Quantitative approximation theorems for scattering neural operators

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Abstract

In this work, we study the learning of a nonlinear operator for the scattering problem based on neural operator architectures. In most inverse scattering problems, the forward operator mapping from the refractive index to the far-field pattern is commonly used measurement. In many numerical methods for constructing the refractive index from the knowledge of the far-field pattern need to evaluate the forward operator, which involves solving PDEs and taking asymptotics. Such procedure is time consuming and not effective. It is therefore a favorable practice to construct a surrogate to replace this forward operator. The main purpose of this paper is to demonstrate that, under certain conditions, the "parametric complexity" of neural scattering operators grows at most logarithmically with respect to the desired accuracy. This result makes the application of these neural operators rather promising in practice.

1 Introduction

Neural operators have emerged as a powerful extension of traditional neural networks from finite-dimensional spaces to infinite-dimensional ones, i.e., function spaces to function spaces, see, for example, [1, 2, 17, 26] to name a few. In solving PDEs problems, while traditional PDEs solvers often require substantial computational resources and time due to high dimensionality or nonlinearity, once trained, neural operators serve as surrogate models, providing significantly faster inference compared to traditional numerical solvers. An additional advantage of neural operators lies in their applicability to Bayesian inverse problems, where the construction of efficient surrogate models can greatly facilitate the computational process. Despite neural operator being universal approximators for continuous operators, their theoretical foundations, particularly in PDEs applications, remain under-explored.

One of the most fundamental questions for any neural network is the universal approximation property. For neural operators, universality has been established in a variety of architectures such as [7, 27, 21] (DeepONets), [15] (FNOs), and [20] (ANOs). Since neural operators map the infinite-dimensional space to the infinite-dimensional one, having manageable size of learnable parameters is crucial in actual applications. Unfortunately, general neural operators suffer from the "curse of parametric complexity" [22]. The focus of this paper is to beat this curse for the scattering operator.

1.1 Related works

Neural operators introduced in [17] as one of the operator learning methods which satisfy the important discretization-invariant property. As mentioned above, neural operators serve as surrogates for the operators mapping from an infinite-dimensional space into another infinite-dimensional space. Other operator learning neural networks were already introduced such as DeepONet [8, 26] and PCA-Net [2], [10]. Various neural operator architectures related to [17] have been proposed, differing primarily in the choice of basis functions within non-local operators. Notable examples include Graph Neural Operators [25], Fourier Neural Operators [24], Wavelet Neural Operators [32, 13], Spherical Fourier Neural Operators [3], and Laplace Neural Operators [5]. These architectures have demonstrated empirical success as the surrogate models of simulators across a wide range of PDEs, as benchmarked in [31]. Even in inverse problems, e.g., Calderón's problem, neural operators (precisely, DeepONets) are rigorously shown to be good approximators of the forward and inverse Calderón maps [4]. One of critical theoretical foundations of neural operators is the universal approximation theorems. This theorem establishes that, for any target operator and desired level of accuracy, there exists a neural operator with sufficiently large learnable parameters such that it approximates the target operators with desired accuracy. This indicates the capacity of the class of neural operators to approximate a wide range of operators. Universal approximation theorems for operator learning were established for neural operators [15, 17, 20, 18], DeepONet [26, 21], and PCA-Net [19]. A nice summary about recent progress on neural operators is given [16].

Our objective here is to establish the quantitative universal approximation theorem, which provides the upper bounds for the numbers of learnable parameters required to achieve a given level of approximation accuracy. Recently, [22] discussed that the operator learning for general operators suffers from "the curse of parametric complexity", where the number of learnable parameters grows exponentially as the desired approximation accuracy increases. At first glance, this complexity may hinder the applicability of neural operators. To further address this issue, we restrict general operators to the solution operators of specific PDEs. Recently, several quantitative approximation theorems have been established for the solution operators of specific PDEs without experiencing exponential growth in model complexity. For instance, [15, 19] developed quantitative approximation theorems for the Darcy and Navier-Stokes equations using Fourier neural operators and PCA-Net, respectively. Additionally, [22] analyzed the Hamilton-Jacobi equations with Hamilton-Jacobi neural operators, while [12] addressed nonlinear parabolic equations. Further studies, such as [6, 21, 28], investigated quantitative approximation theorems using DeepONet for a range of PDEs, including elliptic, parabolic, and hyperbolic equations, while [11] focused on advection-diffusion equations.

1.2 Our results and contributions

In this paper, we present a quantitative approximation theorem for the solution operator of scattering problem using neural operators. Our aim is to establish a quantitative approximation theorem for neural operators which approximate the *far-field pattern* to any desired accuracy. The far-field pattern (aka the scattering amplitude) is the most common measurement used in the inverse scattering problems. In Theorem 4.1, we show that for any given accuracy, the depth and the number of neurons of the neural operators do not grow exponentially. Notably, the depth grows at most logarithmically with respect to the accuracy, while the number of neurons at each layer has a fixed upper bound. From application perspective, the logarithmic growth rate is important. For example, neural operators are useful in the Ensemble Kalman Inverse (EKI), which is a derivative-free Kalman filter method [14], [29], [30], or nonparametric Bayesian inverse problems. In both methods, it is required to evaluate the forward map at each step. It is clear that the process will be more efficient if we replace the forward map by a neural operator.

The idea of the proof is similar to that used in [12] in which it relies on the contraction fixed-point method. It is helpful to note that we can express the solution operator and the far-field pattern in terms of the integral operators. This structure of the paper is as follows. In Section 2, we review some theoretical results of the scattering problem. In Section 3, we give the precise definition of scattering neural operators. The main quantitative approximation theorem and its proof are presented in detailed in Section 4. In Section 5, we provide an application of neural operators to the inverse scattering problem using the EKI.

2 Scattering problem

In this section, we would like to review some theoretical results of the acoustic scattering problem with inhomogeneous medium. Let $D \subset \mathbb{R}^d$ with $d = 2, 3$ be an open bounded smooth domain and denote the function space

$$L^\infty_Q(D;\mathbb{C}) := \{n \in L^\infty(\mathbb{R}^d;\mathbb{C}) : 0 < \mathrm{Re}(n),\ 0 \leq \mathrm{Im}(n),\ \mathrm{supp}(n-1) \subset D,\ |n(x)-1| \leq Q \text{ a.e.}\}. \tag{1}$$

Sometimes, it is more convenient to denote $n = 1+q$ and, by an abuse of notation, we say that $q \in L^\infty_Q(D;\mathbb{C})$ if $n = 1+q$ and $n \in L^\infty_Q(D;\mathbb{C})$. Now, let $q \in L^\infty_Q(D;\mathbb{C})$ and $u_q := u^{\mathrm{inc}} + u_q^{\mathrm{sca}}$ satisfy (assume that u^{inc} solves the Helmholtz equation in $\mathbb{R}^d$ and $u^{\mathrm{inc}} \in C(\overline{D};\mathbb{C})$)

$$\Delta u_q + k^2(1+q)u_q = 0 \quad \text{in} \quad \mathbb{R}^d \tag{2}$$

with the Sommerfeld radiation condition

$$\lim_{|x|\to\infty} |x|^{\frac{d-1}{2}} \left(\frac{\partial u_q^{\mathrm{sca}}}{\partial |x|} - \mathbf{i} k u_q^{\mathrm{sca}} \right) = 0. \tag{3}$$

It is well-known that the scattered field u_q^{sca} possesses the asymptotic behavior

$$u_q^{\mathrm{sca}}(x) = \frac{e^{\mathbf{i}k|x|}}{|x|^{\frac{d-1}{2}}} \left(u_q^\infty(\hat{x}) + O\left(\frac{1}{|x|}\right)\right) \quad \text{as} \quad |x| \to \infty, \tag{4}$$

where $\hat{x} = x/|x| \in \mathbb{S}^{d-1}$ and $u_q^\infty(\hat{x})$ is called the far-field pattern and the scattering amplitude. Our aim is to approximate the forward map $q \mapsto u_q^\infty$ by neural operators. Combining the unique continuation property and the Rellich lemma, one can show that $u_q^\infty(\hat{x})$, $\forall\, \hat{x} \in \mathbb{S}^{d-1}$, uniquely determines the scattered field $u_q^{\mathrm{sca}}(x)$ in $\mathbb{R}^d$.

It is not hard to see that the far-field $u_q^\infty(\hat{x})$ can be expressed explicitly by

$$u_q^\infty(\hat{x}) = c_d \int_D e^{-\mathbf{i}k\hat{x}\cdot y} q(y) u_q(y)\,\mathrm{d}y \tag{5}$$

with

$$c_d = \begin{cases} e^{\mathbf{i}\frac{\pi}{4}} \sqrt{\dfrac{k^3}{8\pi}} & \text{for} \quad d = 2, \\ \dfrac{k^2}{4\pi} & \text{for} \quad d = 3, \end{cases}$$

where the total field u_q is the solution of the *Lippmann-Schwinger integral equation*

$$u_q(x) = u^{\mathrm{inc}}(x) + k^2 \int_D \Phi(x,y) q(y) u_q(y)\mathrm{d}y, \ \ \forall\, x \in \mathbb{R}^d, \tag{6}$$

where $\Phi(x,y)$ denotes the outgoing fundamental solution of the Helmholtz equation in $\mathbb{R}^d$, i.e., for $x \neq y$,

$$\Phi(x,y) := \begin{cases} \dfrac{\mathbf{i}}{4} H_0^{(1)}(k|x-y|) & \text{if} \quad d=2, \\ \dfrac{1}{4\pi} \dfrac{e^{\mathbf{i}k|x-y|}}{|x-y|} & \text{if} \quad d=3, \end{cases} \tag{7}$$

where $H_0^{(1)}(z)$ is the Hankel function of the first kind of order zero.

2.1 The scattered solution and the far-field pattern

When $q \in L_Q^\infty(D;\mathbb{C})$, for each $k > 0$, the solvability of the Lippmann-Schwinger integral equation (6) and hence the well-posedness of the scattering (2), (3), has been proved, see [9, Theorem 8.7]. In view of the formula of the far-field pattern (5), it suffices to consider (6) locally. Let u_q be the solution of (6), then it also satisfies

$$u_q(x) = u^{\mathrm{inc}}(x) + k^2 \int_D \Phi(x,y) q(y) u_q(y) \mathrm{d}y, \quad \forall\, x \in D. \tag{8}$$

Let us now write

$$u_q = \Psi_q(u_q), \tag{9}$$

where $\Psi_q : L^2(D;\mathbb{C}) \to L^2(D;\mathbb{C})$ is defined by

$$\Psi_q(u)(x) := u^{\mathrm{inc}}(x) + k^2 \int_D \Phi(x,y) q(y) u(y) \mathrm{d}y, \quad \forall\, x \in D. \tag{10}$$

This map between $L^2(D;\mathbb{C})$ is well-defined, thanks to $\Phi \in L^2(D \times D;\mathbb{C})$ (Note that the spatial dimensions are now three). In later use, we will consider the case where Ψ_q is a contraction map. Therefore, we impose

Assumption 2.1. *We assume that the wavenumber $k > 0$ and upper bound $Q > 0$ satisfies that*

$$k^2 Q \|\Phi\|_{L^2(D\times D)} \leq \rho < 1.$$

Proposition 2.1. *Under* Assumption 2.1*, $\Psi_q : L^2(D;\mathbb{C}) \to L^2(D;\mathbb{C})$ satisfies*

$$\|\Psi_q(u) - \Psi_q(v)\|_{L^2(D)} \leq \rho \|u - v\|_{L^2(D)}$$

for all $u, v \in L^2(D;\mathbb{C})$, which implies that u_q is a fixed point of Ψ_q.

Proof. By (10), one has

$$\Psi_q(u)(x) - \Psi_q(v)(x) = k^2 \int_D \Phi(x,y) q(y) [u(y) - v(y)] \mathrm{d}y$$

and hence

$$\begin{aligned} \int_D \Big| \Psi_q(u)(x) - \Psi_q(v)(x) \Big|^2 \mathrm{d}x &= k^4 \int_D \Big| \int_D \Phi(x,y) q(y) [u(y) - v(y)] \mathrm{d}y \Big|^2 \mathrm{d}x \\ &\leq k^4 Q^2 \|\Phi\|_{L^2(D\times D)}^2 \|u - v\|_{L^2(D)}^2 \\ &\leq \rho^2 \|u - v\|_{L^2(D)}^2. \end{aligned}$$

$\square$

Corollary 2.1. *Suppose that* Assumption 2.1 *holds and* u^{inc} *satisfies*

$$M := k^2 \Big\| \int_D \Phi(x,y) u^{\text{inc}}(y) q(y) \mathrm{d}y \Big\|_{L^2(D)} < \infty.$$

Assume that

$$\frac{M}{1-\rho} \leq S$$

and let $B(u^{\text{inc}}, S) := \{v \in L^2(D; \mathbb{C}) : \|v - u^{\text{inc}}\|_{L^2(D)} \leq S\}$. *Then there exists a unique fixed point* $u \in B(u^{\text{inc}}, S)$ *of* (10).

Proof. Since Ψ_q is a contraction map, to prove the result, it suffices to show that if $u \in B_R(u^{\text{inc}})$, then $\Psi_q(u) \in B_R(u^{\text{inc}})$. To this end, we estimate

$$\begin{aligned}
\|\Psi_q(u) - u^{\text{inc}}\|_{L^2(D)} &\leq \|\Psi_q(u) - \Psi_q(u^{\text{inc}})\|_{L^2(D)} + \|\Psi_q(u^{\text{inc}}) - u^{\text{inc}}\|_{L^2(D)} \\
&\leq \rho \|u - u^{\text{inc}}\|_{L^2(D)} + k^2 \Big\| \int_D \Phi(x,y) u^{\text{inc}}(y) q(y) \mathrm{d}y \Big\|_{L^2(D)} \\
&\leq \rho S + M \leq S.
\end{aligned}$$

□

Remark 2.1. For simplicity, we could consider a weaker result. Let us set

$$M' := k^2 Q \|\Phi\|_{L^2(D \times D)} \|u^{\text{inc}}\|_{L^2(D)}$$

and choose S' satisfying

$$\frac{M'}{1-\rho} \leq S'.$$

Now if we take

$$R = S' + \|u^{\text{inc}}\|_{L^2(D)}, \tag{11}$$

then (10) has a unique fixed point in $B(0, R)$.

2.2 Complex-valued to Real-valued vector

Since the far-field pattern $u_q^\infty(\hat{x})$ is complex-valued (even if the potential q is real-valued), it is more convenient to work in the real-valued setting. Note that

$$L^2(D; \mathbb{C}) \cong L^2(D; \mathbb{R}) \times L^2(D; \mathbb{R}) = L^2(D; \mathbb{R})^2$$

and

$$L^2(\mathbb{S}^{d-1}; \mathbb{C}) \cong L^2(\mathbb{S}^{d-1}; \mathbb{R}) \times L^2(\mathbb{S}^{d-1}; \mathbb{R}) = L^2(\mathbb{S}^{d-1}; \mathbb{R})^2.$$

In what follow, we consider these identifications.

We define the integral operator $\vec{\Psi}_q : L^2(D; \mathbb{R})^2 \to L^2(D; \mathbb{R})^2$ by, for $u = (u_1, u_2)^T \in L^2(D; \mathbb{R})^2$ and $q = (q_1, q_2)^T \in L^\infty_Q(D; \mathbb{C})$ is understood that $q = q_1 + \mathbf{i} q_1 \in L^\infty_Q(D; \mathbb{C})$,

$$\vec{\Psi}_q(u)(x) = \vec{u}^{\text{inc}}(x) + k^2 \int_D \vec{\Phi}(x,y) M(u(y), q(y)) \mathrm{d}y,$$

where the mapping $M : \mathbb{R}^4 \to \mathbb{R}^2$ is defined by

$$M(u, q) := (u_1 q_1 - u_2 q_2, u_1 q_2 + u_2 q_1)^T \in \mathbb{R}^2$$

and

$$\vec{u}^{\mathrm{inc}}(x) = (\mathrm{Re}(u^{\mathrm{inc}}(x)), \mathrm{Im}(u^{\mathrm{inc}}(x)))^T, \quad \vec{\Phi}(x,y) = \begin{pmatrix} \mathrm{Re}(\Phi(x,y)) & -\mathrm{Im}(\Phi(x,y)) \\ \mathrm{Im}(\Phi(x,y)) & \mathrm{Re}(\Phi(x,y)) \end{pmatrix} \in \mathbb{R}^{2\times 2}.$$

Using these notations, we can write

$$\vec{\Psi}_q(u)(x) = \begin{pmatrix} \mathrm{Re}(\Psi_{q_1+\mathbf{i}q_2}(u_1+\mathbf{i}u_2)(x)) \\ \mathrm{Im}(\Psi_{q_1+\mathbf{i}q_2}(u_1+\mathbf{i}u_2)(x)) \end{pmatrix}.$$

We now define the forward map $F^+ : L^\infty_Q(D;\mathbb{C}) \to L^\infty(\mathbb{S}^{d-1};\mathbb{R})^2$ by

$$F^+(q)(\hat{x}) := (\mathrm{Re}(u^\infty_{q_1+\mathbf{i}q_2}(\hat{x})), \mathrm{Im}(u^\infty_{q_1+\mathbf{i}q_2}(\hat{x})))^T, \quad \hat{x} \in \mathbb{S}^{d-1},\ q = (q_1,q_2)^T \in L^\infty_Q(D;\mathbb{C}).$$

Equivalently, we can write

$$F^+(q)(\hat{x}) = c_d \int_D \vec{e}(\hat{x},y) M(u_q(y), q(y))\mathrm{d}y =: \vec{\Pi}_q(u_q)(\hat{x})$$

where

$$\vec{e}(\hat{x},y) = \begin{pmatrix} \mathrm{Re}(e^{-\mathbf{i}k\hat{x}\cdot y}) & -\mathrm{Im}(e^{-\mathbf{i}k\hat{x}\cdot y}) \\ \mathrm{Im}(e^{-\mathbf{i}k\hat{x}\cdot y}) & \mathrm{Re}(e^{-\mathbf{i}k\hat{x}\cdot y}) \end{pmatrix} \in \mathbb{R}^{2\times 2},$$

and $u_q \in L^2(D;\mathbb{R})^2$ is a fixed point of ρ-contraction map $\vec{\Psi}_q$, i.e., $\vec{\Psi}_q(u_q) = u_q$.

We now define a sequence $(u^{(J)})_{J\in\mathbb{N}} \subset L^2(D;\mathbb{R})^2$ by

$$u^{(0)} = 0 \in L^2(D;\mathbb{R})^2, \quad u^{(J)} := \vec{\Psi}_q(u^{(J-1)}) = \vec{\Psi}_q^{[J]}(u^{(0)})$$

then, $u^{(J)} \to u_q$ as $J \to \infty$. We will mimic this procedure by neural operators defined below.

3 Neural operators for the scattering problem

3.1 Motivation

Our aim is to construct an "approximate operator" (neural operator) that serves an a surrogate for the forward operator F^+. As explained in the Introduction, we would like to study some quantitative approximation of parameters in neural operators such as the length of layers, the width of the neurons, and the rank, and so on, in terms of the desired accuracy. Our idea here is similar to that in [12] in which neural operators are constructed for nonlinear parabolic equations. The main idea is the fixed point argument. The iteration scheme is given by

$$u^{(\ell+1)} = \vec{\Psi}_q(u^{(\ell)})(x) = \vec{u}^{\mathrm{inc}}(x) + k^2 \int_D \vec{\Phi}(x,y) M(u^{(\ell)}(y), q(y))\mathrm{d}y$$

and $u^{(\ell)} \to u_q$ in $L^2(D;\mathbb{R})^2$ provided Assumption 2.1 holds. Let $\{\varphi_n\}_{n=1}^\infty$ be a complete orthonormal basis of $L^2(D;\mathbb{R})^2$. Then $\vec{\Phi}(x,y)$ can be written as an infinite series

$$\vec{\Phi}(x,y) = \sum_{n,m} c_{n,m}\varphi_n(x) \otimes \varphi_m(y)$$

where $c_{n,m} \in \mathbb{R}^{2\times 2}$ for all $n,m \geq 1$ and the series converges in $L^2(D\times D;\mathbb{R})^2$. Let Λ be an index set that is either finite or countably infinite. Denote Λ_N a subset of Λ whose cardinality $|\Lambda_N| = N$ and $\Lambda_N \subset \Lambda_{N'}$ when $N \subset N'$. We now write the partial sum

$$\vec{\Phi}_N(x,y) = \sum_{n,m\in\Lambda_N} c_{n,m}\varphi_n(x) \otimes \varphi_m(y)$$

and thus $\vec{\Phi}_N \to \vec{\Phi}$ in $L^2(D \times D; \mathbb{R})^2$. With the partial sum $\vec{\Phi}_N$, we define the approximate map

$$\vec{\Psi}_{q,N}(v)(x) := \vec{u}^{\mathrm{inc}}(x) + k^2 \int_D \vec{\Phi}_N(x,y) M(v(y), q(y)) \mathrm{d}y.$$

Therefore, it is legitimate to consider the following approximation scheme

$$\hat{u}^{(\ell+1)} = \vec{\Psi}_{q,N}(\hat{u}^{(\ell)})(x) = \vec{u}^{\mathrm{inc}}(x) + k^2 \int_D \vec{\Phi}_N(x,y) M(\hat{u}^{(\ell)}(y), q(y)) \mathrm{d}y$$

and we expect that $\vec{\Pi}_q(\hat{u}^{(L+1)})(\hat{x})$ is a good approximation of $F^+(q)(\hat{x})$ within any desired accuracy when L and N are sufficiently large. We now give a formal definition of neural operators.

3.2 Definition of neural operators

Let X be a set. For an operator $A : X \to X$ and $j \in \mathbb{N}$, we denote by $A^{[j]}$ the j times compositions of A (or the j times products of A): $A^{[0]}$ means the identity operator on X and $A^{[J]} := \underbrace{A \circ \cdots \circ A}_{J \text{ times}}$. We now give a formal definition of neural operators.

Definition 3.1 (Neural operators, [12, 17, 20])**.** *Let $\varphi := \{\varphi_n\}_{n\in\Lambda}$ and $\psi := \{\psi_m\}_{m\in\Gamma}$ be ONBs in $L^2(D;\mathbb{R})^2$ and $L^2(\mathbb{S}^{d-1};\mathbb{R})^2$, respectively. Here, Λ and Γ are index sets that are either finite or countably infinite. We define a neural operator $G : L^\infty_Q(D;\mathbb{C}) \to L^2(\mathbb{S}^{d-1};\mathbb{R})^2$ by*

$$G : q \mapsto \hat{u}^{(L+1)},$$

where the output function $\hat{u}^{(L+1)}$ is determined inductively as follows:

1. **(Hidden layers)** *For $0 \le \ell \le L-1$, $\hat{u}^{(\ell+1)} = (\hat{u}_1^{(\ell+1)}, \hat{u}_2^{(\ell+1)}, \ldots, \hat{u}_{d_{\ell+1}}^{(\ell+1)}) \in L^2(D;\mathbb{R})^{d_{\ell+1}}$ are iteratively given by*

$$\hat{u}^{(\ell+1)}(x) = \sigma\left(W^{(\ell)}\hat{u}^{(\ell)}(x) + (K_N^{(\ell)}\hat{u}^{(\ell)})(x) + b_N^{(\ell)}(x)\right), \quad 0 \le \ell \le L-1,$$

where $\hat{u}^{(0)} = (q_1, q_2) \in L^\infty_Q(D;\mathbb{C})$ ($d_0 = 2$), and $\sigma : \mathbb{R} \to \mathbb{R}$ is a nonlinear activation operating element-wise, and $W^{(\ell)} \in \mathbb{R}^{d_{\ell+1}\times d_\ell}$ is a weight matrix of the ℓ-th hidden layer, and $K_N^{(\ell)} : L^2(D;\mathbb{R})^{d_\ell} \to L^2(D;\mathbb{R})^{d_{\ell+1}}$ and $b_N^{(\ell)} \in L^2(D;\mathbb{R})^{d_{\ell+1}}$ are defined by

$$(K_N^{(\ell)}u)(x) := \sum_{m,n\in\Lambda_N} C_{n,m}^{(\ell)} \langle \varphi_m, u\rangle \varphi_n(x) \quad \textit{with } C_{n,m}^{(\ell)} \in \mathbb{R}^{d_{\ell+1}\times d_\ell},$$
$$b_N^{(\ell)}(x) := \sum_{n\in\Lambda_N} c_N^{(\ell)} \varphi_n(x) \quad \textit{with } c_N^{(\ell)} \in \mathbb{R}^{d_{\ell+1}},$$

where Λ_N is a subset of Λ with its cardinality $|\Lambda_N| = N \in \mathbb{N}$ and the monotonicity $\Lambda_N \subset \Lambda_{N'}$ for any $N \le N'$. Here, we have used the notation

$$\langle \varphi_m, u\rangle := \left(\langle \varphi_m, u_1\rangle_{L^2(D;\mathbb{R})}, \ldots, \langle \varphi_m, u_{d_\ell}\rangle_{L^2(D;\mathbb{R})}\right) \in \mathbb{R}^{d_\ell},$$

for $u = (u_1, \ldots, u_{d_\ell}) \in L^2(D;\mathbb{R})^{d_\ell}$.

2. **(Output layer)** *$\hat{u}^{(L+1)}$ is given by*

$$\hat{u}^{(L+1)}(\hat{x}) = (K_N^{(L+1)}\hat{u}^{(L)})(\hat{x}) + b_N^{(L+1)}(\hat{x}).$$

where $K_N^{(L+1)} : L^2(D;\mathbb{R})^{d_L} \to L^2(\mathbb{S}^{d-1};\mathbb{R})^2$ *and* $b_N^{(L+1)} \in L^2(\mathbb{S}^{d-1};\mathbb{R})^2$ *are defined by*

$$(K_N^{(L+1)}u)(\hat{x}) := \sum_{m\in\Lambda_N, n\in\Gamma_N} C_{n,m}^{(L+1)} \langle \varphi_m, u\rangle \psi_n(\hat{x}) \quad \text{with } C_{n,m}^{(L+1)} \in \mathbb{R}^{2\times d_L},$$
$$b_N^{(L+1)}(\hat{x}) := \sum_{n\in\Gamma_N} c_n^{(L+1)} \psi_n(\hat{x}) \quad \text{with } c_n^{(L+1)} \in \mathbb{R}^2.$$

We denote by $\mathcal{NO}_{N,\varphi,\psi}^{L,\mathbf{d},\sigma}$ *the class of neural operators defined as above, associated with the depth* L*, the width* $\mathbf{d} = (d_1, ..., d_L)$*, the rank* N*, the activation function* σ*, and the ONBs* φ, ψ*.*

4 Quantitative approximation theorem

In this section, we would like to discuss the main theme of this work. For neural operators, we are interested in deriving the upper bound estimates of the depth L, the number of neurons H, and the rank N, in terms of the desired accuracy. In other words, we will investigate the quantitative approximation theorem.

4.1 ReQU activation function

We define the ReQU activation function $ReQU : \mathbb{R} \to \mathbb{R}$ by

$$ReQU(t) := \max\{0, t\}^2, \quad t \in \mathbb{R}.$$

ReQU neural network and exactly represents the polynomial (see e.g., [23, Theorem 2.2]).

4.2 Main result

Our main result is the following quantitative approximation theorem.

Theorem 4.1. *Assume that* Assumption 2.1 *is satisfied. Let* $u^{\mathrm{inc}} \in L^2(D;\mathbb{C})$ *and* $R > 0$ *such that* (11) *holds true. For any given* $\epsilon \in (0, 1)$*, there exist a depth* L*, a width* $\mathbf{d}$*, a rank* N*, and* $G \in \mathcal{NO}_{N,\varphi,\psi}^{L,\mathbf{d},ReQU}$ *such that*

$$\sup_{q\in L^2_Q(D;\mathbb{R})^2} \|F^+(q) - G(q)\|_{L^2(\mathbb{S};\mathbb{R})^2} \le \epsilon.$$

Moreover, $L = L(G)$ *and* $\mathbf{d} = \mathbf{d}(G) = (d_1(G), ..., d_L(G))$ *satisfy*

$$L(G) \le C(\log(\epsilon^{-1})) \tag{12}$$

and

$$d_\ell(G) \le C, \tag{13}$$

where $C > 0$ *is a constant depending on* d, k, D, Q, M, R*, and* $N = N(G)$ *satisfies*

$$C_{\vec{\Phi}}(N(G)) \le C\epsilon \quad \text{and} \quad C_{\vec{e}}(N(G)) \le C\epsilon \quad \text{and} \quad C_{\vec{u}^{\mathrm{inc}}}(N(G)) \le C\epsilon$$

where

$$C_{\vec{\Phi}}(N) := \|\vec{\Phi}_N - \vec{\Phi}\|_{L^2(D\times D;\mathbb{R}^{2\times 2})}, C_{\vec{e}}(N) := \|\vec{e}_N - \vec{e}\|_{L^2(\mathbb{S}^2\times D;\mathbb{R}^{2\times 2})}, C_{\vec{u}^{\mathrm{inc}}}(N) := \|\vec{u}_N^{\mathrm{inc}} - \vec{u}^{\mathrm{inc}}\|_{L^2(D;\mathbb{R})^2}.$$

To achieve the desired accuracy of the approximation, the logarithmically increasing of the layers, the estimate (12), is expected in view of the exponential convergence rate of the fixed point iteration step. On the other hand, combining (12) and (13), we see that the number of neurons defined by $H(G) := \sum_{\ell=1}^{L} d_\ell(G)$ satisfies

$$H(G) \leq C(\log(\epsilon^{-1}))^2,$$

which is reasonable since the number of neurons at each layer is upper bounded by a fixed constant.

4.3 Proof of Theorem 4.1

Here we will give a detailed proof of Theorem 4.1. The proof is based on the techniques developed in [12], where the nonlinear parabolic equation is treated. The argument is divided into several steps.

Step 1. We define the approximate operators $\vec{\Psi}_{q,N}$, $\vec{\Pi}_{q,N}$ by

$$\begin{aligned}
\vec{\Psi}_{q,N}(u)(x) &:= \vec{u}_N^{\mathrm{inc}}(x) + k^2 \int_D \vec{\Phi}_N(x,y) M(u(y), q(y)) \mathrm{d}y, \\
\vec{\Pi}_{q,N}(u)(\hat{x}) &:= c_d \int_D \vec{e}_N(\hat{x}, y) M(u(y), q(y)) \mathrm{d}y,
\end{aligned}$$

where $\vec{\Phi}_N$, $\vec{e}_N$, and $\vec{u}_N^{\mathrm{inc}}$ are given by

$$\begin{aligned}
\vec{\Phi}_N(x,y) &:= \sum_{n,m \in \Lambda_N} C_{n,m}(\vec{\Phi}) \varphi_n(x) \varphi_m(y), \\
\vec{e}_N(\hat{x}, y) &:= \sum_{n \in \Gamma_N, m \in \Lambda_N} C_{n,m}(\vec{e}) \psi_n(\hat{x}) \varphi_m(y), \\
\vec{u}_N^{\mathrm{inc}}(x) &:= \sum_{n \in \Gamma_N} c_n(\vec{u}^{\mathrm{inc}}) \varphi_n(x).
\end{aligned}$$

Here the components $C_{n,m}(\vec{\Phi}), C_{n,m}(\vec{e}) \in \mathbb{R}^{2\times 2}$, and $c_n(\vec{u}^{\mathrm{inc}}) \in \mathbb{R}^2$ are defined by

$$\begin{aligned}
C_{n,m}(\vec{\Phi}) &:= \begin{pmatrix} \langle \mathrm{Re}(\Phi(x,y)), \varphi_n(x)\varphi_m(y) \rangle & -\langle \mathrm{Im}(\Phi(x,y)), \varphi_n(x)\varphi_m(y) \rangle \\ \langle \mathrm{Im}(\Phi(x,y)), \varphi_n(x)\varphi_m(y) \rangle & \langle \mathrm{Re}(\Phi(x,y)), \varphi_n(x)\varphi_m(y) \rangle \end{pmatrix}, \\
C_{n,m}(\vec{e}) &:= \begin{pmatrix} \langle \mathrm{Re}(e^{-\mathbf{i}k\hat{x}\cdot y}), \psi_n(\hat{x})\varphi_m(y) \rangle & -\langle \mathrm{Im}(e^{-\mathbf{i}k\hat{x}\cdot y}), \psi_n(\hat{x})\varphi_m(y) \rangle \\ \langle \mathrm{Im}(e^{-\mathbf{i}k\hat{x}\cdot y}), \psi_n(\hat{x})\varphi_m(y) \rangle & \langle \mathrm{Re}(e^{-\mathbf{i}k\hat{x}\cdot y}), \psi_n(\hat{x})\varphi_m(y) \rangle \end{pmatrix}, \\
c_n(\vec{u}^{\mathrm{inc}}) &= (\langle \mathrm{Re}(u^{\mathrm{inc}}(x)), \varphi_n(x) \rangle, \langle \mathrm{Im}(u^{\mathrm{inc}}(x)), \varphi_n(x) \rangle).
\end{aligned}$$

Since φ and ψ are ONBs, we see that as $N \to \infty$

$$\begin{aligned}
C_{\vec{\Phi}}(N) &:= \|\vec{\Phi}_N - \vec{\Phi}\|_{L^2(D\times D;\mathbb{R}^{2\times 2})} \to 0, \\
C_{\vec{e}}(N) &:= \|\vec{e}_N - \vec{e}\|_{L^2(\mathbb{S}^{d-1}\times D;\mathbb{R}^{2\times 2})} \to 0, \\
C_{\vec{u}^{\mathrm{inc}}}(N) &:= \|\vec{u}_N^{\mathrm{inc}} - \vec{u}^{\mathrm{inc}}\|_{L^2(D;\mathbb{R})^2} \to 0.
\end{aligned}$$

Lemma 4.1.

$$\begin{aligned}
\|\vec{\Psi}_q(u) - \vec{\Psi}_{q,N}(u)\|_{L^2(D;\mathbb{R})^2} &\leq C_{\vec{u}^{\mathrm{inc}}}(N) + k^2 Q C_{\vec{\Phi}}(N) \|u\|_{L^2(D;\mathbb{R})^2}, \\
\|\vec{\Pi}_q(u) - \vec{\Pi}_{q,N}(u)\|_{L^2(\mathbb{S}^{d-1},\mathbb{R})^2} &\leq c_d Q C_{\vec{e}}(N) \|u\|_{L^2(D;\mathbb{R})^2},
\end{aligned} \tag{14}$$

and

$$\begin{aligned} &\|\vec{\Psi}_{q,N}(u) - \vec{\Psi}_{q,N}(v)\|_{L^2(D;\mathbb{R})^2} \leq k^2 Q \left(C_{\vec{\Phi}}(N) + \|\vec{\Phi}\|_{L^2(D\times D;\mathbb{R}^{2\times 2})} \right) \|u-v\|_{L^2(D;\mathbb{R})^2}, \\ &\|\vec{\Pi}_{q,N}(u) - \vec{\Pi}_{q,N}(v)\|_{L^2(\mathbb{S}^{d-1};\mathbb{R})^2} \leq c_d Q \left(C_{\vec{e}}(N) + \|\vec{e}\|_{L^2(\mathbb{S}^{d-1}\times D;\mathbb{R}^{2\times 2})} \right) \|u-v\|_{L^2(D;\mathbb{R})^2}. \end{aligned} \tag{15}$$

Also, if $u^{\mathrm{inc}} \in L^2(D;\mathbb{C})$ *and* $R>0$ *satisfy* (11)*, then we have that, for all* $N\in\mathbb{N}$*,*

$$\vec{\Psi}_{q,N} : B(0,R) \to B(0,R)$$

(*see* Remark 2.1).

Proof. We note that

$$\vec{\Psi}_q(u)(x) - \vec{\Psi}_{q,N}(u)(x) = \vec{u}^{\mathrm{inc}}(x) - \vec{u}_N^{\mathrm{inc}}(x) + k^2 \int_D (\vec{\Phi} - \vec{\Phi}_N)(x,y) M(q(y),u(y)) \mathrm{d}y$$

and

$$\vec{\Pi}_q(u)(\hat{x}) - \vec{\Pi}_{q,N}(u)(\hat{x}) = c_d \int_D (\vec{e} - \vec{e}_N)(\hat{x},y) M(q(y),u(y)) \mathrm{d}y.$$

The estimates (14) then follows easily. On the other hand, we can write

$$\begin{aligned} &\vec{\Psi}_{q,N}(u)(x) - \vec{\Psi}_{q,N}(v)(x) \\ &= k^2 \int_D \vec{\Phi}_N(x,y) M(q(y),(u-v)(y)) \mathrm{d}y \\ &= k^2 \int_D (\vec{\Phi}_N - \vec{\Phi})(x,y) M(q(y),(u-v)(y)) \mathrm{d}y + k^2 \int_D \vec{\Phi}(x,y) M(q(y),(u-v)(y)) \mathrm{d}y \end{aligned}$$

and

$$\begin{aligned} &\vec{\Pi}_{q,N}(u)(\hat{x}) - \vec{\Pi}_{q,N}(v)(\hat{x}) \\ &= c_d \int_D \vec{e}_N(\hat{x},y) M(q(y),(u-v)(y)) \mathrm{d}y \\ &= c_d \int_D (\vec{e}_N - \vec{e})(\hat{x},y) M(q(y),(u-v)(y)) \mathrm{d}y + c_d \int_D \vec{e}(\hat{x},y) M(q(y),(u-v)(y)) \mathrm{d}y \end{aligned}$$

and so (15) can be derived directly.

Observe that

$$\|\vec{u}_N^{\mathrm{inc}}\|_{L^2(D;\mathbb{R})^2} \leq \|\vec{u}^{\mathrm{inc}}\|_{L^2(D;\mathbb{R})^2} \quad \text{and} \quad \|\vec{\Phi}_N\|_{L^2(D\times D;\mathbb{R}^2\times\mathbb{R}^2)} \leq \|\vec{\Phi}\|_{L^2(D\times D;\mathbb{R}^2\times\mathbb{R}^2)}$$

for all N. For R satisfying (11), we conclude that $\vec{\Psi}_{q,N} : B(0,R) \to B(0,R)$ from Remark 2.1. □

Step 2. Next, we define the map $G : L_Q^\infty(D;\mathbb{C}) \to L^2(\mathbb{S}^{d-1};\mathbb{R})^2$ by

$$G(q) := \vec{\Pi}_{q,N} \circ \vec{\Psi}_{q,N}^{[J]}(u^{(0)}), \tag{16}$$

where $u^{(0)} \in B(0,R)$. Recall that $\vec{\Psi}_{q,N}^{[J]} := \underbrace{\vec{\Psi}_{q,N} \circ \cdots \circ \vec{\Psi}_{q,N}}_{J \text{ times}}$. For any $\epsilon>0$, we can choose an $N_\epsilon \in \mathbb{N}$, depending on ϵ, such that

$$C_{\vec{\Phi}}(N) \leq \epsilon, \;\; C_{\vec{e}}(N) \leq \epsilon, \;\; \text{and} \;\; C_{\vec{u}^{\mathrm{inc}}}(N) \leq \epsilon \tag{17}$$

for all $N \geq N_\epsilon$.

Lemma 4.2. *Let $J = \lceil \frac{\log(1/\epsilon)}{\log(1/\rho)} \rceil \in \mathbb{N}$. Then there exists a constant $C > 0$ such that for any $q \in L^\infty_Q(D;\mathbb{C})$*

$$\|F^+(q) - G(q)\|_{L^2(\mathbb{S}^{d-1};\mathbb{R})^2} \le C\epsilon,$$

where $C > 0$ depends on d, k, D, Q, R.

Proof. Note that $F^+(q)$ has the form

$$F^+(q) = \vec{\Pi}_q(u_q).$$

By the triangle inequality and using Lemma 4.1, we have

$$\begin{aligned}
\|F^+(q) - G(q)\|_{L^2(\mathbb{S}^{d-1};\mathbb{R})^2} &\le \|\vec{\Pi}_q(u_q) - \vec{\Pi}_{q,N}(u_q)\|_{L^2(\mathbb{S}^{d-1};\mathbb{R})^2} + \|\vec{\Pi}_{q,N}(u_q) - \vec{\Pi}_{q,N} \circ \vec{\Psi}^{[J]}_{q,N}(u^{(0)})\|_{L^2(\mathbb{S}^{d-1};\mathbb{R})^2} \\
&\le c_d Q \|u_q\|_{L^2(D;\mathbb{R})^2} C_{\vec{e}}(N) \\
&\quad + c_d Q \left(C_{\vec{e}}(N) + \|\vec{e}\|_{L^2(\mathbb{S}^2 \times D;\mathbb{R}^{2\times 2})} \right) \|u_q - \vec{\Psi}^{[J]}_{q,N}(u^{(0)})\|_{L^2(D;\mathbb{R})^2}.
\end{aligned}$$

Since $\vec{\Psi}_q : L^2(D;\mathbb{R})^2 \to L^2(D;\mathbb{R})^2$ is ρ-contractive and $u_q = \vec{\Psi}_q(u_q)$ is the fixed point of $\vec{\Psi}_q$, i.e., $u_q = \vec{\Psi}^{[J]}_q(u_q)$ for all J, we have

$$\begin{aligned}
\|u_q - \vec{\Psi}^{[J]}_{q,N}(u^{(0)})\|_{L^2(D;\mathbb{R})^2} &\le \|\vec{\Psi}^{[J]}_q(u_q) - \vec{\Psi}^{[J]}_q(u^{(0)})\|_{L^2(D;\mathbb{R})^2} + \|\vec{\Psi}^{[J]}_q(u^{(0)}) - \vec{\Psi}^{[J]}_{q,N}(u^{(0)})\|_{L^2(D;\mathbb{R})^2} \\
&\le \rho^J \|u_q - u^{(0)}\|_{L^2(D;\mathbb{R})^2} + \|\vec{\Psi}^{[J]}_q(u^{(0)}) - \vec{\Psi}^{[J]}_{q,N}(u^{(0)})\|_{L^2(D;\mathbb{R})^2}.
\end{aligned}$$

To estimate the second term above, we derive that from the first estimate of (14)

$$\begin{aligned}
&\|\vec{\Psi}^{[J]}_q(u^{(0)}) - \vec{\Psi}^{[J]}_{q,N}(u^{(0)})\|_{L^2(D;\mathbb{R})^2} \\
&\le \sum_{j=1}^{J} \left\| \left(\vec{\Psi}^{[J-j+1]}_q \circ \vec{\Psi}^{[j-1]}_{q,N} \right)(u^{(0)}) - \left(\vec{\Psi}^{[J-j]}_q \circ \vec{\Psi}^{[j]}_{q,N} \right)(u^{(0)}) \right\|_{L^2(D;\mathbb{R})^2} \\
&\le \sum_{j=1}^{J} \rho^{J-j} \left\| \left(\vec{\Psi}_q \circ \vec{\Psi}^{[j-1]}_{q,N} \right)(u^{(0)}) - \vec{\Psi}^{[j]}_{q,N}(u^{(0)}) \right\|_{L^2(D;\mathbb{R})^2} \\
&= \sum_{j=1}^{J} \rho^{J-j} \left(C_{\vec{u}^{\mathrm{inc}}}(N) + k^2 Q C_{\vec{\Phi}}(N) \underbrace{\|\vec{\Psi}^{[j-1]}_{q,N}(u^{(0)})\|_{L^2(D;\mathbb{R})^2}}_{\le R} \right).
\end{aligned}$$

Putting all estimates together, we obtain that

$$\|F^+(q) - G(q)\|_{L^2(\mathbb{S}^{d-1};\mathbb{R})^2} \le C(C_{\vec{e}}(N) + C_{\vec{u}^{\mathrm{inc}}}(N) + C_{\vec{\Phi}}(N) + \rho^J) \le C\epsilon,$$

where C depends on d, k, Q, D, R. □

Step 3. Finally, it is sufficient to represent the approximate operator G as a neural operator in the form of Definition 3.1 and to provide its quantitative estimates.

Lemma 4.3. *Let*

$$G \in \mathcal{NO}^{L,H,ReQU}_{N,\varphi,\psi}.$$

Then

$$L(G) \le C \log(\epsilon^{-1}) \quad \text{and} \quad d_\ell(G) \le C,$$

where $C > 0$ is a constant depending on k, D, Q, R, and $N = N(G)$ satisfies

$$C_{\vec{\Phi}}(N(G)) \le C\epsilon, \quad C_{\vec{e}}(N(G)) \le C\epsilon, \quad \text{and} \quad C_{\vec{u}^{\mathrm{inc}}}(N(G)) \le C\epsilon.$$

Proof. Since $q = (q_1, q_2)^T \in L^\infty_Q(D;\mathbb{C})$, it is obvious that $q \in L^2(D;\mathbb{R})^2$. We define $\vec{\Psi} : L^2(D;\mathbb{R})^4 \to L^2(D;\mathbb{R})^4$ by

$$\vec{\Psi}(u,q) = \begin{pmatrix} \vec{\Psi}_{q,N}(u) \\ q \end{pmatrix},$$

where $\begin{pmatrix} u \\ q \end{pmatrix} \in L^2(D;\mathbb{R})^4$. Similarly, we define $\vec{\Pi} : L^2(D;\mathbb{R})^4 \to L^2(\mathbb{S}^{d-1};\mathbb{R})^2$ by

$$\vec{\Pi}(u,q) := \vec{\Pi}_{q,N}(u).$$

Using these notations, we denote

$$G_{J,N}(q) := \vec{\Pi} \circ \vec{\Psi}^{[J]} \circ W_1(q)$$

where

$$W_1 := \begin{pmatrix} 0 \\ I_2 \end{pmatrix} \in \mathbb{R}^{4\times 2}$$

(Note that since the initial guess $u^{(0)} \in B(0,R)$ of the fixed-point iteration can be arbitrary, it is simple to choose $u^{(0)} = 0$.)

We now write

$$\begin{aligned}\vec{\Psi}(u,q)(x) &= b_N(x) + W_2\hat{M}(u(x),q(x)) + \sum_{n,m\in\Lambda_N} C_{n,m}\langle\varphi_m, \hat{M}(u(y),q(y))\rangle\varphi_n(x) \\ &= (W_2 + K_N)\circ\hat{M}(u,q)(x) + b_N(x),\end{aligned}$$

where

$$b_N(x) = \begin{pmatrix} \vec{u}^{\mathrm{inc}}_N \\ 0 \end{pmatrix} \in L^2(D;\mathbb{R})^4,$$

$$W_2 = \begin{pmatrix} 0 & 0 \\ 0 & I_2 \end{pmatrix} \in \mathbb{R}^{4\times 4},$$

$$K_N u(x) := \sum_{n,m\in\Lambda_N} C_{n,m}\langle\varphi_m, u\rangle\varphi_n(x), \text{ where } C_{n,m} := \begin{pmatrix} k^2 C_{n,m}(\vec{\Phi}) & 0 \\ 0 & 0 \end{pmatrix} \in \mathbb{R}^{4\times 4},$$

and $\hat{M} : \mathbb{R}^4 \to \mathbb{R}^4$ is given by

$$\hat{M}(u,q) := \begin{pmatrix} M(u,q) \\ q \end{pmatrix}.$$

Here, in an abuse of notation, we write $\varphi_n \in L^2(D;\mathbb{R})^4$ as $\begin{pmatrix} \varphi_n \\ 0 \end{pmatrix}$. Also $W_2 \circ \hat{M}(u,q)$ is interpreted as the matrix-vector multiplication $W_2\hat{M}(u,q)$.

On the other hand, we can derive that

$$\begin{aligned}\vec{\Pi}(u,q)(\hat{x}) &= \vec{\Pi}_{q,N}(u)(\hat{x}) \\ &= c_d \int_D \vec{e}_N(\hat{x},y) M(u(y),q(y))\mathrm{d}y, \\ &= c_d \sum_{n\in\Gamma_N, m\in\Lambda_N} C_{n,m}(\vec{e})\langle\varphi_m(y), M(u(y),q(y))\rangle\psi_n(\hat{x}) \\ &= \widetilde{K}_N \circ M(u,q)(\hat{x})\end{aligned}$$

where

$$\widetilde{K}_N u(\hat{x}) := \sum_{n\in\Gamma_N, m\in\Lambda_N} \widetilde{C}_{n,m}\langle\varphi_m, u\rangle\psi_n(\hat{x}), \quad \widetilde{C}_{n,m} := c_d C_{n,m}(\vec{e}) \in \mathbb{R}^{2\times 2}.$$

Thus,

$$\begin{aligned} G_{J,N}(q) &= \vec{\Pi}\circ\vec{\Psi}^{[J]}\circ W_1(q) \\ &= \widetilde{K}_N \circ M \circ \left[\underbrace{((W_2+K_N)\circ\hat{M}+b_N)\circ\cdots\circ((W_2+K_N)\circ\hat{M}+b_N)}_{J}\right]\circ W_1(q). \end{aligned} \tag{18}$$

We would like to remark that since b_N is a fixed function, the composition $b_N \circ W_1(q)$ is simply b_N.

Since functions $\hat{M} : \mathbb{R}^4 \to \mathbb{R}^4$ and $M : \mathbb{R}^4 \to \mathbb{R}^2$ are polynomials, they can be *exactly* represented as ReQU neural networks, see [23, Theorem 3.1]. So their depth and width are constant regardless of ϵ. We now check that (18) can be written in a form of neural operators defined in Definition 3.1. By [23, Theorem 3.1], in the first iteration step $\vec{\Psi}^{[1]}$, we have

$$\hat{M}\circ W_1(q)(x) = \begin{pmatrix} M(u^{(0)}, q) \\ q \end{pmatrix} = \mathrm{ReQU}(u^{(0)}, q) := \hat{u}^{(1)}(x),$$

which can seen as the first hidden layer. The first iteration step gives

$$\vec{\Psi}^{[1]}\circ W_1(q) = (W_2 + K_N)\hat{u}^{(1)} + b_N.$$

Next, the $\hat{M}$ operator in $\vec{\Psi}^{[2]}$ gives rise to

$$\hat{M}\circ((W_2+K_N)\hat{u}^{(1)} + b_N) = \mathrm{ReQU}((W_2+K_N)\hat{u}^{(1)} + b_N) := \hat{u}^{(2)}.$$

Finally, the output layer will be

$$\tilde{K}_N\,\mathrm{ReQU}((W_2+K_N)\hat{u}^{(J)} + b_N).$$

In other words, the above construction ensures that $G \in \mathcal{NO}^{L,\mathbf{d},\mathrm{ReQU}}_{N,\varphi,\psi}$. Moreover, in view of Lemma 4.2, the depth $L(G)$ and the width $\mathbf{d}(G)$ of the neural operator G can be estimated as

$$L(G) \lesssim J \lesssim \log(\epsilon^{-1}), \quad d_\ell(G) \lesssim 1$$

Thus, the proof of Theorem 4.1 is now complete. □

5 Application to the inverse scattering problem

In this section, we would like to demonstrate how to use the neural operator G constructed above to solve the inverse scattering problem in which we want to determine the refractive index $1+q$ (or q) from the far-field pattern. We consider the plane incident field $u^{\mathrm{inc}}(x) = e^{ik\theta\cdot x}$, where $\theta \in \mathbb{S}^{d-1}$, and the corresponding far-field pattern $u_q^\infty(\theta, \hat{x})$. The inverse problem is to determine q from $u_q^\infty(\theta, \hat{x})$ for all $\theta, \hat{x} \in \mathbb{S}^{d-1}$. The unique determination of q by such $u_q^\infty(\theta, \hat{x})$ is well-known, see for example, [9, Chapter 10].

Here we are interested in the reconstruction of q from $u_q^\infty(\theta, \hat{x})$ for all $\theta, \hat{x} \in \mathbb{S}^{d-1}$. Our method is based on the Ensemble Kalman Inversion (EKI) [14], [29], [30]. EKI is known to be a derivative-free Bayesian inference method. In theory, in each prediction step, we have to evaluate the forward map $q \mapsto u_q^\infty$, which is rather time consuming. It is therefore reasonable to replace the mapping $q \mapsto u_q^\infty$ by its surrogate G.

We now describe EKI in detailed. To begin, assume that we are given a far-field pattern $u_q^\infty(\theta, \hat{x})$ generated by an unknown q. Suppose that G has been trained by a collection of data $\{q_t^{(j)}, u^\infty_{q_t^{(j)}}\}_{j=1}^N$ with a sufficiently large $N \in \mathbb{N}$. Let $q_t^{(j_0)}$ be given by

$$q_t^{(j_0)} = \underset{q_t^{(j)}, 1 \le j \le N}{\operatorname{argmin}} \|u_q^\infty - u^\infty_{q_t^{(j)}}\|_{L^2(\mathbb{S}^{d-1} \times \mathbb{S}^{d-1})}. \tag{19}$$

Roughly speaking, $q_t^{(j_0)}$ is an estimator of q. In EKI, we consider an augmented state space. Let $Z = X \times Y$, where $X = C_Q(D; \mathbb{C})$ and $Y = L^2(\mathbb{S}^{d-1} \times \mathbb{S}^{d-1})$. Here we say that $q \in C_Q(D; \mathbb{C})$ if $n = 1 + q$ and n belongs to the set

$$\{n \in C(\mathbb{R}^d; \mathbb{C}) : 0 < \operatorname{Re}(n),\ 0 \le \operatorname{Im}(n),\ \operatorname{supp}(n-1) \subset D,\ |n(x) - 1| \le Q\}.$$

Define the forward map $\mathcal{G} : Z \mapsto Z$ by

$$\mathcal{G}(z) = \begin{pmatrix} q \\ G(q) \end{pmatrix} \quad \text{for } z = \begin{pmatrix} q \\ w \end{pmatrix} \in Z.$$

We consider the inverse problem as an inference problem with noisy data given by

$$y = G(q) + \eta, \tag{20}$$

where $\eta \sim N(0, \Gamma)$ is a mean-zero Gaussian random variable with known covariance Γ on Y. Let us define the artificial dynamics

$$z_{k+1} = \mathcal{G}(z_k). \tag{21}$$

Related to the artificial dynamics, (20) is written as

$$y_{k+1} = \mathcal{H} z_{k+1} + \eta_{k+1}, \tag{22}$$

where the projection operator $\mathcal{H} : Z \to Y$ is defined by $\mathcal{H} = (0, I)$ and $\{\eta_k\}$ is an iid sequence with $\eta_1 \sim N(0, \Gamma)$ and Γ is given above.

The scheme requires an initial (or first guess) ensemble of particles $\{z_0^{(j)}\}_{j=1}^J$ which will be iteratively updated with the ensemble Kalman filter method. The ensemble $\{z_0^{(j)}\}_{j=1}^J$ can be defined by constructing an ensemble $\{q^{(j)}\}_{j=1}^J$ in X. To be precise, let μ_0 be a probability measure on X with mean $q_t^{(j_0)}$. We then choose $q_0^{(1)}, \cdots, q_0^{(J)} \overset{iid}{\sim} \mu_0$ and define $\mathcal{A} = \operatorname{span}\{q_0^{(j)}\}_{j=1}^J$. Once $\{q_0^{(j)}\}_{j=1}^J$ is specified, we can simply define

$$z_0^{(j)} = \begin{pmatrix} q_0^{(j)} \\ G(q_0^{(j)}) \end{pmatrix}$$

which consists of particles in Z. At any k-th step, we set the estimator

$$\bar{q}_k \equiv \frac{1}{J} \sum_{j=1}^J q_k^{(j)} = \frac{1}{J} \sum_{j=1}^J \mathcal{H}^\perp z_k^{(j)} \quad k = 0, 1, \cdots,$$

where $\mathcal{H}^\perp = (I, 0)$.

We now describe the iterative ensemble Kalman filter method for (21), (22).

Algorithm. Let $\{z_0^{(j)}\}_{j=1}^J$ be the initial ensemble. For $k = 0, 1, 2, \cdots$

(i) *Prediction step.* We first propagate particles under the dynamics (21):

$$\widetilde{z}_{k+1}^{(j)} = \begin{pmatrix} \widetilde{q}_{k+1}^{(j)} \\ \widetilde{w}_{k+1}^{(j)} \end{pmatrix} = \mathcal{G}(z_k^{(j)}) = \begin{pmatrix} q_k^{(j)} \\ G(q_k^{(j)}) \end{pmatrix}.$$

Compute the empirical mean and covariance:

$$\widehat{z}_{k+1} = \frac{1}{J}\sum_{j=1}^{J} \widetilde{z}_{k+1}^{(j)}$$

$$\mathcal{C}_{k+1} = \frac{1}{J}\sum_{j=1}^{J} \widetilde{z}_{k+1}^{(j)}(\widetilde{z}_{k+1}^{(j)})^T - \widehat{z}_{k+1}(\widehat{z}_{k+1})^T.$$

(ii) *Analysis step.* Define the *Kalman gain* $\mathcal{K}_{k+1}$ by

$$\mathcal{K}_{k+1} = \mathcal{C}_{k+1}\mathcal{H}^T(\mathcal{H}\mathcal{C}_{k+1}\mathcal{H}^T + \Gamma)^{-1}.$$

Update each ensemble particle by

$$z_{k+1}^{(j)} = \widetilde{z}_{k+1}^{(j)} + \mathcal{K}_{k+1}(y_{k+1}^{(j)} - \mathcal{H}\widetilde{z}_{k+1}^{(j)}) = (I - \mathcal{K}_{k+1}\mathcal{H})\widetilde{z}_{k+1}^{(j)} + \mathcal{K}_{k+1}y_{k+1}^{(j)},$$

where $y_{k+1}^{(j)} = y + \eta_{k+1}^{(j)}$ with $\eta_{k+1}^{(j)} \sim N(0, \Gamma)$. Here y is the observation data and $y_{k+1}^{(j)}$ is obtained by artificially perturbing the observation data, see (22).

(iii) Finally, we compute the mean of the parameter update

$$\bar{q}_{k+1} = \frac{1}{J}\sum_{j=1}^{J} \mathcal{H}^{\perp} z_{k+1}^{(j)} = \frac{1}{J}\sum_{j=1}^{J} q_{k+1}^{(j)}.$$

Here $\bar{q}_{k+1}$ is a refined estimator of q.

It is important to point out that for every $(k, j) \in \mathbb{N} \times \{1, 2, \cdots, J\}$ we have $q_{k+1}^{(j)} \in \mathcal{A}$ and hence $\bar{q}_{k+1} \in \mathcal{A}$ for all $k \in \mathbb{N}$, see [14, Theorem 2.1].

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References

[1] Anima Anandkumar, Kamyar Azizzadenesheli, Kaushik Bhattacharya, Nikola Kovachki, Zongyi Li, Burigede Liu, and Andrew Stuart. Neural operator: Graph kernel network for partial differential equations. In *ICLR 2020 Workshop on Integration of Deep Neural Models and Differential Equations*, 2020.

[2] Kaushik Bhattacharya, Bamdad Hosseini, Nikola B Kovachki, and Andrew M Stuart. Model reduction and neural networks for parametric pdes. *The SMAI journal of computational mathematics*, 7:121–157, 2021.

[3] Boris Bonev, Thorsten Kurth, Christian Hundt, Jaideep Pathak, Maximilian Baust, Karthik Kashinath, and Anima Anandkumar. Spherical fourier neural operators: Learning stable dynamics on the sphere. In *International conference on machine learning*, pages 2806–2823. PMLR, 2023.

[4] Javier Castro, Claudio Muñoz, and Nicolás Valenzuela. The calderón's problem via deeponets. *Vietnam Journal of Mathematics*, pages 1–32, 2024.

[5] Gengxiang Chen, Xu Liu, Qinglu Meng, Lu Chen, Changqing Liu, and Yingguang Li. Learning neural operators on Riemannian manifolds. *arXiv preprint arXiv:2302.08166*, 2023.

[6] Ke Chen, Chunmei Wang, and Haizhao Yang. Deep operator learning lessens the curse of dimensionality for PDEs. *Transactions on Machine Learning Research*, 2023.

[7] Tianping Chen and Hong Chen. Approximation capability to functions of several variables, nonlinear functionals, and operators by radial basis function neural networks. *IEEE Transactions on Neural Networks*, 6(4):904–910, 1995.

[8] Tianping Chen and Hong Chen. Universal approximation to nonlinear operators by neural networks with arbitrary activation functions and its application to dynamical systems. *IEEE transactions on neural networks*, 6(4):911–917, 1995.

[9] D. Colton and R. Kress. *Inverse Acoustic and Electromagnetic Scattering Theory*, volume 93. Springer Nature, 2019.

[10] Maarten V de Hoop, Daniel Zhengyu Huang, Elizabeth Qian, and Andrew M Stuart. The cost-accuracy trade-off in operator learning with neural networks. *arXiv preprint arXiv:2203.13181*, 2022.

[11] Beichuan Deng, Yeonjong Shin, Lu Lu, Zhongqiang Zhang, and George Em Karniadakis. Approximation rates of deeponets for learning operators arising from advection–diffusion equations. *Neural Networks*, 153:411–426, 2022.

[12] Takashi Furuya, Koichi Taniguchi, and Satoshi Okuda. Quantitative approximation for neural operators in nonlinear parabolic equations. *arXiv preprint arXiv:2410.02151*, 2024.

[13] Gaurav Gupta, Xiongye Xiao, and Paul Bogdan. Multiwavelet-based operator learning for differential equations. *Advances in neural information processing systems*, 34:24048–24062, 2021.

[14] Marco A Iglesias, Kody JH Law, and Andrew M Stuart. Ensemble kalman methods for inverse problems. *Inverse Problems*, 29(4):045001, 2013.

[15] Nikola Kovachki, Samuel Lanthaler, and Siddhartha Mishra. On universal approximation and error bounds for Fourier neural operators. *Journal of Machine Learning Research*, 22(290):1–76, 2021.

[16] Nikola B Kovachki, Samuel Lanthaler, and Andrew M Stuart. Operator learning: Algorithms and analysis. *arXiv preprint arXiv:2402.15715*, 2024.

[17] Nikola B Kovachki, Zongyi Li, Burigede Liu, Kamyar Azizzadenesheli, Kaushik Bhattacharya, Andrew M Stuart, and Anima Anandkumar. Neural operator: Learning maps between function spaces with applications to PDEs. *J. Mach. Learn. Res.*, 24(89):1–97, 2023.

[18] Anastasis Kratsios, Takashi Furuya, Matti Lassas, Maarten de Hoop, et al. Mixture of experts soften the curse of dimensionality in operator learning. *arXiv preprint arXiv:2404.09101*, 2024.

[19] Samuel Lanthaler. Operator learning with pca-net: upper and lower complexity bounds. *Journal of Machine Learning Research*, 24(318):1–67, 2023.

[20] Samuel Lanthaler, Zongyi Li, and Andrew M Stuart. The nonlocal neural operator: Universal approximation. *arXiv preprint arXiv:2304.13221*, 2023.

[21] Samuel Lanthaler, Siddhartha Mishra, and George E Karniadakis. Error estimates for deeponets: A deep learning framework in infinite dimensions. *Transactions of Mathematics and Its Applications*, 6(1):tnac001, 2022.

[22] Samuel Lanthaler and Andrew M Stuart. The curse of dimensionality in operator learning. *arXiv preprint arXiv:2306.15924*, 2023.

[23] Shanshan Li, BoTang and Haijun Yu. Better approximations of high dimensional smooth functions by deep neural networks with rectified power units. *Communications in Computational Physics*, 27(2):379–411, 2019.

[24] Zongyi Li, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. Fourier neural operator for parametric partial differential equations. *arXiv preprint arXiv:2010.08895*, 2020.

[25] Zongyi Li, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. Neural operator: Graph kernel network for partial differential equations. *arXiv preprint arXiv:2003.03485*, 2020.

[26] Lu Lu, Pengzhan Jin, and George Em Karniadakis. Deeponet: Learning nonlinear operators for identifying differential equations based on the universal approximation theorem of operators. *arXiv preprint arXiv:1910.03193*, 2019.

[27] Lu Lu, Pengzhan Jin, Guofei Pang, Zhongqiang Zhang, and George Em Karniadakis. Learning nonlinear operators via deeponet based on the universal approximation theorem of operators. *Nature machine intelligence*, 3(3):218–229, 2021.

[28] Carlo Marcati and Christoph Schwab. Exponential convergence of deep operator networks for elliptic partial differential equations. *SIAM Journal on Numerical Analysis*, 61(3):1513–1545, 2023.

[29] Claudia Schillings and Andrew M Stuart. Analysis of the ensemble kalman filter for inverse problems. *SIAM Journal on Numerical Analysis*, 55(3):1264–1290, 2017.

[30] Claudia Schillings and Andrew M Stuart. Convergence analysis of ensemble kalman inversion: the linear, noisy case. *Applicable Analysis*, 97(1):107–123, 2018.

[31] Makoto Takamoto, Timothy Praditia, Raphael Leiteritz, Daniel MacKinlay, Francesco Alesiani, Dirk Pflüger, and Mathias Niepert. Pdebench: An extensive benchmark for scientific machine learning. *Advances in Neural Information Processing Systems*, 35:1596–1611, 2022.

[32] Tapas Tripura and Souvik Chakraborty. Wavelet neural operator for solving parametric partial differential equations in computational mechanics problems. *Computer Methods in Applied Mechanics and Engineering*, 404:115783, 2023.