbol{\lambda}, \mathbf{0})]$$
$$\leq 3C_f m_f \epsilon_f^d \cdot \frac{\lambda_f}{m_f} \sum_{i=1}^{m_f} \|\mathcal{L}[h](\mathbf{x}_f^i) - f(\mathbf{x}_f^i)\|^2 + 3\lambda_f \epsilon_f^{2\alpha} [\mathcal{L}[h]]_{\alpha;U}^2$$
$$+ 3\sum_{k=1}^{N_B} C_{b,k} m_{b,k} \epsilon_{b,k}^{d-1} \cdot \frac{\lambda_{b,k}}{m_{b,k}} \sum_{j=1}^{m_{b,k}} \|\mathcal{B}[h](\mathbf{x}_{b,k}^j) - g(\mathbf{x}_{b,k}^j)\|^2 + 3\lambda_f \epsilon_f^{2\alpha} [f]_{\alpha;U}^2$$
$$+ 3\sum_{k=1}^{N_B} \lambda_{b,k} \epsilon_{b,k}^{2\alpha} [\mathcal{B}_k[h]]_{\alpha;\Gamma_k}^2 + 3\sum_{k=1}^{N_B} \lambda_{b,k} \epsilon_{b,k}^{2\alpha} [g_k]_{\alpha;\Gamma_k}^2$$
$$\leq C_{\boldsymbol{m}} \cdot \text{Loss}_{\boldsymbol{m}}(h; \boldsymbol{\lambda}, \mathbf{0}) + 3\lambda_f \epsilon_f^{2\alpha} [\mathcal{L}[h]]_{\alpha;U}^2 + 3\sum_{k=1}^{N_B} \lambda_{b,k} \epsilon_{b,k}^{2\alpha} [\mathcal{B}_k[h]]_{\alpha;\Gamma_k}^2$$
$$+ 3\lambda_f \epsilon_f^{2\alpha} [f]_{\alpha;U}^2 + 3\sum_{k=1}^{N_B} \lambda_{b,k} \epsilon_{b,k}^{2\alpha} [g_k]_{\alpha;\Gamma_k}^2,$$

where

$$C_{\boldsymbol{m}} = 3\max\{C_f m_f \epsilon_f^d, \max_k\{C_{b,k} m_{b,k} \epsilon_{b,k}^{d-1}\}\}.$$

Then, the proof is completed. □

LEMMA B.2. *Let X be a compact subset in $\mathbb{R}^d$ and μ be the probability measure supported on X. Suppose that for any cube $H_\epsilon(\boldsymbol{x})$ of side length ϵ centered at $\boldsymbol{x}$ in $\mathbb{R}^d$, there exists $s \le d$ such that $\forall \boldsymbol{x} \in X$,*

$$c\epsilon^s \le \mu(H_\epsilon(\boldsymbol{x}) \cap X), \qquad \|y - y'\| \le \sqrt{s}\epsilon, \quad \forall \boldsymbol{y}, \boldsymbol{y}' \in H_\epsilon(\boldsymbol{x}) \cap X,$$

where $c > 0$ depends only on (μ, X). Then, with probability at least $1 - \sqrt{n}(1 - 1/\sqrt{n})^n$ over iid n sample points $\{\boldsymbol{x}_i\}_{i=1}^n$ from μ, for any $\boldsymbol{x} \in X$, there exists a point $\boldsymbol{x}_j$ such that $\|\boldsymbol{x} - \boldsymbol{x}_j\| \le \sqrt{s}c^{-\frac{1}{s}}n^{\frac{1}{2s}}$.

Proof. Since X is compact in $\mathbb{R}^d$, let $\{H_\epsilon(\mathbf{z}_i)\}_{i=1}^K$ be the set of K almost disjoint cubes of side length ϵ centered at $\mathbf{z}_i$ that cover X. From the condition on μ, K can be at most $\frac{1}{c\epsilon^s}$. Given Z_K, let $V_{\mathbf{z}_i}$ be the Voronoi cell associated with $\mathbf{z}_i$, i.e.,

$$V_{\mathbf{z}_i} = \{\mathbf{x} \in X \,|\, \|\mathbf{x} - \mathbf{z}_i\| = \min_{\mathbf{z} \in Z_K} \|\mathbf{x} - \mathbf{z}\|\} = H_\epsilon(\mathbf{z}_i) \cap X.$$

Note that $\mu(V_{\mathbf{z}_i} \cap V_{\mathbf{z}_j}) = 0$ for $i \ne j$ and $\mu(\cup_{j=1}^K V_{\mathbf{z}_j}) = 1$. Let $p_i = \mu(V_{\mathbf{z}_i})$ that is the probability that a random sample from μ falls in the Voronoi cell $V_{\mathbf{z}_i}$. Moreover, by the property of μ, we have $p_i \ge c\epsilon^s$.

For a positive integer n satisfying $n \ge \frac{1}{c\epsilon^s} \ge K$, let A_n be the event that for randomly drawn n points, each $V_{\mathbf{z}_i}$ contains at least one point. Then,

$$\mu(A_n) = \sum_{i_j \ge 1, |\boldsymbol{i}| = n} \binom{n}{i_1, \cdots, i_K} p_1^{i_1} \cdots p_K^{i_K},$$

where $\boldsymbol{i} = (i_1, \cdots, i_K)$ and $|\boldsymbol{i}| = \sum_{j=1}^K i_j$. Let $p_{\min} = \min_i p_i$. Then we have

$$1 - \mu(A_n) \le \sum_{j=1}^K (1 - p_i)^n \le K(1 - p_{\min})^n \le c^{-1}\epsilon^{-s}(1 - c\epsilon^s)^n.$$

Note that if two points are in $V_{\mathbf{z}_i}$, the distance between these two points is at most $\sqrt{s}\epsilon$. Thus, with probability at least $1 - c^{-1}\epsilon^{-s}(1 - c\epsilon^s)^n$ over iid n samples $\Omega_n = \{\mathbf{x}_i\}_{i=1}^n$, for any $\mathbf{x} \in X$, there exists a point $\mathbf{x}_i$ such that $\|\mathbf{x} - \mathbf{x}_i\|_2 \le \sqrt{s}\epsilon$. By letting $\frac{1}{c^2\epsilon^{2s}} = n \ge \frac{1}{c\epsilon^s}$, the proof is completed. Note that the probability in the above statement becomes $1 - \sqrt{n}(1 - \frac{1}{\sqrt{n}})^n$ that goes to 1 as $n \to \infty$. □

Proof of Theorem 3.2. Let $\mathcal{T}_f^{m_f} = \{\mathbf{x}_f^i\}_{i=1}^{m_f}$ be iid samples from μ_f on U and $\mathcal{T}_b^{m_b} = \{\mathbf{x}_b^i\}_{i=1}^{m_b}$ be iid samples from μ_b on Γ.

By Lemma B.2, with probability at least

(B.3) $$\left(1 - \sqrt{m_f}(1 - 1/\sqrt{m_f})^{m_f}\right) \prod_{k=1}^{N_B} \left(1 - \sqrt{m_{b,k}}(1 - 1/\sqrt{m_{b,k}})^{m_{b,k}}\right),$$

$\forall \mathbf{x}_f \in U$ and $\forall \mathbf{x}_b \in \Gamma$, there exists $\mathbf{x}_f' \in \mathcal{T}_f^{m_f}$ and $\mathbf{x}_b' \in \mathcal{T}_f^{m_b}$ such that $\|\mathbf{x}_f - \mathbf{x}_f'\| \le \sqrt{d}c_f^{-\frac{1}{d}}m_f^{-\frac{1}{2d}}$ and $\|\mathbf{x}_{b,k} - \mathbf{x}_{b,k}'\| \le \sqrt{d-1}c_{b,k}^{-\frac{1}{d-1}}m_{b,k}^{-\frac{1}{2(d-1)}}$. By letting $\epsilon_f = \sqrt{d}c_f^{-\frac{1}{d}}m_f^{-\frac{1}{2d}}$

and $\epsilon_{b,k} = \sqrt{d-1} c_{b,k}^{-\frac{1}{d-1}} m_{b,k}^{-\frac{1}{2(d-1)}}$, it follows from Lemma B.1 that with probability at least (B.3),

$$\text{Loss}^{\text{PINN}}(h; \boldsymbol{\lambda})$$

$$\leq C_{\boldsymbol{m}} \cdot \left[\text{Loss}_{\boldsymbol{m}}^{\text{PINN}}(h; \boldsymbol{\lambda}) + \lambda_{f,\boldsymbol{m}}^R \cdot \left[\mathcal{L}[h]\right]_{\alpha;U}^2 + \sum_{k=1}^{N_B} \lambda_{b,k,\boldsymbol{m}}^R \cdot \left[\mathcal{B}_k[h]\right]_{\alpha;\Gamma_k}^2 \right] + Q,$$

where for $k = 1, \cdots, N_B$,

$$C_{\boldsymbol{m}} = 3 \max\left\{ \frac{C_f}{c_f} \sqrt{d}^d m_f^{\frac{1}{2}}, \max_k \left\{ \frac{C_{b,k}}{c_{b,k}} \sqrt{d-1}^{d-1} m_{b,k}^{\frac{1}{2}} \right\} \right\},$$

$$\lambda_{f,\boldsymbol{m}}^R = \frac{3\lambda_f \sqrt{d}^{2\alpha} c_f^{-\frac{2\alpha}{d}} m_f^{-\frac{\alpha}{d}}}{C_{\boldsymbol{m}}}, \qquad \lambda_{b,k,\boldsymbol{m}}^R = \frac{3\lambda_{b,k} \sqrt{d-1}^{2\alpha} c_{b,k}^{-\frac{2\alpha}{d-1}} m_{b,k}^{-\frac{\alpha}{d-1}}}{C_{\boldsymbol{m}}},$$

$$Q = 3\lambda_f d^\alpha c_f^{-\frac{2\alpha}{d}} m_f^{-\frac{\alpha}{d}} [f]_{\alpha;U}^2 + 3 \sum_{k=1}^{N_B} \lambda_{b,k} (d-1)^\alpha c_{b,k}^{-\frac{2\alpha}{d-1}} m_{b,k}^{-\frac{\alpha}{d-1}} [g_k]_{\alpha;U}^2.$$

Let $C' = 3 \max\{\lambda_f d^\alpha c_f^{-\frac{2\alpha}{d}} m_f^{-\frac{\alpha}{d}}, \max_k \{\lambda_{b,k}(d-1)^\alpha c_{b,k}^{-\frac{2\alpha}{d-1}} m_{b,k}^{-\frac{\alpha}{d-1}}\}\}$. Then, we have

$$\text{Loss}^{\text{PINN}}(h; \boldsymbol{\lambda}) \leq C_{\boldsymbol{m}} \cdot \text{Loss}_{\boldsymbol{m}}(h; \boldsymbol{\lambda}, \boldsymbol{\lambda}_{\boldsymbol{m}}^R) + C'(m_f^{-\frac{\alpha}{d}} + N_B \max_k m_{b,k}^{-\frac{\alpha}{d-1}}),$$

where $\boldsymbol{\lambda}_{\boldsymbol{m}}^R = (\lambda_{f,\boldsymbol{m}}^R, \lambda_{b,1,\boldsymbol{m}}^R, \cdots, \lambda_{b,N_B,\boldsymbol{m}}^R)$. Then, the proof is completed. □

Appendix C. Proof of Theorem 3.4.

Proof of Theorem 3.4. Suppose $m_f = \mathcal{O}(m_{b,k}^{\frac{d}{d-1}})$ for all k. It then can be checked that $\hat{\lambda}_{f,\boldsymbol{m}}^R = \hat{\lambda}_{b,k,\boldsymbol{m}}^R = \mathcal{O}(m_f^{-\frac{1}{2}-\frac{\alpha}{d}})$ for all k, where $\hat{\lambda}_{f,\boldsymbol{m}}$ and $\hat{\lambda}_{b,k,\boldsymbol{m}}$ are defined in (3.1). Let $\boldsymbol{\lambda}$ be a vector independent of $\boldsymbol{m}$ and $\boldsymbol{\lambda}_{\boldsymbol{m}}^R$ be a vector satisfying (3.2).

Let $h_m \in \mathcal{H}_{\boldsymbol{m}}$ be a function that minimizes $\text{Loss}_{\boldsymbol{m}}(\cdot; \boldsymbol{\lambda}, \boldsymbol{\lambda}_{\boldsymbol{m}}^R)$. First, note that since $u_{\boldsymbol{m}}^* \in \mathcal{H}_{\boldsymbol{m}}$,

(C.1)

$$\min_j (\boldsymbol{\lambda}_{\boldsymbol{m}}^R)_j \left(R_f(h_m) + \sum_{k=1}^{N_B} R_{b,k}(h_m) \right) \leq \text{Loss}_m(h_m; \boldsymbol{\lambda}, \boldsymbol{\lambda}_{\boldsymbol{m}}^R)$$

$$\leq \text{Loss}_m(u_{\boldsymbol{m}}^*; \boldsymbol{\lambda}, \boldsymbol{\lambda}_{\boldsymbol{m}}^R) \leq \text{Loss}_m(u_{\boldsymbol{m}}^*; \boldsymbol{\lambda}, \boldsymbol{0}) + \|\boldsymbol{\lambda}_{\boldsymbol{m}}^R\|_\infty \left(R_f(u_{\boldsymbol{m}}^*) + \sum_{k=1}^{N_B} R_{b,k}(u_{\boldsymbol{m}}^*) \right).$$

Since $\boldsymbol{\lambda}_{\boldsymbol{m}}^R \geq \hat{\boldsymbol{\lambda}}_{\boldsymbol{m}}^R$ and $\|\boldsymbol{\lambda}_{\boldsymbol{m}}^R\|_\infty = \mathcal{O}(\|\hat{\boldsymbol{\lambda}}_{\boldsymbol{m}}^R\|_\infty)$, we have $\frac{\max_j (\boldsymbol{\lambda}_{\boldsymbol{m}}^R)_j}{\min_j (\boldsymbol{\lambda}_{\boldsymbol{m}}^R)_j} = \mathcal{O}(1)$. Let $R^* = \sup_{\boldsymbol{m}} (R_f(u_{\boldsymbol{m}}^*) + \sum_{k=1}^{N_B} R_b(u_{\boldsymbol{m}}^*))$. By the third assumption in 3.3, we have $R^* < \infty$.

The second assumption of 3.3 can be relaxed to the following condition:

- For each m_f, $\mathcal{H}_{m_f}$ contains a function $u_{m_f}^*$ satisfying $\text{Loss}_{m_f}^{\text{PINN}}(u_{m_f}^*; \boldsymbol{\lambda}) = \mathcal{O}(m_f^{-\frac{1}{2}-\frac{\alpha}{d}})$.

We then have $R_f(h_m), R_{b,k}(h_m) \leq \mathcal{O}(R^*)$ for all m. Since $R_f(h_m) = \left[\mathcal{L}[h_m]\right]_{\alpha;U}^2$ and $R_{b,k}(h_m) = \left[\mathcal{B}_k[h_m]\right]_{\alpha;U}^2$, the Hölder coefficients of $\mathcal{L}[h_m]$ and $\mathcal{B}_k[h_m]$ are uniformly bounded above. With the first assumption of (3.3), $\{\mathcal{L}[h_m]\}$ and $\{\mathcal{B}_k[h_m]\}$ are uniformly bounded and uniformly equicontinuous sequences of functions in $C^{0,\alpha}(U)$ and

$C^{0,\alpha}(\Gamma_k)$, respectively. By invoking the Arzela-Ascoli Theorem, there exists a subsequence h_{m_j} and functions $G \in C^{0,\alpha}(U)$ and $B_k \in C^{0,\alpha}(\Gamma_k)$ such that $\mathcal{L}[h_{m_j}] \to G$ and $\mathcal{B}_k[h_{m_j}] \to B_k$ in $C^0(U)$ and $C^0(\Gamma_k)$, respectively, as $j \to \infty$.

Since $\text{Loss}_m(h_m; \boldsymbol{\lambda}, \boldsymbol{\lambda}_{\boldsymbol{m}}^R) = \mathcal{O}(m_f^{-\frac{1}{2}-\frac{\alpha}{d}})$, by combining it with Theorem 3.2, we have that with probability at least $(1 - \sqrt{m_f}(1 - c_f/\sqrt{m_f})^{m_f}) \prod_{k=1}^{N_B}(1 - \sqrt{m_{b,k}}(1 - c_{b,k}/\sqrt{m_{b,k}})^{m_{b,k}})$,

$$\text{Loss}(h_m; \boldsymbol{\lambda}, \boldsymbol{0}) = \mathcal{O}(m^{-\frac{\alpha}{d}}).$$

Hence, the probability of $\lim_{m \to \infty} \text{Loss}(h_m; \boldsymbol{\lambda}, \boldsymbol{0}) = 0$ is one. Thus, with probability 1,

$$
\begin{aligned}
0 &= \lim_{j \to \infty} \text{Loss}(h_{m_j}; \boldsymbol{\lambda}, \boldsymbol{0}) \\
&= \lim_{j \to \infty} \lambda_f \int_U \|\mathcal{L}[h_{m_j}](\mathbf{x}_f) - f(\mathbf{x}_f)\|^2 d\mu_f(\mathbf{x}_f) \\
&\quad + \sum_{k=1}^{N_B} \lambda_{b,k} \int_{\Gamma_k} \|\mathcal{B}_k[h_{m_j}](\mathbf{x}_{b,k}) - g_k(\mathbf{x}_{b,k})\|^2 d\mu_{b,k}(\mathbf{x}_{b,k}) \\
&= \lambda_f \int_U \|G(\mathbf{x}_f) - f(\mathbf{x}_f)\|^2 d\mu_f(\mathbf{x}_f) \\
&\quad + \sum_{k=1}^{N_B} \lambda_{b,k} \int_{\Gamma_k} \|B_k(\mathbf{x}_{b,k}) - g_k(\mathbf{x}_{b,k})\|^2 d\mu_{b,k}(\mathbf{x}_{b,k}),
\end{aligned}
$$

which shows that $G = f$ in $L^2(U; \mu_f)$ and $B_k = g_k$ in $L^2(\Gamma_k; \mu_{b,k})$. Note that since $\mathcal{L}[h_{m_j}]$ and $\mathcal{B}_k[h_{m_j}]$ are uniformly bounded above and uniformly converge to G and B_k, respectively, the third equality holds by Lebesgue's Dominated Convergence Theorem. Since the subsequence was arbitrary, we conclude that $\mathcal{L}[h_m] \to f$ in $L^2(U; \mu_f)$ and $\mathcal{B}_k[h_m] \to g_k$ in $L^2(\Gamma_k; \mu_{b,k})$ as $m \to \infty$. Furthermore, since $\{\mathcal{L}[h_m]\}$ and $\{\mathcal{B}_k[h_m]\}$ are equicontinuous, its convergence mode is improved to C^0. $\qquad\square$

Appendix D. Proof of Theorem 3.6. For readability, the existence and the uniqueness of the classical solution to (3.6) is stated as follow.

THEOREM D.1 (Theorem 6.13 of [9]). *For $0 < \alpha < 1$, let U satisfy an exterior sphere condition at every boundary point. Let the operator $\mathcal{L}$ be strictly elliptic in U with coefficients in $C^\alpha(U)$ and $\tilde{c}(\boldsymbol{x}) \leq 0$. Then, the Dirichlet problem of (3.6) has a unique solution in $C^{2,\alpha}(U) \cap C^0(\bar{U})$ for all $f \in C^\alpha(U)$ and all $g \in C^0(\partial U)$.*

LEMMA D.2. *Suppose Assumption 3.5 holds and $\tilde{c}(\boldsymbol{x}) \leq 0$. Then, there exists the unique classical solution u^* to the PDE (3.6). Furthermore, there exists a positive constant C that depends only on U, $\tilde{\boldsymbol{b}}(\boldsymbol{x})$, λ_0 and v such that*

(D.1) $$\|u^* - h\|_{C^0(U)} \leq C(\|f - \mathcal{L}[h]\|_{C^0(U)} + \|g - h\|_{C^0(\partial U)}),$$

for any $h \in C^0(U)$ satisfying $\mathcal{L}[h] \in C^{0,\alpha}(U)$ and $h \in C^{0,\alpha}(\partial U)$.

Proof of Lemma D.2. By Theorem D.1, there exists a unique classical solution $\xi \in C^{2,\alpha}(U) \cap C^0(\bar{U})$ to

$$\mathcal{L}[\xi] = 0, \text{ on } U, \qquad \xi|_{\partial U} = h|_{\partial U} - g.$$

Since $\xi \in C^{2,\alpha}(U) \cap C^0(\bar{U})$, $\tilde{c}(\mathbf{x}) \leq 0$ and Assumption 3.5 holds, one can apply the Weak Maximum principle (e.g. Corollary 3.11 in [9]) to have

$$\|\xi\|_{C^0(U)} \leq \|h - g\|_{C^0(\partial U)}.$$

By Theorem D.1, the PDE (3.6) has a unique classical solution u^*. Let $\tilde{e} = u^* - h + \xi$. Then, $\tilde{e}$ satisfies $\mathcal{L}[\tilde{e}] = f - \mathcal{L}[h]$ in U and $\tilde{e}|_{\partial U} = 0$. From an apriori bound of the elliptic equation (e.g. Theorem 3.7. of [9]), we have

$$\|\tilde{e}\|_{C^0(U)} \leq \frac{C}{\lambda_0}\|f - \mathcal{L}[h]\|_{C^0(U)},$$

where C is a constant depending only on $\operatorname{diam}(U)$ and $\sup_U \frac{\|\tilde{\boldsymbol{b}}(\mathbf{x})\|}{\lambda_0}$. Hence,

$$\|u^* - h\|_{C^0(U)} \leq \|\tilde{e}\|_{C^0(U)} + \|\xi\|_{C^0(U)} \leq \frac{C}{\lambda_0}\|f - \mathcal{L}[h]\|_{C^0(U)} + \|h - g\|_{C^0(\partial U)},$$

which completes the proof. □

Proof of Theorem 3.6. Let $\{h_m\}_{m \geq 1}$ be the sequence of the minimizers from Theorem 3.4. It follows from Theorem 3.4 that $\|h_m - g\|_{C^0(\partial U)} \to 0$ and $\|f - \mathcal{L}[h_m]\|_{C^0(U)} \to 0$. By Assumption 3.3, $\mathcal{L}[h] \in C^{0,\alpha}(U)$ and $h \in C^{0,\alpha}(\partial U)$ for all $h \in \mathcal{H}_{\boldsymbol{m}}$. Lemma D.2 shows $h_m \to u^*$ in $C^0(U)$, which completes the proof. □

Appendix E. Proof of Theorem 3.7.

Proof. The proof continues from the proof of Lemma D.2. Since $\tilde{e}|_{\partial U} = 0$, it follows from Assumption 3.5 that

$$-\langle \mathcal{L}[\tilde{e}], \tilde{e} \rangle_{L^2(U)} \geq \frac{\lambda}{2}\|D\tilde{e}\|_{L^2(U)}^2 - \lambda v^2 \|\tilde{e}\|_{L^2(U)}^2.$$

Thus,

$$\begin{aligned} \|D\tilde{e}\|_{L^2(U)}^2 &\leq \|\mathcal{L}[\tilde{e}]\|_{L^2(U)}\|\tilde{e}\|_{L^2(U)} + 2v^2\|\tilde{e}\|_{L^2(U)}^2 \\ &\leq C' \left[\|\mathcal{L}[\tilde{e}]\|_{L^2(U)}^2 + \|\tilde{e}\|_{L^2(U)}^2 \right], \end{aligned}$$

where C' is a constant independent of h. Therefore,

$$\|\tilde{e}\|_{H^1(U)}^2 = \|D\tilde{e}\|_{L^2(U)}^2 + \|\tilde{e}\|_{L^2(U)}^2 \leq C'' \left[\|\mathcal{L}[\tilde{e}]\|_{L^2(U)}^2 + \|\tilde{e}\|_{L^2(U)}^2 \right],$$

for some constant C''. Then,

$$\begin{aligned} \|u^* - h\|_{H^1(U)}^2 &\leq 2\|\tilde{e}\|_{H^1(U)}^2 + 2\|\xi\|_{H^1(U)}^2 \\ &\leq C''' \left(\|f - \mathcal{L}[h]\|_{C^0(U)} + \|g - h\|_{C^0(\partial U)} \right) + 2\|\xi\|_{H^1(U)}^2, \end{aligned}$$

for some constant C'''. Since $\xi = 0$ and $h_m = g$ on ∂U, the proof is completed by Theorem 3.4 as $\|f - \mathcal{L}[h_m]\|_{C^0(U)} \to 0$. □

Appendix F. Proof of Theorem 3.10. For reader's convenience, let us recall a result on the existence of the classical solution to the parabolic equation.

THEOREM F.1 (Corollary 2 in Chapter 3 of [8]). *Suppose Assumption* (3.9) *holds. suppose further that for every point* $x' \in \partial U$, *there exists a closed ball* $\bar{B}$ *in* $\mathbb{R}^n$ *such that* $\bar{B} \cap \bar{U} = \{x'\}$. *Then, for any continuous function* φ *on* $\partial U \times (0, T]$ *and* g *on* $U \times \{t = 0\}$, *there exists a unique classical solution* u^* *to* (3.7).

LEMMA F.2. *Suppose Assumption 3.3 and 3.9 hold and $\tilde{c}(\boldsymbol{x}, t) \leq 0$. Let u^* be the solution to the PDE (3.7) and let $\psi(\boldsymbol{x}, t)$ be the combined boundary and initial conditions on $\Gamma_T = \overline{U}_T - U_T$. Then, there exists a positive universal constant C that depends only on U and the PDE (3.7) such that*

$$\|h - u^*\|_{C^0(0,T;C^0(U))} \leq C \left[\|f + h_t - \mathcal{L}[h]\|_{C^0(0,T;C^0(U))} + \|h - \psi\|_{C^0(\Gamma_T)}\right],$$

for any $h \in C^{2,\alpha}$.

Proof. Let us combine the boundary and the initial conditions into one condition:

$$u(x, t) = \psi(x, t) \quad \text{on } \Gamma_T = \overline{U}_T - U_T.$$

For a fixed $h \in C^{2,\alpha}(U_T)$, let ξ be the solution to

$$\begin{cases} -\xi_t + \mathcal{L}[\xi] = 0, & \text{in } U_T \\ \xi = \psi - h, & \text{on } \Gamma_T \end{cases}$$

We note that since $\psi - h$ is continuous on Γ_T, the existence of ξ is guaranteed by Theorem F.1. Note that since $\tilde{c}(\mathbf{x}, t) \leq 0$ in U_T, ξ is continuous, and $\mu(U_T) > 0$, it follows from the Weak Maximum Principle that

$$\|\xi\|_{C^0(D)} \leq \|\psi - h\|_{C^0(\Gamma_T)}.$$

Let u^* be a unique classical solution to the PDE (3.7), and let $\tilde{e} = u^* - h - \xi$. Since Assumption 3.9 holds and $\tilde{c}(\mathbf{x}, t) \leq 0$, it follows from a consequence of the weak maximum principle (e.g. p 42, Chapter 2 of Freidman) that

$$\|\tilde{e}\|_{C^0(0,T;C^0(U))} \leq C'\|f + h_t - \mathcal{L}[h]\|_{C^0(0,T;C^0(U))},$$

for some constant C'. Therefore,

$$\begin{aligned} \|h - u^*\|_{C^0(0,T;C^0(U))} &\leq \|\tilde{e}\|_{C^0(0,T;C^0(U))} + \|\xi\|_{C^0(0,T;C^0(U))} \\ &\leq C'' \left[\|f + h_t - \mathcal{L}[h]\|_{C^0(0,T;C^0(U))} + \|\psi - h\|_{C^0(\Gamma_T)}\right]. \end{aligned}$$

Here C'' is a positive universal constant that is independent of h. ☐

Proof of Theorem 3.10. Let $\{h_m\}_{m \geq 1}$ be the sequence of minimizers of (2.4). Note that from Theorem 3.4, we have

$$\lim_{m \to \infty} \|(h_m)_t - \mathcal{L}[h_m] + f\|_{C^0(D)} = 0, \qquad \lim_{m \to \infty} \|h_m - \psi\|_{C^0(\Gamma_T)} = 0.$$

By Lemma F.2, it readily follows that $\lim_{m \to \infty} \|h_m - u^*\|_{C^0(0,T;C^0(U))} = 0$. ☐

Appendix G. Proof of Theorem 3.11.

Proof. The proof continues from the proof of Lemma F.2. Note that $\frac{d}{dt}\tilde{e}_m + \mathcal{L}[\tilde{e}_m] = f + (h_m)_t - \mathcal{L}[h_m]$ on U_T and $\tilde{e}_m|_{\Gamma_T} = 0$. For a fixed t, by the integration by parts, one obtains

$$\begin{aligned} \langle (\tilde{e}_m)_t - \mathcal{L}[\tilde{e}_m], \tilde{e}_m \rangle_{L^2(U)} &= \frac{1}{2}\frac{d}{dt}\|\tilde{e}_m\|_{L^2(U)}^2 - \langle \mathcal{L}[\tilde{e}_m], \tilde{e}_m \rangle_{L^2(U)} \\ &\geq \frac{1}{2}\frac{d}{dt}\|\tilde{e}_m(t)\|_{L^2(U)}^2 + \beta\|\tilde{e}_m(t)\|_{H^1(U)}^2 - \gamma\|\tilde{e}_m(t)\|_{L^2(U)}^2, \end{aligned}$$

for some $\beta > 0$ and $\gamma \geq 0$. Also, note that

$$\langle (\tilde{e}_m)_t - \mathcal{L}[\tilde{e}_m], \tilde{e}_m \rangle_{L^2(U)} \leq \frac{1}{2}\|f + (h_m)_t - \mathcal{L}[h_m]\|^2_{L^2(U)} + \frac{1}{2}\|\tilde{e}_m(t)\|^2_{L^2(U)}.$$

By combining the above two inequalities, we have

$$\frac{d}{dt}\|\tilde{e}_m(t)\|^2_{L^2(U)} + \beta'\|\tilde{e}_m(t)\|^2_{H^1(U)} \leq C_1\|\tilde{e}_m(t)\|^2_{L^2(U)} + C_2\|f + (h_m)_t - \mathcal{L}[h_m]\|^2_{L^2(U)},$$

for some positive constants β', C_1, C_2 that are independent of m. By integrating it with respect to t from 0 to T,

$$\|\tilde{e}_m(T)\|^2_{L^2(U)} - \|\tilde{e}_m(0)\|^2_{L^2(U)} + \beta'\|\tilde{e}_m\|^2_{L^2(0,T;H^1(U))}$$
$$\leq C_1\|\tilde{e}_m\|^2_{L^2(0,T;L^2(U))} + C_2\|f + (h_m)_t - \mathcal{L}[h_m]\|^2_{L^2(0,T;L^2(U))}.$$

Since $\tilde{e}_m|_{\Gamma_T} = 0$, we have $\|\tilde{e}_m(0)\|^2_{L^2(U)} = 0$. Hence,

$$\|\tilde{e}_m\|^2_{L^2(0,T;H^1(U))} \leq C_1'\|\tilde{e}_m\|^2_{L^2(0,T;L^2(U))} + C_2'\|f + (h_m)_t - \mathcal{L}[h_m]\|^2_{L^2(0,T;L^2(U))}.$$

By Lemma F.2, we have

$$\|\tilde{e}_m\|^2_{L^2(0,T;H^1(U))} \leq C''\|f + (h_m)_t - \mathcal{L}[h_m]\|^2_{C^0(0,T;C^0(U))},$$

for some constant C''. Hence, $\lim_{m\to\infty}\|\tilde{e}_m\|_{L^2(0,T;H_0^1(U))} = 0$. Therefore, $h_m \to u^*$ in $L^2(0,T;H^1(U))$. □

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