

Neural and gpc operator surrogates: construction and expression rate bounds

L. Herrmann and Ch. Schwab and J. Zech

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Eidgenössische Technische Hochschule
CH-8092 Zürich
Switzerland

Neural and gpc operator surrogates: construction and expression rate bounds

Lukas Herrmann¹, Christoph Schwab², and Jakob Zech³

Abstract Approximation rates are analyzed for deep surrogates of maps between infinite-dimensional function spaces, arising e.g. as data-to-solution maps of linear and nonlinear partial differential equations. Specifically, we study approximation rates for *Deep Neural Operator* and *Generalized Polynomial Chaos (gpc) Operator* surrogates for nonlinear, holomorphic maps between infinite-dimensional, separable Hilbert spaces. Operator in- and outputs from function spaces are assumed to be parametrized by stable, affine representation systems. Admissible representation systems comprise orthonormal bases, Riesz bases or suitable tight frames of the spaces under consideration. Algebraic expression rate bounds are established for both, deep neural and gpc operator surrogates acting in scales of separable Hilbert spaces containing domain and range of the map to be expressed, with finite Sobolev or Besov regularity. We illustrate the abstract concepts by expression rate bounds for the coefficient-to-solution map for a linear elliptic PDE on the torus.

Key words: Neural Networks, generalize polynomial chaos, operator learning

1 Introduction

In recent years, deep learning (DL) based numerical methods have started to impact the numerical solution of (parametric) partial differential equations (PDEs) at every stage of the solution process. Deep Neural Networks (DNNs) have been promoted as efficient approximation architectures for PDE solutions and parametric PDE response manifolds. However, the theoretical understanding of the methodology re-

¹Johann Radon Institute for Computational and Applied Mathematics, Austrian Academy of Sciences, Altenbergerstrasse 69, 4040 Linz, Austria, e-mail: lukas.herrmann@ricam.oeaw.ac.at

²Seminar for Applied Mathematics, ETH Zürich, Rämistrasse 101, 8092 Zurich, Switzerland, e-mail: christoph.schwab@sam.math.ethz.ch

³Interdisziplinäres Zentrum für wissenschaftliches Rechnen, Universität Heidelberg, Im Neuenheimer Feld 205, 69120 Heidelberg, Germany, e-mail: jakob.zech@uni-heidelberg.de

mains underdeveloped; quoting [2, Sec. 4.1.1]: “applying deep learning to infinite dimensional spaces is associated with a number of fundamental questions regarding convergence..., if it converges, in what sense?”

1.1 Existing results

Recent successful examples of deployment of DL surrogates in numerical PDE solution algorithms (e.g. [42, 52, 56, 21], has promoted *neural network approximation architectures for PDE solution approximation*. The related question of approximation rates of NN based PDE discretizations has been answered in a number of settings. We mention only [39, 35, 53, 33, 7, 6] and the references there. These approximation rate results were developed in function spaces on finite-dimensional domains.

A more recent and distinct development addresses *neural networks for operator learning*, i.e. for the neural network emulation of maps between infinite dimensional function spaces, such as solution operators of PDEs, coefficient-to-solution and shape-to-solution maps for elliptic PDEs, to name but a few. These have been promulgated under the acronym “Neural operators”, “O-Nets”, “operator learning”, see, e.g., [34, 31] and the references there. Versions of the *DNN universal approximation theorems for operator learning* have been established, following the pioneering work [8], recently in [54, 20, 31, 30, 1]. In these references, generic approximation properties of operators for several architectures of DNNs of in principle arbitrary large depth and width have been established. These results are analogous to the early, universal approximation results of DNNs for function approximation from the 90s of the previous century, as e.g., [27] and [41] and the references there.

Contrary to the mentioned universality theorems, proofs of *operator expression rate bounds* tend to be problem-specific, including assumptions on regularity of input and output data of the operators of interest, and some structural assumptions on the operator mappings. With domains and/or ranges of the operators of interest being infinite-dimensional, as a rule, overcoming the *curse of dimensionality* (CoD) in the proofs of operator emulation bounds is necessary. The results in the present paper leverage progress in recent years on approximation rate bounds for gpc representations of such maps for DNN approximation. This line of research was initiated in [45], building on earlier results on gpc emulation rates in [5] and the references there.

For coefficient-to-solution maps of elliptic PDEs, *on domains consisting of smooth coefficient functions*, it was shown recently in [36] that *exponential expression rates of solution operators* is possible with certain deep ReLU NNs. This result leverages the exponential encoding and decoding of smooth (analytic) functions with tensorized polynomials by spectral collocation, combined with a ReLU NN which emulates a Gaussian Elimination Method for regular matrices of size N in NN size $O(N^4)$, and scaling polylogarithmically in terms of the target accuracy ε of the solution vector.

1.2 Contributions

We establish expression rate bounds for DNN emulations of holomorphic maps between subsets of (scales of) infinite-dimensional spaces \mathcal{X} and \mathcal{Y} . We focus in particular on maps between scales $\{\mathcal{X}^s\}_{s \geq 0}$ and $\{\mathcal{Y}^t\}_{t \geq 0}$ of spaces of finite regularity, such as function spaces of Sobolev- or Besov-type on “physical domains”, being for example bounded subsets D of Euclidean space. Mappings between function spaces on manifolds \mathcal{M} are also covered by the present operator expression rate bounds, upon introduction of stable bases in suitable function spaces on \mathcal{M} , or also on space-time cylinders $\mathcal{M} \times [0, T]$.

A typical example is the (nonlinear) coefficient-to-solution map for linear, elliptic or parabolic partial differential equations of second order which we develop for illustration in some detail in Section 6 ahead. In this “linear elliptic PDE” case, the (nonlinear) coefficient-to-solution map is holomorphic between suitable subsets of $L^\infty(D)$ (accounting for positivity) and $H^1(D)$ (accounting for homogeneous essential boundary conditions on ∂D). The notion of operator holomorphy requires complexifications of the domain and range spaces, in the (common) case that physical modelling will initially comprise only spaces of real-valued functions in D . To simplify technicalities of exposition, we develop the theory for separable, real Hilbert spaces \mathcal{X} . Then, complexification is a standard process resulting in a (canonical) extension [37].

Our results show that for data with finite Sobolev- or Besov regularity, there exist operator surrogates of either deep neural network or of generalized polynomial chaos type such that approximation rates afforded by linear approximation schemes are essentially preserved by the surrogate operators. This generalizes the recent result in [36] where analyticity of inputs was exploited in an essential fashion to the more realistic, finite regularity setting, in rather general classes of function spaces. In addition, our *proofs of these results are constructive* allowing for a *deterministic construction of the surrogate maps with a set budget of pre-defined, numerical operator queries*. Our main results, Theorems 1 and 3, ensure *worst case and mean square generalization error bounds for neural operator surrogates* thus computed. The algebraic operator expression rates are limited by the approximation rates of the encoding and decoding operators entering into the construction of the surrogates. Theorem 6 then has corresponding results for the gpc operator surrogate.

We note that alternative approaches to analyzing the generalization error of operator surrogates, such as methods from statistical learning theory (e.g. [32] and the references there), deliver lower approximation rates (these results do not require holomorphy of \mathcal{G} , however).

1.3 Outline

In Section 2, we present an abstract function space setting, in which the operators and their surrogates will be analyzed. We precise in particular the notion of stable

bases in smoothness scales via isomorphisms to sequence spaces, comprising orthonormal bases in separable Hilbert spaces of Fourier and Karhunen-Loève type, as well as biorthogonal bases of spline and wavelet type. Examples are furnished by Sobolev and Besov spaces, and by reproducing kernel Hilbert spaces of covariance operators in statistics (e.g. [50] and [47] and the references there).

Section 3 gives a succinct statement of our main results in Theorems 1 and 3; these theorems provide expression rate bounds of Deep Neural Network operator emulations and of generalized polynomial chaos emulations for holomorphic maps between separable Hilbert spaces admitting *stable, biorthogonal bases*. There, a key role in building appropriate encoding and decoding operators for neural operator networks is taken by *dual bases*, which must, to some extent, be available explicitly in order to construct the encoders and decoders. Section 4 provides the proof of Theorem 1 which asserts the *existence* of operator emulations which preserve algebraic encoding and decoding error bounds of input and output data.

In Section 5, we discuss in further detail the second, novel class of operator emulations dubbed *generalized polynomial chaos operator (“gpc operator”) surrogates*. Its deterministic construction is via finitely truncated gpc expansions of holomorphic parametric maps, resulting from suitable encoders and decoders in the domain and range, respectively. Sparse gpc operator surrogates provide a construction (via “stochastic collocation”) for operator emulations, i.e., the proof of Theorem 6 on gpc operator expression rates yields an explicit deterministic construction procedure realizing the proposed operator emulations.

Finally, in Section 6 we illustrate the abstract theory with an example.

1.4 Notation

We write $\mathbb{N} = \{1, 2, \dots\}$ and $\mathbb{N}_0 = \{0, 1, 2, \dots\}$. Throughout, $C \lesssim D$ means that C can be bounded by a multiple of D , independently of parameters which C and D may depend on. $C \gtrsim D$ is defined as $D \lesssim C$, and $C \simeq D$ as $C \lesssim D$ and $C \gtrsim D$.

For a Hilbert space \mathcal{X} , the inner product of v and $w \in \mathcal{X}$ is denoted by $\langle v, w \rangle$. The space of real-valued square integrable sequences indexed over \mathbb{N} is denoted by $\ell^2(\mathbb{N})$. Complex valued, square summable sequences shall be denoted with $\ell^2(\mathbb{N}, \mathbb{C})$.

2 Setting

We fix notation and introduce, following established practice in statistical learning theory, encoder and decoder operators as stipulated in [8, 30]. Throughout, \mathcal{X} , \mathcal{Y} denote two separable Hilbert spaces over \mathbb{R} .

2.1 Framework

“Operator learning” refers, in the present paper, to procedures of emulation of (not necessarily linear) maps $\mathcal{G} : \mathcal{X} \rightarrow \mathcal{Y}$. We will address *existence and error bounds of surrogate maps* $\tilde{\mathcal{G}}$, subject to a finite number N of parameters defining $\tilde{\mathcal{G}}$. If we wish to emphasize the dependence on N , we also write $\tilde{\mathcal{G}}_N = \tilde{\mathcal{G}}$.

On suitable subsets $S \subseteq \mathcal{X}$ of admissible input data, we will consider convergence rates in N either in terms of the *worst case error*

$$\sup_{a \in S} \|\mathcal{G}(a) - \tilde{\mathcal{G}}_N(a)\|_{\mathcal{Y}} \quad (1)$$

or the *mean square error*

$$\left(\int_{a \in S} \|\mathcal{G}(a) - \tilde{\mathcal{G}}_N(a)\|_{\mathcal{Y}}^2 d\zeta(a) \right)^{1/2}, \quad (2)$$

for a measure ζ on S equipped with the Borel sigma algebra.

As in [31, 20] and the references there, we seek surrogates $\tilde{\mathcal{G}}_N$ of the form

$$\tilde{\mathcal{G}}_N := \mathcal{D} \circ \tilde{\mathbf{G}}_N \circ \mathcal{E}, \quad (3)$$

where $\mathcal{E} : \mathcal{X} \rightarrow \ell^2(\mathbb{N})$ and $\mathcal{D} : \ell^2(\mathbb{N}) \rightarrow \mathcal{Y}$ denote the so-called *encoder* and *decoder* maps. The encoder allows to express elements in \mathcal{X} in a certain (efficient) representation system. For example, \mathcal{E} could map vectors in \mathcal{X} to their Fourier coefficients w.r.t. some fixed orthonormal basis in \mathcal{X} , and \mathcal{D} could perform the opposite operation w.r.t. another fixed orthonormal basis in \mathcal{Y} . While we restrict ourselves to linear encoders/decoders, we will give a more general framework and further details in the next subsections. The parametric approximations $\tilde{\mathbf{G}}_N : \ell^2(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$ in (3) belong to hypothesis classes comprising N -term polynomial chaos expansions or deep neural networks depending on N parameters.

2.2 Representation systems

We discuss several representation systems and corresponding pairs of encoder/decoder maps. Specifically, we will admit (possibly redundant) biorthogonal systems such as Riesz bases realized by Multiresolution Analyses (MRAs) or by wavelet frames, which offer additional flexibility over mere orthogonal bases. This framework also comprises Karhunen-Loève eigenfunctions, Fourier bases and other, fully orthogonal families as particular cases. See e.g. [50, Chap. 2,5,6.3] for general discussion and constructions.

2.2.1 Frames

Constructions of concrete representation systems are often simplified when one insists on stability, but the basis property is relaxed. This leads to the concept of *frames*, which we now shortly recall. It comprises biorthogonal wavelet bases as a particular case, and allows in particular also iterative realization on unstructured simplicial partitions of polyhedra via the so-called BPX multi-level iteration [22].

Definition 1. A collection $\Psi = \{\psi_j : j \in \mathbb{N}\} \subset \mathcal{X}$ is called a *frame for \mathcal{X}* , if the *analysis operator*

$$F : \mathcal{X} \rightarrow \ell^2(\mathbb{N}) : v \mapsto (\langle v, \psi_j \rangle)_{j \in \mathbb{N}}$$

is boundedly invertible between \mathcal{X} and $\text{range}(F) \subset \ell^2(\mathbb{N})$.

The adjoint F' of the analysis operator is called the *synthesis operator*. It is given by

$$F' : \ell^2(\mathbb{N}) \rightarrow \mathcal{X} : \mathbf{v} \mapsto \mathbf{v}^\top \Psi. \quad (4)$$

The *numerical stability of frames* is quantified by the *frame bounds*

$$\Lambda_\Psi := \|F\|_{\mathcal{X} \rightarrow \ell^2}, \quad \lambda_\Psi := \inf_{0 \neq v \in \mathcal{X}} \frac{\|Fv\|_{\ell^2}}{\|v\|_{\mathcal{X}}}. \quad (5)$$

Remark 1. Since $\|F'\|_{\ell^2 \rightarrow \mathcal{X}} = \|F\|_{\mathcal{X} \rightarrow \ell^2}$, (5) implies that for all $\mathbf{v} \in \ell^2(\mathbb{N})$

$$\left\| \sum_{j \in \mathbb{N}} v_j \psi_j \right\|_{\mathcal{X}}^2 = \|F'\mathbf{v}\|_{\mathcal{X}}^2 \leq \Lambda_\Psi^2 \sum_{j \in \mathbb{N}} v_j^2. \quad (6)$$

The *frame operator* $S := F'F : \mathcal{X} \rightarrow \mathcal{X}$ is boundedly invertible, self-adjoint and positive (e.g. [12, 17, 23]) with $\|F'F\|_{\mathcal{X} \rightarrow \mathcal{X}} = \Lambda_\Psi^2$ and $\|(F'F)^{-1}\|_{\mathcal{X} \rightarrow \mathcal{X}} = \lambda_\Psi^{-2}$, [12, Lemma 5.1.5]. The collection $\tilde{\Psi} := S^{-1}\Psi$ is a frame for \mathcal{X} which is referred to as the *canonical dual frame* of Ψ . Its analysis operator is $\tilde{F} := F(F'F)^{-1}$, and its frame bounds (5) are $\lambda_{\tilde{\Psi}}^{-1}$ and $\Lambda_{\tilde{\Psi}}^{-1}$, respectively.

Crucially, we have [12, 23]

$$F'\tilde{F} = I \quad \text{on} \quad \mathcal{X}. \quad (7)$$

Whence every $v \in \mathcal{X}$ has the representation $v = \mathbf{v}^\top \tilde{\Psi}$ with $\mathbf{v} = \tilde{F}(v) \in \ell^2(\mathbb{N})$, and

$$\Lambda_{\tilde{\Psi}}^{-1} \leq \frac{\|\mathbf{v}\|_{\ell^2}}{\|v\|_{\mathcal{X}}} \leq \lambda_{\tilde{\Psi}}^{-1}. \quad (8)$$

Property (8) is in fact equivalent to $\tilde{\Psi}$ being a frame for \mathcal{X} (see, e.g., [23, Thm. 8.29 (b)]). Unless Ψ is a Riesz basis, representation of $v \in \mathcal{X}$ as $v = \mathbf{v}^\top \tilde{\Psi}$ is generally not unique: there holds $\ell^2(\mathbb{N}) = \text{ran}(F) \oplus^\perp \ker(F')$ and $\mathbf{Q} := \tilde{F}F'$ is the orthoprojector onto $\text{ran}(F)$. We refer to [12, 23] and the references there for more details.

2.2.2 Riesz Bases

Riesz bases are special cases of frames. They are defined as follows.

Definition 2. A sequence $\Psi = \{\psi_j\}_{j \in \mathbb{N}} \subset \mathcal{X}$ is a Riesz-basis of \mathcal{X} if there exists a bounded bijective operator $A : \mathcal{X} \rightarrow \mathcal{X}$ and an orthonormal basis $(e_j)_{j \in \mathbb{N}}$ such that $\psi_j = Ae_j$ for all $j \in \mathbb{N}$.

Remark 2. A frame Ψ is a Riesz basis, iff it is a basis of \mathcal{X} . Moreover, a frame Ψ is a Riesz basis of \mathcal{X} iff $\ker(F) = \{0\}$. Equivalently, $\text{ran}(F) = \ell^2$.

Every Riesz basis is a basis of \mathcal{X} , and is also a frame for \mathcal{X} : there exist *Riesz constants* $0 < \lambda_\Psi \leq \Lambda_\Psi < \infty$ such that for all $(c_j)_{j \in \mathbb{N}} \in \ell^2(\mathbb{N})$

$$\lambda_\Psi \sum_{j \in \mathbb{N}} |c_j|^2 \leq \left\| \sum_{j \in \mathbb{N}} c_j \psi_j \right\|_{\mathcal{X}}^2 \leq \Lambda_\Psi \sum_{j \in \mathbb{N}} |c_j|^2. \quad (9)$$

The canonical dual frame $\tilde{\Psi} = \{\tilde{\psi}_j\}_{j \in \mathbb{N}}$ of Ψ is also a Riesz basis of \mathcal{X} , and is referred to as the *dual basis* or the *biorthogonal system* to Ψ , since for all j , and all $k \in \mathbb{N}$ holds $\langle \psi_j, \tilde{\psi}_k \rangle = \delta_{kj}$. We refer to [12, Sec. 5] for further details and proofs.

Remark 3. Constructions of piecewise polynomial Riesz bases for Sobolev spaces in polytopal domains $D \subset \mathbb{R}^d$ are available (e.g. [19, 48] and the references there).

2.2.3 Orthonormal Bases

Orthonormal bases (ONBs) are particular instances of frames and Riesz bases: if Ψ is an orthonormal basis of \mathcal{X} , then $\tilde{\Psi} = \Psi$. This includes, for example, Fourier-bases [23], Daubechies - type wavelets [18] and orthogonal polynomials [49]. It also includes orthonormal bases obtained by principal component analyses associated with a covariance operator corresponding to a Gaussian measure on \mathcal{X} as commonly used in statistical learning theory (e.g. [47]). Such bases are generally not explicitly available, but may be approximately calculated in practice.

Example 1. Denote by \mathbb{T}^d the d -dimensional torus. The Fourier basis Ψ is an ONB of $\mathcal{X} = L^2(\mathbb{T}^d)$. The analysis and synthesis operators F, F' are in this case the Fourier transform and its inverse transform.

2.3 Encoder and decoder

In the following we use the notation

$$\Psi_{\mathcal{X}} = (\psi_j)_{j \in \mathbb{N}}, \quad \tilde{\Psi}_{\mathcal{X}} = (\tilde{\psi}_j)_{j \in \mathbb{N}}, \quad \Psi_{\mathcal{Y}} = (\eta_j)_{j \in \mathbb{N}}, \quad \tilde{\Psi}_{\mathcal{Y}} = (\tilde{\eta}_j)_{j \in \mathbb{N}}. \quad (10)$$

to denote frames and their dual frames of \mathcal{X} , \mathcal{Y} respectively. With the corresponding analysis operators $F_{\mathcal{X}}$, $F_{\mathcal{Y}}$ the encoder/decoder pair in (3) is defined by the analysis and synthesis operators which are given by

$$\mathcal{E} := \tilde{F}_{\mathcal{X}} = \begin{cases} \mathcal{X} \rightarrow \ell^2(\mathbb{N}) \\ x \mapsto (\langle x, \tilde{\Psi}_j \rangle)_{j \in \mathbb{N}}, \end{cases} \quad \mathcal{D} := F'_{\mathcal{Y}} = \begin{cases} \ell^2(\mathbb{N}) \rightarrow \mathcal{Y} \\ (y_j)_{j \in \mathbb{N}} \mapsto \sum_{j \in \mathbb{N}} y_j \eta_j. \end{cases} \quad (11)$$

Remark 4. If $\Psi_{\mathcal{X}}$, $\Psi_{\mathcal{Y}}$ are Riesz bases of \mathcal{X} , \mathcal{Y} , respectively, then the encoder $\mathcal{E} : \mathcal{X} \rightarrow \ell^2(\mathbb{N})$ and decoder $\mathcal{D} : \ell^2(\mathbb{N}) \rightarrow \mathcal{Y}$ in (11) are boundedly invertible operators.

Remark 5. Encoders and decoders with rate-optimal performance for subsets $\mathcal{X}^s \subset \mathcal{X}$ are obtained from *n-term truncation*. In the most straight forward case, *linear n-term truncation* of representations $u \in \mathcal{X}$ will ensure rate-optimal approximations for \mathcal{X}^s being classical Sobolev or Besov spaces with summability index $p \geq 2$. It is well-known that MRAs which constitute Riesz bases in \mathcal{X} afford *nonlinear encoding by coefficient thresholding*. This could also be referred to as *adaptive encoding*. Such encoders are known to ensure rate-optimal approximations for a given budget of n coefficients for considerably larger set $\mathcal{X}^s \subset \mathcal{X}$, comprising in particular Besov spaces in \mathbb{D} with summability indices $q \in (0, 1]$ (see, e.g., [50, 51]).

2.4 Smoothness scales

Our analysis will require subspaces of \mathcal{X} and \mathcal{Y} exhibiting ‘‘extra smoothness’’. Typical instances are Sobolev and Besov spaces with ‘‘ s -th weak derivatives bounded’’. It is well-known, that membership in such function classes can be encoded via weighted summability of expansion coefficients.

To formalize this, for a fixed strictly positive, monotonically decreasing weighted sequence $\mathbf{w} = (w_j)_{j \in \mathbb{N}}$ such that $\mathbf{w}^{1+\varepsilon} \in \ell^1(\mathbb{N})$ for all $\varepsilon > 0$, we introduce scales of Hilbert spaces $\mathcal{X}^s \subseteq \mathcal{X}$, $\mathcal{Y}^t \subseteq \mathcal{Y}$ for $s, t \geq 0$ with norms¹

$$\|x\|_{\mathcal{X}^s}^2 := \sum_{j \in \mathbb{N}} \langle x, \tilde{\Psi}_j \rangle^2 w_j^{-2s}, \quad \|y\|_{\mathcal{Y}^t}^2 := \sum_{j \in \mathbb{N}} \langle y, \tilde{\eta}_j \rangle^2 w_j^{-2t}. \quad (12)$$

Lemma 1. *Let $s \geq 0$. The space $\mathcal{X}^s = \{x \in \mathcal{X} : \|x\|_{\mathcal{X}^s} < \infty\}$ is a Hilbert space with inner product $\langle x, x' \rangle_{\mathcal{X}^s} = \sum_{j \in \mathbb{N}} \langle x, \tilde{\Psi}_j \rangle \langle x', \tilde{\Psi}_j \rangle w_j^{-2s}$.*

Proof. Clearly $\langle \cdot, \cdot \rangle_{\mathcal{X}^s}$ defines an inner product on the set \mathcal{X}^s compatible with the norm $\|\cdot\|_{\mathcal{X}^s}$. We need to show that \mathcal{X}^s is closed w.r.t. this norm.

Denote $\mathcal{E} = \tilde{F}_{\mathcal{X}}$, $\mathcal{D} = F'_{\mathcal{Y}}$ and recall that $\mathcal{E}(\mathcal{X})$ is a closed subspace of $\ell^2(\mathbb{N})$ due to the property $\|\mathcal{E}(x)\|_{\ell^2(\mathbb{N})} \geq \lambda_{\mathcal{X}} \|x\|_{\mathcal{X}}$. Furthermore, denote in the following

¹ All of the following remains valid if we use distinct weight sequences $(w_{\mathcal{X},j})_{j \in \mathbb{N}}$ and $(w_{\mathcal{Y},j})_{j \in \mathbb{N}}$ to define \mathcal{X}^s , \mathcal{Y}^t respectively. We refrain from doing so for simplicity of presentation.

by $\ell_s^2(\mathbb{N})$ the sequence space of $\mathbf{x} \in \ell^2(\mathbb{N})$ such that $\|\mathbf{x}\|_{\ell_s^2}^2 := \sum_{j \in \mathbb{N}} x_j^2 w_j^{-2s} < \infty$. Note that $\ell_s^2(\mathbb{N})$ is closed, and $\|\mathcal{E}(x)\|_{\ell_s^2} = \|x\|_{\mathcal{X}^s}$.

Take a Cauchy sequence $(x_n)_{n \in \mathbb{N}} \subseteq \mathcal{X}^s$ w.r.t. $\|\cdot\|_{\mathcal{X}^s}$. Then $(\mathcal{E}(x_n))_{n \in \mathbb{N}} \subseteq \ell^2(\mathbb{N})$ is a Cauchy-sequence w.r.t. $\ell_s^2(\mathbb{N})$, and since $\ell_s^2(\mathbb{N})$ is closed, there exists $\mathbf{x} \in \ell_s^2(\mathbb{N}) \subseteq \ell^2(\mathbb{N})$ such that $\mathcal{E}(x_n) \rightarrow \mathbf{x} \in \ell_s^2(\mathbb{N})$. Since $\mathcal{E}(\mathcal{X}) \subseteq \ell^2(\mathbb{N})$ is closed, \mathbf{x} belongs to $\mathcal{E}(\mathcal{X}) \subseteq \ell^2(\mathbb{N})$. Since \mathcal{D} maps from $\ell^2(\mathbb{N})$ to \mathcal{X} , $\tilde{x} := \mathcal{D}(\mathbf{x}) \in \mathcal{X}$ is well-defined and belongs to \mathcal{X}^s since

$$\|\tilde{x}\|_{\mathcal{X}^s} = \|\mathbf{x}\|_{\ell_s^2} < \infty.$$

Moreover, using that $\mathcal{E} \circ \mathcal{D}$ is the identity on $\mathcal{E}(\mathcal{X})$ (cp. (7))

$$\|x_n - \tilde{x}\|_{\mathcal{X}^s} = \|\mathcal{E}(x_n) - \mathcal{E}(\tilde{x})\|_{\ell_s^2} = \|\mathcal{E}(x_n) - \mathcal{E}(\mathcal{D}(\mathbf{x}))\|_{\ell_s^2} = \|\mathcal{E}(x_n) - \mathbf{x}\|_{\ell_s^2} \rightarrow 0$$

as $n \rightarrow \infty$. This shows that \mathcal{X}^s is closed w.r.t. $\|\cdot\|_{\mathcal{X}^s}$. \square

Remark 6. For ONBs $\Psi_{\mathcal{X}} = \{\psi_j\}_{j \in \mathbb{N}}$ and $\Psi_{\mathcal{Y}} = \{\eta_j\}_{j \in \mathbb{N}}$ of \mathcal{X} and \mathcal{Y} , the sequences $(w_j^s \psi_j)_{j \in \mathbb{N}}$ and $(w_j^t \eta_j)_{j \in \mathbb{N}}$ form ONBs of \mathcal{X}^s , \mathcal{Y}^t respectively.

The Hilbert spaces \mathcal{X}^s and \mathcal{Y}^t are included in their (unique, [37]) complexified versions $\mathcal{X}_{\mathbb{C}}^s = \{1, i\} \otimes \mathcal{X}^s$ and $\mathcal{Y}_{\mathbb{C}}^t = \{1, i\} \otimes \mathcal{Y}^t$, for which the encoder and decoder in (11) act on weighted, complex sequence spaces.

Remark 7. The results of this paper can be extended to the case where \mathcal{X} and \mathcal{Y} are separable Hilbert spaces over the coefficient field \mathbb{C} . We do not elaborate details in order to avoid having to distinguish between two cases in the following.

3 Main results

Our goal is to approximate maps \mathcal{G} from (subsets of) \mathcal{X} into \mathcal{Y} . In the following denote by $\Psi_{\mathcal{X}}$, $\Psi_{\mathcal{Y}}$ fixed frames of the separable Hilbert spaces \mathcal{X} , \mathcal{Y} as in (10), and let the encoder $\mathcal{E} : \mathcal{X} \rightarrow \ell^2(\mathbb{N})$, decoder $\mathcal{D} : \ell^2(\mathbb{N}) \rightarrow \mathcal{Y}$ be as in (11). With

$$U := [-1, 1]^{\mathbb{N}},$$

and \mathbf{w} as in Section 2.4, for $s > \frac{1}{2}$, set

$$\sigma_r^s := \begin{cases} U \rightarrow \mathcal{X} \\ \mathbf{y} \mapsto r \sum_{j \in \mathbb{N}} w_j^s y_j \Psi_j. \end{cases} \quad (13)$$

The condition $s > \frac{1}{2}$ ensures that the coefficient sequence $(r w_j^s y_j)_{j \in \mathbb{N}}$ belongs to $\ell^2(\mathbb{N})$ so that σ_r^s is well-defined as a mapping from U to \mathcal{X} (cp. (4)). For $s > \frac{1}{2}$ we then introduce the following ‘‘Cubes’’ in \mathcal{X}

$$\tilde{C}_r^s(\mathcal{X}) := \{\sigma_r^s(\mathbf{y}) : \mathbf{y} \in U\}$$

and additionally for $s \geq 0$

$$\begin{aligned} C_r^s(\mathcal{X}) &:= \{a \in \mathcal{X} : \mathcal{E}(a) \in \times_{j \in \mathbb{N}} [-rw_j^s, rw_j^s]\} \\ &= \left\{ a \in \mathcal{X} : \sup_{j \in \mathbb{N}} |\langle a, \tilde{\Psi}_j \rangle| w_j^{-s} \leq r \right\}. \end{aligned} \quad (14)$$

The sets $C_r^s(\mathcal{X})$ will serve as the domains on which \mathcal{G} is to be approximated.

Remark 8. Note that $C_r^s(\mathcal{X}) \subseteq \tilde{C}_r^s(\mathcal{X})$. If $\Psi_{\mathcal{X}} = (\psi_j)_{j \in \mathbb{N}}$ is a Riesz-basis, then (due to the basis property) the $\ell^2(\mathbb{N})$ -sequence of expansion coefficients of any element $a \in \mathcal{X}$ w.r.t. $\Psi_{\mathcal{X}}$ is unique. Due to (7) and (13) it thus must hold $\mathcal{E}(\sigma_r^s(\mathbf{y})) = (rw_j^s y_j)_{j \in \mathbb{N}}$ for all $\mathbf{y} \in U$. This implies $\tilde{C}_r^s(\mathcal{X}) = C_r^s(\mathcal{X})$. For general frames, this does not hold, since $\mathcal{E}(\sigma_r^s(\mathbf{y}))$ need not belong to $\times_{j \in \mathbb{N}} [-rw_j^s, rw_j^s]$ for $\mathbf{y} \in U$.

Remark 9. Let $s' \geq 0$ and $s > s' + 1/2$. Then $C_r^s(\mathcal{X}) \subset \mathcal{X}^{s'}$, since for $a \in C_r^s(\mathcal{X})$

$$\|a\|_{\mathcal{X}^{s'}}^2 = \sum_{j \in \mathbb{N}} \langle a, \tilde{\Psi}_j \rangle^2 w_j^{-2s'} \leq r^2 \sum_{j \in \mathbb{N}} w_j^{2(s-s')} < \infty,$$

due to $(w_j)_{j \in \mathbb{N}} \in \ell^{1+\varepsilon}(\mathbb{N})$ for any $\varepsilon > 0$.

We shall work under the *assumption that \mathcal{G} allows a complex differentiable extension to some open superset of $\tilde{C}_r^s(\mathcal{X})$ in $\mathcal{X}_{\mathbb{C}}$* :

Assumption 1. *There exist $s > 1$, $t > 0$ and an open set $O_{\mathbb{C}} \subseteq \mathcal{X}_{\mathbb{C}}$ containing $\tilde{C}_r^s(\mathcal{X})$ such that $\mathcal{G} : O_{\mathbb{C}} \rightarrow \mathcal{Y}_{\mathbb{C}}$ is holomorphic and $\sup_{a \in O_{\mathbb{C}}} \|\mathcal{G}(a)\|_{\mathcal{Y}_{\mathbb{C}}} \leq M$.*

We emphasize that holomorphy, i.e. Fréchet differentiability of $\mathcal{G} : O_{\mathbb{C}} \rightarrow \mathcal{Y}_{\mathbb{C}}$, in Assumption 1 is understood w.r.t. the topologies of $\mathcal{X}_{\mathbb{C}}$ and $\mathcal{Y}_{\mathbb{C}}$ (and *not* some stronger topologies such as $\mathcal{X}_{\mathbb{C}}^{s-1/2}$ and $\mathcal{Y}_{\mathbb{C}}^t$).

3.1 Worst-case error for NN operator surrogates

Our first main result states that a holomorphic operator \mathcal{G} as in Assumption 1 can be uniformly approximated on $C_r^s(\mathcal{X})$ by a NN surrogate of the form $\mathcal{D} \circ \tilde{\mathbf{G}} \circ \mathcal{E}$, where $\tilde{\mathbf{G}}$ is a ReLU NN. More precisely, $\tilde{\mathbf{G}}$ is a function of the form

$$\tilde{\mathbf{G}} = A_L \circ \text{ReLU} \circ A_{L-1} \cdots \circ A_1 \circ \text{ReLU} \circ A_0 \quad (15)$$

where the application of $\text{ReLU}(x) := \max\{0, x\}$ is understood componentwise, and each $A_j : \mathbb{R}^{n_j} \rightarrow \mathbb{R}^{n_{j+1}}$ is an affine transformation of the form $A_j(x) = W_j x + b_j$ with $W_j \in \mathbb{R}^{n_{j+1} \times n_j}$, $b_j \in \mathbb{R}^{n_{j+1}}$. The entries of the weights W_j and the biases b_j are parameters that determine the NN. It is common practice to determine these

parameters by NN “training”, where some regression procedure on input-output data pairs with the map induced by $\tilde{\mathbf{G}}$ of the form (15) is used to find choices of the weights and biases. Alternatively, concrete constructions of the NN parameters W_j , b_j based on *a-priori specified samples of input-output data pairs* are sometimes proposed (e.g. [25]). The presently developed, constructive proofs are of this type. We refer to the number of nonzero entries of all W_j and b_j , i.e.

$$\text{size}(\tilde{\mathbf{G}}) := \sum_{0 \leq j \leq L} \|W_j\|_0 + \|b_j\|_0 \quad (16)$$

as the *size of the NN in (15)*. In other words, the “size” of the network is the number of trainable network parameters.

Remark 10. Any realization of a NN $\tilde{\mathbf{G}}$ of the form (15) represents a map from $\mathbb{R}^{n_0} \rightarrow \mathbb{R}^{n_{L+1}}$. Throughout we will also understand $\tilde{\mathbf{G}}$ as a function from $\ell^2(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$: Formally replacing A_0 with an infinite matrix in $\mathbb{R}^{n_1 \times \infty}$ and A_L with an infinite matrix in $\mathbb{R}^{\infty \times n_L}$ by filling up the (infinitely many) entries with zeros, $\tilde{\mathbf{G}}$ becomes a mapping from $\ell^2(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$. This new network is of the same size as the original one, since we only add zero entries (cp. (16)). Note that the function it realizes is simply obtained by padding the original network input and output with zeros.

The composition $\mathcal{D} \circ \tilde{\mathbf{G}} \circ \mathcal{E}$ is well-defined in the sense of Rmk. 10.

Theorem 1. *Let Assumption 1 be satisfied with $s > 1$, $t > 0$. Fix $\delta > 0$ (arbitrarily small) and $r > 0$. Then there exists a constant $C > 0$ such that for every $N \in \mathbb{N}$ there exists a ReLU NN $\tilde{\mathbf{G}}_N$ of size $O(N)$ such that*

$$\sup_{a \in C_r^s(\mathcal{X})} \|\mathcal{G}(a) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathcal{E}(a)))\|_{\mathcal{Y}} \leq CN^{-\min\{s-1, t\} + \delta}. \quad (17)$$

Next, introduce the closed ball of radius r in \mathcal{X}^s

$$B_r(\mathcal{X}^s) := \{a \in \mathcal{X}^s : \|a\|_{\mathcal{X}^s} \leq r\}.$$

Since for any $\varepsilon > 0$, we have

$$B_r(\mathcal{X}^s) \subseteq C_r^s(\mathcal{X}) \subseteq B_{r_\varepsilon}(\mathcal{X}^{s-\frac{1}{2}-\varepsilon})$$

with $r_\varepsilon := r(\sum_{j \in \mathbb{N}} w_j^{1+2\varepsilon})^{1/2} < \infty$ (cp. (12), (14) and Rmk. 9), we trivially get the following:

Corollary 1. *Consider the setting of Theorem 1. Then there exists a constant $C > 0$ such that for every $N \in \mathbb{N}$ there exists a ReLU NN $\tilde{\mathbf{G}}_N$ of size $O(N)$ such that*

$$\sup_{a \in B_r(\mathcal{X}^s)} \|\mathcal{G}(a) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathcal{E}(a)))\|_{\mathcal{Y}} \leq CN^{-\min\{s-1, t\} + 1 + \delta}.$$

Remark 11. Clearly $B_r(\mathcal{X}^s)$ is a proper subset of $C_r^s(\mathcal{X})$. However, in general there is no $s' > s$ and $r' > 0$ such that $B_{r'}(\mathcal{X}^{s'}) \subseteq C_r^s(\mathcal{X})$, thus we cannot use Theorem 1 to improve the convergence rate on the ball $B_r(\mathcal{X}^s) \subset \mathcal{X}^s$.

Our results provide sufficient conditions under which operator nets can overcome the curse of dimensionality, since we allow the operators to have infinite dimensional domains. The proof hinges on certain ‘‘sparsity’’ properties of the encoded coefficients. Neural networks are able to exploit this form of intrinsic low-dimensionality and in this way elude the curse of dimension. However, we emphasize that it is the intrinsic sparsity of the considered functions, rather than specific properties of NNs that lead to these statements. The same convergence rate can be obtained with other methods such as sparse-grid polynomial interpolation or low-rank tensor approximation, as we discuss in Section 3.3 ahead.

3.2 Mean-square error for NN operator surrogates

We can improve the operator approximation rate of Theorem 1, if we measure the error in a mean-square sense. To this end assume that $\Psi_{\mathcal{X}}$ is a Riesz-basis, and let $\mu := \otimes_{j \in \mathbb{N}} \frac{\lambda}{2}$ be the uniform probability measure on $U := \times_{j \in \mathbb{N}} [-1, 1]$ equipped with its product Borel sigma algebra, where λ stands for the Lebesgue measure in \mathbb{R} . By Rmk. 8, the pushforward $(\sigma_r^s)_\# \mu$ of μ under σ_r^s then constitutes a measure on $C_r^s(\mathcal{X})$.

Theorem 2. *Assume that $\Psi_{\mathcal{X}}$ is a Riesz basis. Let Assumption 1 be satisfied with $s > 1$, $t > 0$. Fix $\delta > 0$ (arbitrarily small) and $r > 0$. Then there exists a constant $C > 0$ such that for every $N \in \mathbb{N}$ there exists a ReLU NN $\tilde{\mathbf{G}}_N$ of size $O(N)$ such that*

$$\|\mathcal{G} - \mathcal{D} \circ \tilde{\mathbf{G}}_N \circ \mathcal{E}\|_{L^2(C_r^s(\mathcal{X}), (\sigma_r^s)_\# \mu; \mathcal{D})} \leq CN^{-\min\{s-\frac{1}{2}, t\} + \delta}. \quad (18)$$

3.3 Worst-case error for gpc operator surrogates

For our third main result, instead of a NN $\tilde{\mathbf{G}}_N$ we use a multivariate polynomial $p_N : \mathbb{R}^n \rightarrow \mathbb{R}^m$. The operator surrogate then takes the form $\mathcal{D} \circ p_N \circ \mathcal{E}$, where the composition is again understood as truncating the output of \mathcal{E} after the first n parameters, and padding the output of p_N with infinitely many zeros (cp. Rmk. 10). The advantage over the NN operator surrogate in Theorem 1 is, that, while we achieve the same convergence rate, the proof is entirely constructive, and one can explicitly compute p_N as an interpolation polynomial. Hence no ‘‘training’’ is required, and one obtains (higher-order) deterministic generalizations bounds, rather than (low-order) probabilistic bounds as is common in statistical learning theory.

Contrary to Section 3.2, we now allow for $\Psi_{\mathcal{X}}$ again to be a general frame.

Theorem 3. Consider the setting of Theorem 1. Then there is a constant $C > 0$ such that for every $N \in \mathbb{N}$ there exists a multivariate polynomial p_N such that

$$\sup_{a \in C_r^s(\mathcal{X})} \|\mathcal{G}(a) - \mathcal{D}(p_N(\mathcal{E}(a)))\|_{\mathcal{Y}} \leq CN^{-\min\{s-1,t\}+\delta}.$$

Furthermore, p_N belongs to an N -dimensional space of multivariate polynomials. Its components are interpolation polynomials, whose computation requires the evaluation of $\langle \mathcal{G}(a), \tilde{\eta}_j \rangle$ at at most N tuples $(a, j) \in C_r^s(\mathcal{X}) \times \mathbb{N}$.

Before coming to the proofs, let us make one further remark. Corollary 1 states that we can *uniformly* approximate any holomorphic \mathcal{G} as in Assumption 1 with a NN operator surrogate on the ball $B_r(\mathcal{X}^s)$; an analogous corollary also holds for gpc operator surrogates. Since \mathcal{X}^s is an infinite dimensional Hilbert space, $B_r(\mathcal{X}^s)$ is not compact in \mathcal{X}^s . Thus the image of $B_r(\mathcal{X}^s)$ will in general also not be compact in \mathcal{Y}^t , for example in case $\mathcal{X} = \mathcal{Y}^t$ and $\mathcal{G} : \mathcal{X} \rightarrow \mathcal{Y}^t$ is the identity (which satisfies Assumption 1). Therefore it seems counterintuitive that we can uniformly approximate \mathcal{G} using a NN with only *finitely* many parameters (or a polynomial of finite degree). This is possible, because the approximation rate is stated not in the norm of \mathcal{Y}^t , but in the weaker norm of \mathcal{Y} , and in fact a ball in \mathcal{Y}^t is compact in \mathcal{Y} :

Lemma 2. For every $0 \leq t' < t < \infty$, the set $B_r(\mathcal{Y}^t)$ is compact in $\mathcal{Y}^{t'}$.

Proof. Let $(a_n)_{n \in \mathbb{N}}$ be a sequence in $B_r(\mathcal{Y}^t)$ and denote $\mathbf{x}_n = \mathcal{E}(a_n)$, where $\mathbf{x}_n = (x_{n,j})_{j \in \mathbb{N}} \in \ell^2(\mathbb{N})$. Then, due to $a_n \in B_r(\mathcal{Y}^t)$ holds $\sum_{j \in \mathbb{N}} x_{n,j}^2 w_j^{-2t} \leq r$ for all $n \in \mathbb{N}$ and, in particular,

$$x_{n,j} \in [-rw_j^t, rw_j^t] \quad \forall n, j \in \mathbb{N}.$$

Compactness of $[-rw_1^t, rw_1^t]$ implies the existence of a subsequence $(\mathbf{x}_{1,n})_{n \in \mathbb{N}}$ of $(\mathbf{x}_n)_{n \in \mathbb{N}}$, such that $(x_{1,n,1})_{n \in \mathbb{N}}$ is a Cauchy sequence in $[-rw_1^t, rw_1^t]$. Inductively, let $(\mathbf{x}_{k,n})_{n \in \mathbb{N}}$ be a subsequence of $(\mathbf{x}_{k-1,n})_{n \in \mathbb{N}}$ such that $(x_{k,n,k})_{n \in \mathbb{N}}$ is a Cauchy sequence in $[-rw_k^t, rw_k^t]$. Then $\tilde{\mathbf{x}}_n := \mathbf{x}_{n,n}$ defines a subsequence of $(\mathbf{x}_n)_{n \in \mathbb{N}}$ with the property that $(\tilde{x}_{n,j})_{n \in \mathbb{N}}$ is a Cauchy sequence for each $j \in \mathbb{N}$. Denote the corresponding sequence in $\mathcal{Y}^{t'}$ by $(\tilde{a}_n)_{n \in \mathbb{N}}$.

Now fix $\varepsilon > 0$ arbitrary. Let $N(\varepsilon) \in \mathbb{N}$ be so large that $w_{N(\varepsilon)}^{2(t-t')} < \frac{\varepsilon}{4r^2}$. Then for all $n \in \mathbb{N}$

$$\sum_{j > N(\varepsilon)} x_{n,j}^2 w_j^{-2t'} \leq w_{N(\varepsilon)}^{2(t-t')} \sum_{j > N(\varepsilon)} x_{n,j}^2 w_j^{-2t} \leq \frac{\varepsilon}{4}.$$

Next, since $(\tilde{x}_{n,j})_{n \in \mathbb{N}}$ is a Cauchy sequence for each $j \leq N(\varepsilon)$, there exists $M(\varepsilon) \in \mathbb{N}$ so large that

$$\sum_{j=1}^{N(\varepsilon)} |x_{m,j} - x_{n,j}|^2 w_j^{-2t'} < \frac{\varepsilon}{2} \quad \forall m, n \geq M(\varepsilon).$$

Then for all $m, n \geq M(\varepsilon)$ we have

$$\|\tilde{a}_n - \tilde{a}_m\|_{\mathcal{Y}^{t'}} \leq \sum_{j=1}^{N(\varepsilon)} |x_{m,j} - x_{n,j}|^2 w_j^{-2t'} + 2 \sum_{j>N(\varepsilon)} (x_{m,j}^2 + x_{n,j}^2) w_j^{-2t'} \leq \varepsilon.$$

Thus $(\tilde{a}_n)_{n \in \mathbb{N}}$ is a Cauchy sequence in $\mathcal{Y}^{t'}$. This concludes the proof. \square

4 Proof of Theorem 1 and Theorem 2

With $s > 1$ and σ_r^s as in (13) let in the following

$$\mathbf{G} := \tilde{\mathbf{F}}_{\mathcal{Y}} \circ \mathcal{G} \circ \sigma_r^s. \quad (19)$$

Since $\sigma_r^s : U \rightarrow \mathcal{X}$, $\mathcal{G} : \mathcal{X} \rightarrow \mathcal{Y}$ and $\tilde{\mathbf{F}}_{\mathcal{Y}} : \mathcal{Y} \rightarrow \ell^2(\mathbb{N})$ we have $\mathbf{G} : U \rightarrow \ell^2(\mathbb{N})$. Moreover, due to $\mathcal{D} = \mathbf{F}'_{\mathcal{Y}}$ and (7) we have that $\mathcal{D} \circ \tilde{\mathbf{F}}_{\mathcal{Y}}$ is the identity on \mathcal{Y} and thus

$$u(\mathbf{y}) := (\mathcal{D} \circ \mathbf{G})(\mathbf{y}) = \mathcal{G}(\sigma_r^s(\mathbf{y})) \quad (20)$$

is well-defined for $\mathbf{y} \in U$. To prove Theorem 1 we first show that $\mathbf{G} : U \rightarrow \mathcal{X}$ can be approximated.

4.1 Auxiliary results

The following lemma states that the holomorphic function $\mathcal{G} : O_{\mathbb{C}} \rightarrow \mathcal{Y}$ from Assumption 1, is actually also holomorphic as a mapping to the more regular space $\mathcal{Y}^{t'}$ for any $t' < t$:

Lemma 3. *Let Assumption 1 be satisfied. Then for every $t' \in [0, t)$, the map $\mathcal{G} : O_{\mathbb{C}} \rightarrow \mathcal{Y}^{t'}$ is holomorphic.*

Proof. By Assumption 1, for every $a \in O_{\mathbb{C}}$

$$\|\mathcal{G}(a)\|_{\mathcal{Y}^{t'}}^2 = \sum_{j \in \mathbb{N}} |\langle \mathcal{G}(a), \tilde{\eta}_j \rangle|^2 w_j^{-2t'} \leq M^2$$

and for every $\tilde{\eta}_j \in \tilde{\Psi}$, $j \in \mathbb{N}$, the map

$$O_{\mathbb{C}} \rightarrow \mathbb{C} : a \mapsto \langle \mathcal{G}(a), \tilde{\eta}_j \rangle$$

is holomorphic. Thus for each $n \in \mathbb{N}$

$$\mathcal{G}_n : O_{\mathbb{C}} \rightarrow \mathcal{Y}^{t'} : a \mapsto \sum_{j=1}^n \langle \mathcal{G}(a), \tilde{\eta}_j \rangle \eta_j$$

is holomorphic. In addition,

$$\begin{aligned}
\limsup_{n \rightarrow \infty} \sup_{a \in O_{\mathbb{C}}} \|\mathcal{G}(a) - \mathcal{G}_n(a)\|_{\mathcal{Y}_{\mathbb{C}}^{t'}}^2 &= \limsup_{n \rightarrow \infty} \sup_{a \in O_{\mathbb{C}}} \sum_{j > n} |\langle \mathcal{G}(a), \tilde{\eta}_j \rangle|^2 w_j^{-2t'} \\
&\leq \limsup_{n \rightarrow \infty} \sup_{j > n} w_j^{2(t-t')} \sup_{a \in O_{\mathbb{C}}} \sum_{j > n} |\langle \mathcal{G}(a), \tilde{\eta}_j \rangle|^2 w_j^{-2t} \\
&\leq \limsup_{n \rightarrow \infty} \sup_{j > n} w_j^{2(t-t')} M^2 = 0.
\end{aligned}$$

Thus we have uniform convergence $\mathcal{G}_n \rightarrow \mathcal{G}$ in the topology of $\mathcal{Y}_{\mathbb{C}}^{t'}$ which implies holomorphy of $\mathcal{G} : O_{\mathbb{C}} \rightarrow \mathcal{Y}_{\mathbb{C}}^{t'}$ as claimed, see [26, Theorem 3.1.5c]. \square

It is well known, that algebraic decay of the ‘‘input’’ sequence $w_j^s \psi_j$ in (13) is inherited by the Legendre coefficients of the ‘‘output’’ $u(\mathbf{y})$, see for example [10] and the earlier works [14, 15] for the analysis for some specific choices of \mathcal{G} , and [13] for the general analysis. To provide a statement of this type, we first introduce some notation and denote by L_n the n -th Legendre polynomial normalized such that $\frac{1}{2} \int_{-1}^1 L_n(x)^2 dx = 1$. For a multiindex

$$\mathbf{v} \in \mathcal{F} := \{(\mathbf{v}_j)_{j \in \mathbb{N}_0} \in \mathbb{N}_0^{\mathbb{N}} : |\mathbf{v}| < \infty\}$$

we write for $\mathbf{y} = (y_j)_{j \in \mathbb{N}} \in U = [-1, 1]^{\mathbb{N}}$

$$L_{\mathbf{v}}(\mathbf{y}) := \prod_{j \in \text{supp } \mathbf{v}} L_{\mathbf{v}_j}(y_j),$$

where an empty product is understood as constant 1. With the infinite product measure $\mu = \otimes_{j \in \mathbb{N}} \frac{\lambda}{2}$ on $U = [-1, 1]^{\mathbb{N}}$, we then have $\|L_{\mathbf{v}}\|_{L^2(U, \mu)} = 1$. As is well known, e.g., [44, Theorem 2.12], $(L_{\mathbf{v}})_{\mathbf{v} \in \mathcal{F}}$ is an orthonormal basis of $L^2(U, \mu)$. Moreover, there holds the bound

$$\|L_{\mathbf{v}}\|_{L^\infty(U)} \leq \prod_{j \in \mathbb{N}} (1 + 2\mathbf{v}_j)^{1/2} \quad (21)$$

for all $\mathbf{v} \in \mathcal{F}$, see [38, §18.2(iii) and §18.3] with our normalization of $L_{\mathbf{v}}$.

We work with the following theorem, which, apart from giving an algebraically decaying upper bound on the Legendre coefficients, additionally provides information on the structure of these upper bounds. It is essentially [55, Theorem 2.2.10] stated in the current setting. To formulate the result, we first introduce an order-relation on multi-indices. For $\boldsymbol{\mu} = (\mu_j)_{j \in \mathbb{N}}$ and $\mathbf{v} = (\mathbf{v}_j)_{j \in \mathbb{N}} \in \mathcal{F}$ we write $\boldsymbol{\mu} \leq \mathbf{v}$ iff $\mu_j \leq \mathbf{v}_j$ for all $j \in \mathbb{N}$. A set $\Lambda \subseteq \mathcal{F}$ is *downward closed* iff $\mathbf{v} \in \Lambda$ implies $\boldsymbol{\mu} \in \Lambda$ whenever $\boldsymbol{\mu} \leq \mathbf{v}$.

Theorem 4. *Let Assumption 1 be satisfied with some $s > 1$ and $t > 0$. Fix $\tau > 0$, $p \in (\frac{1}{s}, 1]$ and $t' \in [0, t)$. For $\mathbf{v} \in \mathcal{F}$, set $\omega_{\mathbf{v}} := \prod_{j \in \text{supp } \mathbf{v}} (1 + 2\mathbf{v}_j)$ for all $\mathbf{v} \in \mathcal{F}$ (empty products are equal to 1). Then there exists $C > 0$ and a sequence $(a_{\mathbf{v}})_{\mathbf{v} \in \mathcal{F}} \in \ell^p(\mathcal{F})$ of positive numbers such that*

(i) for each $\mathbf{v} \in \mathcal{F}$

$$\omega_{\mathbf{v}}^\tau \left\| \int_U L_{\mathbf{v}}(\mathbf{y}) u(\mathbf{y}) d\mu(\mathbf{y}) \right\|_{\mathcal{Y}^{t'}} \leq C a_{\mathbf{v}}, \quad (22)$$

(ii) there exists an enumeration $(\mathbf{v}_i)_{i \in \mathbb{N}}$ of \mathcal{F} such that $(a_{\mathbf{v}_i})_{i \in \mathbb{N}}$ is monotonically decreasing, the set $\Lambda_N := \{a_{\mathbf{v}_i} : i \leq N\} \subseteq \mathcal{F}$ is downward closed for each $N \in \mathbb{N}$, and additionally

$$m(\Lambda_N) = O(\log(|\Lambda_N|)), \quad d(\Lambda_N) = o(\log(|\Lambda_N|)) \quad \text{as } N \rightarrow \infty. \quad (23)$$

(iii) the following expansion holds with absolute and uniform convergence:

$$\forall \mathbf{y} \in U : \quad u(\mathbf{y}) = \sum_{\mathbf{v} \in \mathcal{F}} L_{\mathbf{v}}(\mathbf{y}) \int_U L_{\mathbf{v}}(\mathbf{x}) u(\mathbf{x}) \, d\mu(\mathbf{x}) \in \mathcal{Y}'.$$

Proof. By definition $u(\mathbf{y}) = \mathcal{G}(\sum_{j \in \mathbb{N}} y_j w_j^s \psi_j)$ for all $\mathbf{y} \in U$. Our choice of the sequence \mathbf{w} guarantees $\sum_{j \in \mathbb{N}} \|w_j^s \psi_j\|_{\mathcal{X}}^p \leq \Lambda_{\Psi}^{p/2} \sum_{j \in \mathbb{N}} w_j^{sp} < \infty$, where we used that $\|\psi_j\|_{\mathcal{X}} \leq \Lambda_{\Psi}^{1/2}$ by (6). Moreover by Lemma 3 the map $\mathcal{G} : O_{\mathbb{C}} \rightarrow \mathcal{Y}'_{\mathbb{C}}$ is holomorphic and uniformly bounded in norm by M , where by Assumption 1 the set $\{\sum_{j \in \mathbb{N}} y_j w_j^s \psi_j : \mathbf{y} \in U\}$ is contained in $O_{\mathbb{C}}$. Thus $u(\mathbf{y}) := \mathcal{G}(\sigma_r^s(\mathbf{y}))$ satisfies [55, Assumption 1.3.7].

Now [55, Theorem 2.2.10 (i) and (ii)] with “ $k = 1$ ” give the existence of $(a_{\mathbf{v}})_{\mathbf{v} \in \mathcal{F}} \in \ell^p(\mathcal{F})$ satisfying item (i) of the current theorem. Item (ii) is a consequence of [55, Theorem 2.2.10 (iii)]² and [55, Lemma 1.4.15]. Finally (iii) holds by [55, Corollary 2.2.12]. \square

To approximate the bounded function $u : U \rightarrow \mathcal{Y}$ in (20), we first expand it in the frame $(\eta_j L_{\mathbf{v}}(\mathbf{y}))_{j, \mathbf{v}}$ of $L^2(U, \mu; \mathcal{Y})$:

$$u(\mathbf{y}) = \mathcal{G}(\sigma_r^s(\mathbf{y})) = \sum_{j \in \mathbb{N}} \sum_{\mathbf{v} \in \mathcal{F}} c_{\mathbf{v}, j} \eta_j L_{\mathbf{v}}(\mathbf{y}) \quad (24a)$$

with coefficients

$$c_{\mathbf{v}, j} := \int_U L_{\mathbf{v}}(\mathbf{y}) \langle \mathcal{G}(\sigma_r^s(\mathbf{y})), \tilde{\eta}_j \rangle \, d\mu(\mathbf{y}) \quad (24b)$$

with convergence in $L^2(U, \mu; \mathcal{Y})$. We have the following weighted bound on these coefficients:

Proposition 1. *Consider the setting of Theorem 4. Then for each $\mathbf{v} \in \mathcal{F}$*

$$\omega_{\mathbf{v}}^2 \sum_{j \in \mathbb{N}} w_j^{-2t'} c_{\mathbf{v}, j}^2 \leq C^2 a_{\mathbf{v}}^2.$$

Proof. It holds

$$\left\| \int_U L_{\mathbf{v}}(\mathbf{y}) u(\mathbf{y}) \, d\mu(\mathbf{y}) \right\|_{\mathcal{Y}''}^2 = \sum_{j \in \mathbb{N}} w_j^{-2t'} \left\langle \int_U L_{\mathbf{v}}(\mathbf{y}) u(\mathbf{y}) \, d\mu(\mathbf{y}), \tilde{\eta}_j \right\rangle^2 = \sum_{j \in \mathbb{N}} w_j^{-2t'} c_{\mathbf{v}, j}^2.$$

Together with (22) this gives the statement. \square

² The set \mathfrak{J} occurring in [55, Theorem 2.2.10 (iii)] can for example be chosen as $\{0\} \cup \{2^j : j \in \mathbb{N}_0\}$, but the specific choice is of no significance here.

Before proving the main statement we need one more lemma.

Lemma 4. *Let $\alpha > 1$, $\beta > 0$ and assume given two sequences $(a_i)_{i \geq 1}, (d_j)_{j \geq 1} \subset (0, \infty)^\mathbb{N}$ with $a_i \lesssim i^{-\alpha}$ and $d_j \lesssim j^{-\beta}$ for all $i, j \in \mathbb{N}$. Assume that additionally $(d_j)_{j \in \mathbb{N}}$ is monotonically decreasing. Suppose that there exists $C < \infty$ such that the sequence $(c_{i,j})_{j,i \in \mathbb{N}}$ satisfies*

$$\forall i \in \mathbb{N} : \sum_{j \in \mathbb{N}} c_{i,j}^2 d_j^{-2} \leq C^2 a_i^2.$$

Then for every $\delta > 0$

(i) for every $N \in \mathbb{N}$ exists $(m_i)_{i \in \mathbb{N}} \subseteq \mathbb{N}_0$ monotonically decreasing such that $\sum_{i \in \mathbb{N}} m_i \leq N$ and

$$\sum_{i \in \mathbb{N}} \left(\sum_{j > m_i} c_{i,j}^2 \right)^{1/2} \lesssim N^{-\min\{\alpha-1, \beta\} + \delta},$$

(ii) for every $n \in \mathbb{N}$ exists $(m_i)_{i \in \mathbb{N}} \subseteq \mathbb{N}_0$ monotonically decreasing such that $\sum_{i \in \mathbb{N}} m_i \leq N$ and

$$\left(\sum_{i \in \mathbb{N}} \sum_{j > m_i} c_{i,j}^2 \right)^{1/2} \lesssim N^{-\min\{\alpha-\frac{1}{2}, \beta\} + \delta}.$$

Proof. Fix $n \in \mathbb{N}$. Set $m_i := \lceil (\frac{n}{i})^{(\alpha-1)/\beta} \rceil$ for $i \leq n$ and $m_i := 0$ otherwise. For $i \leq n$, since $(d_j)_{j \in \mathbb{N}}$ was assumed monotonically decreasing,

$$\left(\sum_{j > m_i} c_{i,j}^2 \right)^{1/2} = \left(\sum_{j > m_i} c_{i,j}^2 d_j^2 d_j^{-2} \right)^{1/2} \leq C d_{m_i} a_i \lesssim m_i^{-\beta} i^{-\alpha}$$

and for $i > n$ we have $(\sum_{j > m_i} c_{i,j}^2)^{1/2} = (\sum_{j \geq 1} c_{i,j}^2)^{1/2} \lesssim a_i \lesssim i^{-\alpha}$. Thus

$$\sum_{i \in \mathbb{N}} \left(\sum_{j > m_i} c_{i,j}^2 \right)^{1/2} \lesssim \sum_{i \leq n} m_i^{-\beta} i^{-\alpha} + C \sum_{i > n} i^{-\alpha} \lesssim \sum_{i \leq n} \left(\frac{n}{i} \right)^{-\alpha+1} i^{-\alpha} + n^{-\alpha+1} \lesssim n^{-\alpha+1} \log(n).$$

Moreover

$$\sum_{j \in \mathbb{N}} m_j \lesssim n + n^{\frac{\alpha-1}{\beta}} \int_1^{n+1} x^{-\frac{\alpha-1}{\beta}} dx \lesssim n + n^{\frac{\alpha-1}{\beta}} \begin{cases} 1 & \text{if } \frac{\alpha-1}{\beta} > 1 \\ \log(n) & \text{if } \frac{\alpha-1}{\beta} = 1 \\ n^{1-\frac{\alpha-1}{\beta}} & \text{if } \frac{\alpha-1}{\beta} < 1 \end{cases} \lesssim \begin{cases} n^{\frac{\alpha-1}{\beta}} & \text{if } \frac{\alpha-1}{\beta} > 1 \\ n \log(n) & \text{if } \frac{\alpha-1}{\beta} = 1 \\ n & \text{if } \frac{\alpha-1}{\beta} < 1. \end{cases}$$

With $M := \sum_{j \in \mathbb{N}} m_j$ we get

$$\sum_{i \in \mathbb{N}} \left(\sum_{j > m_i} c_{i,j}^2 \right)^{1/2} \lesssim \begin{cases} M^{-\beta+\delta} & \text{if } \alpha-1 \geq \beta \\ M^{-\alpha+1+\delta} & \text{if } \alpha-1 < \beta. \end{cases}$$

Choosing $n(N)$ appropriately we can guarantee $M(n) \sim N$.

For the second item fix again $n \in \mathbb{N}$ and set $m_i := \lceil (\frac{n}{i})^{(2\alpha-1)/(2\beta)} \rceil$ for $i \leq n$ and $m_i := 0$ otherwise. For $i \leq n$

$$\sum_{j>m_i} c_{i,j}^2 = \sum_{j>m_i} c_{i,j}^2 d_j^2 d_j^{-2} \leq C d_{m_i}^2 a_i^2 \lesssim m_i^{-2\beta} i^{-2\alpha},$$

and for $i > n$ we have $\sum_{j>m_i} c_{i,j}^2 \lesssim a_i^2 \lesssim i^{-2\alpha}$. With the same calculation as in the first case (but with α, β replaced by $2\alpha, 2\beta$ respectively) we get with $M := \sum_{j \in \mathbb{N}} m_j$

$$\sum_{i \in \mathbb{N}} \left(\sum_{j>m_i} c_{i,j}^2 \right) \lesssim \begin{cases} M^{-2\beta+\delta} & \text{if } 2\alpha - 1 \geq 2\beta \\ M^{-2\alpha+1+\delta} & \text{if } 2\alpha - 1 < 2\beta. \end{cases}$$

This concludes the proof. \square

Remark 12. The convergence rates in the above lemma are optimal as can be checked.

4.2 Proof in a particular case

We prove a particular case of Theorem 1, with fixed parameter range $y_j \in [-1, 1]$.

Theorem 5. *Let Assumption 1 be satisfied for some $s > 1$ and $t > 0$. Fix $\delta > 0$ (arbitrarily small).*

Then there exists a constant $C > 0$ such that for every $N \in \mathbb{N}$ exists a ReLU NN $\tilde{\mathbf{G}}_N$ of size $O(N \log(N)^5)$ such that

$$\sup_{\mathbf{y} \in U} \|\mathcal{G}(\sigma_r^s(\mathbf{y})) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathbf{y}))\|_{\mathcal{D}} \leq CN^{-\min\{s-1, t\}+\delta} \quad (25)$$

and

$$\|\mathcal{G}(\sigma_r^s(\mathbf{y})) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathbf{y}))\|_{L^2(U, \mathcal{D})} \leq CN^{-\min\{s-\frac{1}{2}, t\}+\delta}. \quad (26)$$

Proof. Let $(a_{\mathbf{v}})_{\mathbf{v} \in \mathcal{F}}$ and the enumeration $(\mathbf{v}_i)_{i \in \mathbb{N}}$ be as in Theorem 4 (with “ τ ” in this theorem being $1/2$), so that $(a_{\mathbf{v}_i})_{i \in \mathbb{N}}$ is monotonically decreasing and belongs to $\ell^p(\mathbb{N})$, where we fix $p \in (\frac{1}{s}, 1]$ such that $\frac{1}{p} \geq s - \delta/2$. Note that due to $ia_{\mathbf{v}_i}^p \leq \sum_{j \in \mathbb{N}} a_{\mathbf{v}_j}^p < \infty$ this implies $a_{\mathbf{v}_i} \lesssim i^{-1/p} \leq i^{-s+\delta/2}$.

Fix $N \in \mathbb{N}$ and set $\Lambda_N := \{\mathbf{v}_j : j \leq N\} \subset \mathcal{F}$, which is a downward closed set by Theorem 4. By [40, Proposition 2.13], for every $0 < \gamma < 1$ there exists a ReLU NN $(\tilde{L}_{\mathbf{v}})_{\mathbf{v} \in \Lambda_N}$ such that

$$\sup_{\mathbf{y} \in U} \sup_{\mathbf{v} \in \Lambda_N} |L_{\mathbf{v}}(\mathbf{y}) - \tilde{L}_{\mathbf{v}}(\mathbf{y})| \leq \gamma,$$

and using (23) one has the bound

$$\text{size}((\tilde{L}_{\mathbf{v}})_{\mathbf{v} \in \Lambda_N}) = O(N \log(N)^4 \log(1/\gamma)) \quad (27)$$

on the network size. The constant hidden in $O(\cdot)$ is independent of N and γ . In the following fix for $N \in \mathbb{N}$, $N \geq 2$, the accuracy $\gamma := N^{-s+\frac{1}{2}} \in (0, 1)$. With these choices, the right-hand side of (27) is $O(N \log(N)^5)$.

Next fix $t' \in [0, t)$ such that $t' > t - \delta/2$. By Proposition 1 with $\omega_{\mathbf{v}} := \prod_{j \in \text{supp } \mathbf{v}} (1 + 2v_j) \geq 1$ we have for every $i \in \mathbb{N}$

$$\omega_{\mathbf{v}_i}^{1/2} \left(\sum_{j \in \mathbb{N}} w_j^{-2t'} c_{\mathbf{v}_i, j}^2 \right)^{1/2} \lesssim a_{\mathbf{v}_i} \lesssim i^{-s+\frac{\delta}{2}}. \quad (28a)$$

Moreover, due to $(w_j^{t'})_{j \in \mathbb{N}} \in \ell^{1/(t-\delta/2)}(\mathbb{N})$, by the same argument as above (using that $(w_j)_{j \in \mathbb{N}}$ was assumed monotonically decreasing) it holds

$$w_j^{t'} \lesssim j^{-t+\frac{\delta}{2}}. \quad (28b)$$

We now show (25) and (26) separately.

- (i) Due to (28) with $\alpha := s - \delta/2$ and $\beta := t - \delta/2$, by Lemma 4 we can find $(m_i)_{i \in \mathbb{N}} \subset \mathbb{N}_0$ such that $\sum_{i \in \mathbb{N}} m_i \leq N$ and

$$\sum_{i \in \mathbb{N}} \omega_{\mathbf{v}_i}^{1/2} \left(\sum_{j > m_i} c_{\mathbf{v}_i, j}^2 \right)^{1/2} \leq N^{-\min\{s-1, t\}+\delta}. \quad (29)$$

Now define for $j \in \mathbb{N}$ (where an empty sum is equal to 0)

$$\tilde{g}_j(\mathbf{y}) := \sum_{\{i \in \mathbb{N}; m_i \geq j\}} \tilde{L}_{\mathbf{v}_i}(\mathbf{y}) c_{\mathbf{v}_i, j}. \quad (30)$$

Then by (24) with $\tilde{\mathbf{G}}_N = (\tilde{g}_j)_{j \in \mathbb{N}}$ for all $\mathbf{y} \in U$

$$\begin{aligned} \|\mathcal{G}(\sigma_r^s(\mathbf{y})) - \mathcal{D}(\tilde{g}(\mathbf{y}))\|_{\mathcal{Y}} &= \left\| \sum_{i, j \in \mathbb{N}} c_{\mathbf{v}_i, j} L_{\mathbf{v}_i}(\mathbf{y}) \eta_j - \sum_{i \in \mathbb{N}} \sum_{j \leq m_i} c_{\mathbf{v}_i, j} \tilde{L}_{\mathbf{v}_i}(\mathbf{y}) \eta_j \right\|_{\mathcal{Y}} \\ &\leq \left\| \sum_{i \in \mathbb{N}} L_{\mathbf{v}_i}(\mathbf{y}) \sum_{j > m_i} c_{\mathbf{v}_i, j} \eta_j \right\|_{\mathcal{Y}} + \left\| \sum_{i \in \mathbb{N}} (L_{\mathbf{v}_i}(\mathbf{y}) - \tilde{L}_{\mathbf{v}_i}(\mathbf{y})) \sum_{j \leq m_i} \eta_j c_{\mathbf{v}_i, j} \right\|_{\mathcal{Y}} \\ &\leq \Lambda_{\mathcal{Y}} \sum_{i \in \mathbb{N}} \|L_{\mathbf{v}_i}\|_{L^\infty(U)} \left(\sum_{j > m_i} c_{\mathbf{v}_i, j}^2 \right)^{1/2} + \Lambda_{\mathcal{Y}} \gamma \sum_{i \in \mathbb{N}} \left(\sum_{j \leq m_i} c_{\mathbf{v}_i, j}^2 \right)^{1/2}, \end{aligned}$$

where $\Lambda_{\mathcal{Y}}$ denotes the upper frame constant in (5) for the frame $\Psi_{\mathcal{Y}} = (\eta_j)_{j \in \mathbb{N}}$, cp. Rmk. 1. By (21) and (29) the first term is $O(N^{-\min\{s-1, t\}+\delta})$ and the second term is $O(\gamma) = O(N^{-\min\{s-1/2, t\}})$ which shows the error bound (25).

The size of $\tilde{\mathbf{G}}_N = (\tilde{g}_j)_{j \in \mathbb{N}}$ in (30) is bounded by

$$\begin{aligned} \text{size}((\tilde{L}_{\mathbf{v}})_{\mathbf{v} \in \Lambda_N}) + \sum_{j \in \mathbb{N}} |\{i \in \mathbb{N} : m_i \geq j\}| &= O(N \log(N)^5) + \sum_{i \in \mathbb{N}} \sum_{j \leq m_i} 1 \\ &= O(N \log(N)^5), \end{aligned}$$

since $\sum_{i \in \mathbb{N}} m_i \leq N$.

- (ii) Due to (28) with $\alpha := s - \delta/2$ and $\beta := t - \delta/2$, by Lemma 4 we can find $(m_i)_{i \in \mathbb{N}} \subset \mathbb{N}_0$ such that $\sum_{i \in \mathbb{N}} m_i \leq N$ and

$$\sum_{i \in \mathbb{N}} \sum_{j > m_i} c_{\mathbf{v},j}^2 \leq N^{-\min\{s-\frac{1}{2}, t\} + \delta}. \quad (31)$$

The rest of the calculation is similar as in the first case. Let \tilde{g}_j be as in (30). Then by (24) and because $(L_{\mathbf{v}}(\mathbf{y})\eta_j)_{\mathbf{v},j}$ is an ONB of $L^2(U, \mu; \mathscr{Y})$

$$\begin{aligned} \|\mathscr{G}(\sigma_r^s(\mathbf{y})) - \mathscr{D}((\tilde{g}_j(\mathbf{y}))_{j \in \Lambda_{\mathbb{N}, \varepsilon}})\|_{L^2(U, \mathscr{Y})} &\leq \left\| \sum_{i \in \mathbb{N}} \sum_{j > m_i} c_{\mathbf{v},j} L_{\mathbf{v}}(\mathbf{y}) \eta_j \right\|_{L^2(U, \mathscr{Y})} \\ &\quad + \left\| \sum_{i \in \mathbb{N}} \sum_{j \leq m_i} c_{\mathbf{v},j} \eta_j |L_{\mathbf{v}}(\mathbf{y}) - \tilde{L}_{\mathbf{v}}(\mathbf{y})| \right\|_{L^2(U, \mathscr{Y})} \\ &\leq \Lambda_{\mathscr{Y}} \left(\sum_{i \in \mathbb{N}} \sum_{j > m_i} c_{\mathbf{v},j}^2 \right)^{1/2} + \Lambda_{\mathscr{Y}} \gamma \left(\sum_{i \in \mathbb{N}} \sum_{j \leq m_i} c_{\mathbf{v},j}^2 \right)^{1/2}, \end{aligned}$$

where $\Lambda_{\mathscr{Y}}$ denotes again the upper frame constant in (5) for the frame $\Psi_{\mathscr{Y}} = (\eta_j)_{j \in \mathbb{N}}$. By (31) the first term is $O(N^{-\min\{s-1/2, t\} + \delta})$ and the second term is $O(\gamma) = O(N^{-\min\{s-1/2, t\}})$, which shows the error bound (26).

The size of $\tilde{\mathbf{G}}_N$ is bounded in the same way as in the first case. \square

4.3 Proof of Theorem 1 in the general case

We obtain Theorem 1 from Theorem 5 by a scaling argument, via the weight sequences which characterize the admissible input data.

Introduce the scaling

$$S = \times_{j \in \mathbb{N}} [-rw_j^s, rw_j^s] \rightarrow U : (x_j)_{j \in \mathbb{N}} \mapsto \left(\frac{x_j}{rw_j^s} \right)_{j \in \mathbb{N}}, \quad (32)$$

where $U = [-1, 1]^{\mathbb{N}}$. Then (cp. (11) and (14))

$$S \circ \mathscr{E}(a) \in U \quad \forall a \in C_r^s(\mathscr{X}).$$

Let $\tilde{\mathbf{G}}_N : \ell^2(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$ be as in Theorem 5. Since $\sigma_r^s : U \rightarrow \tilde{C}_r^s(\mathcal{X})$ is surjective and $\tilde{C}_r^s(\mathcal{X}) \supseteq C_r^s(\mathcal{X})$ (see Rmk. 8), (25) in Theorem 5 implies with $\hat{\mathbf{G}}_N := \tilde{\mathbf{G}}_N \circ S$

$$\begin{aligned} & \sup_{a \in C_r^s(\mathcal{X})} \|\mathcal{G}(a) - \mathcal{D}(\hat{\mathbf{G}}_N(\mathcal{E}(a)))\|_{\mathcal{Y}} \\ &= \sup_{\{\mathbf{y} \in U : \sigma_r^s(\mathbf{y}) \in C_r^s(\mathcal{X})\}} \|\mathcal{G}(\sigma_r^s(\mathbf{y})) - \mathcal{D}(\tilde{\mathbf{G}}_N(S(\mathcal{E}(\sigma_r^s(\mathbf{y}))))\|_{\mathcal{Y}} \\ &\leq \sup_{\mathbf{y} \in U} \|\mathcal{G}(\sigma_r^s(\mathbf{y})) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathbf{y}))\|_{\mathcal{Y}} = O(N^{-\min\{s-1, t\} + \delta}). \end{aligned}$$

Since S is an infinite linear diagonal transformation, $\hat{\mathbf{G}}_N$ is a network of the same size as $\tilde{\mathbf{G}}_N$ and thus of size $O(N \log(N)^5)$ by Theorem 5 (cp. Rmk. 10 and (15)).

Setting $M = M(N) := N \log(N)^5$ we obtain a network of size $O(M)$ that achieves error $O(N^{-\min\{s-1, t\} + \delta}) = O(M^{-\min\{s-1, t\} + 2\delta})$. Since $\delta > 0$ is arbitrary here, we obtain (17). The calculation for (18) is similar.

4.4 Proof of Theorem 2 in the general case

The argument is similar as in Sec. 4.3 Let S be as in (32). Since $\Psi_{\mathcal{X}}$ is assumed to be a Riesz basis, by Rmk. 8 it holds (cp. (13) and (32))

$$C_r^s(\mathcal{X}) = \{\sigma_r^s(\mathbf{y}) : \mathbf{y} \in U\} \quad \text{and} \quad \mathcal{E}(\sigma_r^s(\mathbf{y})) = S^{-1}(\mathbf{y}) \quad \forall \mathbf{y} \in U.$$

With $\tilde{\mathbf{G}}_N$ as in Thm. 5 and $\hat{\mathbf{G}}_N := \tilde{\mathbf{G}}_N \circ S$ we find with (26)

$$\begin{aligned} \|\mathcal{G}(a) - \mathcal{D}(\hat{\mathbf{G}}_N(\mathcal{E}(a)))\|_{L^2(C_r^s(\mathcal{X}), (\sigma_r^s)_\# \mu)} &= \|\mathcal{G}(\sigma_r^s(\mathbf{y})) - \mathcal{D}(\hat{\mathbf{G}}_N(\mathcal{E}(\sigma_r^s(\mathbf{y})))\|_{L^2(U, \mu)} \\ &= \|\mathcal{G}(\sigma_r^s(\mathbf{y})) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathbf{y}))\|_{L^2(U, \mu)} \\ &= O(N^{-\min\{s-\frac{1}{2}, t\} + \delta}). \end{aligned}$$

The size on the bound of $\hat{\mathbf{G}}_N$ follows by the same argument as in Sec. 4.3.

5 Sparse-grid interpolation

In this section we discuss operator approximation using sparse-grid interpolation instead of NNs. In contrast to neural network approximation, the construction of surrogate operators via sparse-grid gpc interpolation is, in the current setting, an entirely deterministic algorithm of essentially linear complexity, which in particular does *not* rely on solving a (nonconvex) optimization problem. Moreover, for the case of uniform approximation we will prove the same convergence rate as in Theorem 1. Thus, from a theoretical viewpoint, sparse-grid interpolation has significant advantages over NN training in the construction of surrogate operators.

To recall the construction of the Smolyak (sparse-grid) interpolant (e.g. [9]) fix a sequence of distinct points $(\chi_j)_{j \in \mathbb{N}_0} \subseteq [-1, 1]$. For a multiindex $\mathbf{v} \in \mathcal{F}$ and a function $u : U \rightarrow \mathbb{R}$ we define for $\mathbf{y} = (y_j)_{j \in \mathbb{N}} \in U$

$$(I_{\mathbf{v}}u)(\mathbf{y}) = \sum_{\{\boldsymbol{\mu} \in \mathcal{F} : \boldsymbol{\mu} \leq \mathbf{v}\}} u((\chi_{\mu_j})_{j \in \mathbb{N}}) \prod_{j \in \mathbb{N}} \prod_{\substack{i=0 \\ i \neq \mu_j}}^{v_j} \frac{y_j - \chi_i}{\chi_{\mu_j} - \chi_i}, \quad (33)$$

where $\mathbf{v} \leq \boldsymbol{\mu}$ is understood as $\mu_j \leq v_j$ for all $j \in \mathbb{N}$. Note that the sum in (33) is over $\prod_{j \in \mathbb{N}} (1 + v_j)$ indices, which is finite since $\mathbf{v} \in \mathcal{F}$. Moreover we point out that $I_{\mathbf{v}}$ maps from $C^0(U)$ to $\text{span}\{\mathbf{y}^{\boldsymbol{\mu}} : \boldsymbol{\mu} \leq \mathbf{v}\}$. Throughout we assume that the $(\chi_j)_{j \in \mathbb{N}}$ are such that the Lebesgue constant $L((\chi_j)_{j=0}^n)$ of $(\chi_j)_{j=0}^n$ enjoys the property

$$L((\chi_j)_{j=0}^n) \leq (1+n)^\tau \quad \forall n \in \mathbb{N}_0 \quad (34)$$

for some fixed $\tau > 0$. One popular example for such a sequence are the so-called Leja points, see [11] and the references there.

For a finite downward closed set $\Lambda \subseteq \mathcal{F}$ denote

$$\mathbb{P}_\Lambda := \text{span}\{\mathbf{y}^{\mathbf{v}} : \mathbf{v} \in \Lambda\}.$$

The Smolyak interpolant is the map $I_\Lambda : C^0(U) \rightarrow \mathbb{P}_\Lambda$ defined via

$$I_\Lambda := \sum_{\mathbf{v} \in \Lambda} \zeta_{\Lambda, \mathbf{v}} I_{\mathbf{v}}, \quad \zeta_{\Lambda, \mathbf{v}} := \sum_{\{\mathbf{e} \in \{0,1\}^{\mathbb{N}} : \mathbf{v} + \mathbf{e} \in \Lambda\}} (-1)^{|\mathbf{e}|}.$$

Remark 13. It can be checked that the number of function evaluations of u required to compute $I_\Lambda u$ equals $|\Lambda|$.

The Smolyak interpolant has the following well-known properties, see for example [55, Lemma 1.3.3], [9].

Lemma 5. *Let Λ be finite and downward closed. Then with τ as in (34) and $\omega_{\mathbf{v}} := \prod_{j \in \mathbb{N}} (1 + 2v_j)$*

- (i) $I_\Lambda : C^0(U) \rightarrow \mathbb{P}_\Lambda$ and $I_\Lambda p = p$ for all $p \in \mathbb{P}_\Lambda$.
- (ii) $\|I_\Lambda L_{\mathbf{v}}\|_{L^\infty(U)} \leq \omega_{\mathbf{v}}^{3/2+\tau}$ for all $\mathbf{v} \in \mathcal{F}$.

The following theorem shows the same convergence rate as established in Theorem 5 for NNs, for Smolyak interpolation p_N of the components of the parametric map \mathcal{G} :

Theorem 6. *Let Assumption 1 be satisfied for some $s > 1$ and $t > 0$, and let the interpolation points $(\chi_j)_{j \in \mathbb{N}_0}$ be such that (34) holds. Fix $\delta > 0$ (arbitrarily small).*

Then, there exists a constant $C > 0$ (depending on δ, τ, s, t, r) such that, for every $N \in \mathbb{N}$, there exist downward closed index sets $(\Lambda_{N,j})_{j \leq N}$ such that $\sum_{j=1}^N |\Lambda_{N,j}| \leq N$ and with the interpolated coefficients $p_N(\mathbf{y}) = (I_{\Lambda_{N,j}} \langle u(\mathbf{y}), \tilde{\eta}_j \rangle)_{j \leq N}$ holds

$$\sup_{\mathbf{y} \in U} \|\mathcal{G}(\sigma_r^s(\mathbf{y})) - \mathcal{D}(p_N(\mathbf{y}))\|_{\mathcal{Y}} \leq CN^{-\min\{s-1,t\}+\delta}. \quad (35)$$

Remark 14. The convergence rate is in terms of $N \geq \sum_{j=1}^N |\Lambda_{N,j}|$, which is an upper bound of the number of required evaluations of $\langle u(\mathbf{y}), \tilde{\eta}_j \rangle$ for all $j \in \mathbb{N}$ (here u is as in (20)).

Proof.[Proof of Theorem 6] Let $(a_{\mathbf{v}})_{\mathbf{v} \in \mathcal{F}}$ and the enumeration $(\mathbf{v}_i)_{i \in \mathbb{N}}$ be as in Theorem 4 (with “tau” being $\frac{3}{2} + \tau$ for the value in (34)), so that $(a_{\mathbf{v}_i})_{i \in \mathbb{N}}$ is monotonically decreasing and belongs to $\ell^p(\mathbb{N})$, where we fix $p \in (\frac{1}{s}, 1]$ such that $\frac{1}{p} \geq s - \delta/2$. Again we point out that due to $ia_{\mathbf{v}_i}^p \leq \sum_{j \in \mathbb{N}} a_{\mathbf{v}_j}^p < \infty$ this implies $a_{\mathbf{v}_i} \lesssim i^{-1/p} \leq i^{-s+\delta/2}$.

Next fix $t' \in [0, t)$ such that $t' > t - \delta/2$. By Proposition 1 with $\omega_{\mathbf{v}} := \prod_{j \in \text{supp } \mathbf{v}} (1 + 2v_j) \geq 1$ we have for every $i \in \mathbb{N}$

$$\omega_{\mathbf{v}_i}^{3/2+\tau} \left(\sum_{j \in \mathbb{N}} w_j^{-2t'} c_{\mathbf{v}_i, j}^2 \right)^{1/2} \lesssim a_{\mathbf{v}_i} \lesssim i^{-s+\frac{\delta}{2}}. \quad (36a)$$

Moreover, due to $(w'_j)_{j \in \mathbb{N}} \in \ell^{1/(t-\delta/2)}(\mathbb{N})$, by the same argument as above (using that $(w_j)_{j \in \mathbb{N}}$ was assumed monotonically decreasing) it holds

$$w'_j \lesssim j^{-t+\frac{\delta}{2}}. \quad (36b)$$

Due to (36) with $\alpha := s - \delta/2$ and $\beta := t - \delta/2$, by Lemma 4 we can find $(m_i)_{i \in \mathbb{N}} \subset \mathbb{N}_0$ such that $\sum_{i \in \mathbb{N}} m_i \leq N$ and

$$\sum_{i \in \mathbb{N}} \omega_{\mathbf{v}_i}^{3/2+\tau} \left(\sum_{j > m_i} c_{\mathbf{v}_i, j}^2 \right)^{1/2} \leq N^{-\min\{s-1,t\}+\delta}. \quad (37)$$

Now define for $j \leq N$

$$\Lambda_{N,j} := \{\mathbf{v}_i : m_i \geq j\} = \{\mathbf{v}_i : i \leq \max\{r : m_r \geq j\}\},$$

where the equality follows by the fact that $(m_i)_{i \in \mathbb{N}}$ is monotonically decreasing according to Lemma 4. Thus each $\Lambda_{N,j}$ is downward closed by Theorem 4. Moreover

$$\sum_{j \in \mathbb{N}} |\Lambda_{N,j}| = \sum_{j \in \mathbb{N}} \sum_{\{i: m_i \geq j\}} 1 = \sum_{i \in \mathbb{N}} \sum_{\{j: j \leq m_i\}} 1 = \sum_{i \in \mathbb{N}} m_i \leq N.$$

With (24) it holds

$$I_{\Lambda_{N,j}} \langle u, \eta_j \rangle = I_{\Lambda_{N,j}} \sum_{\mathbf{v} \in \mathcal{F}} c_{\mathbf{v}, j} L_{\mathbf{v}} = \sum_{\mathbf{v} \in \Lambda_{N,j}} c_{\mathbf{v}, j} L_{\mathbf{v}} + \sum_{\mathbf{v} \in \mathcal{F} \setminus \Lambda_{N,j}} c_{\mathbf{v}, j} I_{\Lambda_{N,j}} L_{\mathbf{v}},$$

where we used that $I_{\Lambda_{N,j}} L_{\mathbf{v}} = L_{\mathbf{v}}$ for all $\mathbf{v} \in \Lambda_{N,j}$ by Lemma 5 (i).

Thus for all $\mathbf{y} \in U$ with $p_N(\mathbf{y}) = (I_{\Lambda_{N,j}} \langle u, \eta_j \rangle)_{j=1}^N$

$$\begin{aligned}
& \|\mathcal{G}(\sigma_r^s(\mathbf{y})) - \mathcal{D}(p_N(\mathbf{y}))\|_{\mathcal{Y}} \\
&= \left\| \sum_{j \in \mathbb{N}} \sum_{\mathbf{v} \in \mathcal{F}} c_{\mathbf{v},j} L_{\mathbf{v}}(\mathbf{y}) \eta_j - \sum_{j \in \mathbb{N}} \sum_{\mathbf{v} \in \Lambda_{N,j}} c_{\mathbf{v},j} L_{\mathbf{v}}(\mathbf{y}) \eta_j - \sum_{j \in \mathbb{N}} \sum_{\mathbf{v} \in \mathcal{F} \setminus \Lambda_{N,j}} c_{\mathbf{v},j} I_{\Lambda_{N,j}} L_{\mathbf{v}}(\mathbf{y}) \eta_j \right\|_{\mathcal{Y}} \\
&\leq \left\| \sum_{j \in \mathbb{N}} \sum_{\{\mathbf{v}_i: m_i < j\}} c_{\mathbf{v}_i,j} L_{\mathbf{v}_i}(\mathbf{y}) \eta_j \right\|_{\mathcal{Y}} + \left\| \sum_{j \in \mathbb{N}} \sum_{\{\mathbf{v}_i: m_i < j\}} c_{\mathbf{v}_i,j} (L_{\mathbf{v}_i}(\mathbf{y}) - I_{\Lambda_{N,j}} L_{\mathbf{v}_i}(\mathbf{y})) \eta_j \right\|_{\mathcal{Y}} \\
&= \left\| \sum_{i \in \mathbb{N}} \sum_{j > m_i} c_{\mathbf{v}_i,j} L_{\mathbf{v}_i}(\mathbf{y}) \eta_j \right\|_{\mathcal{Y}} + \left\| \sum_{i \in \mathbb{N}} \sum_{j > m_i} c_{\mathbf{v}_i,j} (L_{\mathbf{v}_i}(\mathbf{y}) - I_{\Lambda_{N,j}} L_{\mathbf{v}_i}(\mathbf{y})) \eta_j \right\|_{\mathcal{Y}} \\
&\leq \Lambda_{\mathcal{Y}} \sum_{i \in \mathbb{N}} \left(\sum_{j > m_i} c_{\mathbf{v}_i,j}^2 \|L_{\mathbf{v}_i}\|_{L^\infty(U)}^2 \right)^{1/2} + \left(\sum_{j > m_i} c_{\mathbf{v}_i,j}^2 (\|L_{\mathbf{v}_i}\|_{L^\infty(U)} + \|I_{\Lambda_{N,j}} L_{\mathbf{v}_i}\|_{L^\infty(U)})^2 \right)^{1/2},
\end{aligned}$$

where $\Lambda_{\mathcal{Y}}$ denotes again the upper frame constant in (5) for the frame $\Psi_{\mathcal{Y}} = (\eta_j)_{j \in \mathbb{N}}$, cp. Rmk. 1. By Lemma 5 (ii) and (21) we have

$$\|L_{\mathbf{v}_i}\|_{L^\infty(U)} + \|I_{\Lambda_{N,j}} L_{\mathbf{v}_i}\|_{L^\infty(U)} \leq 2\omega_{\mathbf{v}}^{3/2+\tau}.$$

Thus, using (37) we find

$$\sup_{\mathbf{y} \in U} \|\mathcal{G}(\sigma_r^s(\mathbf{y})) - \mathcal{D}(p_N(\mathbf{y}))\|_{\mathcal{Y}} \leq 3\Lambda_{\mathcal{Y}} N^{-\min\{s-1,t\}+\delta}$$

which concludes the proof. \square

Theorem 3 is now a direct consequence of Theorem 6; specifically the statement of Theorem 3 follows after introducing a scaling to map $\times_{j \in \mathbb{N}} [-rw_j^s, rw_j^s] \rightarrow U$ as in the proof of Theorem 1.

Remark 15. As mentioned above, sparse-grid interpolation is deterministic. In practice, computing the interpolant requires determining the sets $\Lambda_{N,j}$ occurring in Theorem 6. For given weights $(w_j)_{j \in \mathbb{N}}$, this can be achieved in almost linear complexity as is discussed for example in [55, Theorem 2.2.10 and Section 3.1.3].

6 Example: Diffusion equation on the torus

Denote by $\mathbb{T}^d \simeq [0, 1]^d$ the d -dimensional torus, $d \in \mathbb{N}$. In the following all function spaces on \mathbb{T}^d are assumed to be 1-periodic with respect to each variable.

6.1 Operator \mathcal{G}

Given a nominal coefficient $\bar{a} \in L^\infty(\mathbb{T}^d)$, a diffusion coefficient $a \in L^\infty(\mathbb{T}^d)$, and a source $f \in H^{-1}(\mathbb{T}^d)/\mathbb{R}$, we wish to find $u \in H^1(\mathbb{T}^d)$ such that

$$-\nabla \cdot ((\bar{a} + a)\nabla u) = f \text{ on } \mathbb{T}^d \quad \text{and} \quad \int_{\mathbb{T}^d} u(x) \, dx = 0 \quad (38)$$

in a weak sense. Assuming

$$\operatorname{ess\,inf}_{x \in \mathbb{T}^d} (\bar{a}(x) + a(x)) > a_{\min}, \quad (39)$$

for some constant $a_{\min} > 0$, it follows by the Lax-Milgram Lemma that (38) has a unique solution $u \in H^1(\mathbb{T}^d)/\mathbb{R}$ that we denote by $\mathcal{G}(a) := u$. Thus \mathcal{G} is a well-defined map from $\{a \in L^\infty(\mathbb{T}^d) : (39) \text{ holds}\} \rightarrow H^1(\mathbb{T}^d)/\mathbb{R} \hookrightarrow H^1(\mathbb{T}^d)$.

6.2 \mathcal{X}^s and \mathcal{Y}^t

We first construct the usual Fourier basis on $L^2(\mathbb{T}^d)$: Set for $j \in \mathbb{N}$

$$\xi_0 = 1, \quad \xi_{2j}(x) = (2\pi)^{-1/2} \cos(2\pi jx), \quad \xi_{2j-1}(x) = (2\pi)^{-1/2} \sin(2\pi jx),$$

and for $d \geq 2$ and $\mathbf{j} \in \mathbb{N}_0^d$

$$\xi_{\mathbf{j}}(x_1, \dots, x_d) := \prod_{k=1}^d \xi_{j_k}(x_k).$$

Then $\{\xi_{\mathbf{j}} : \mathbf{j} \in \mathbb{N}_0^d\}$ is an ONB of $L^2(\mathbb{T}^d)$. Moreover, recall that for $s \geq 0$, holds

$$H^s(\mathbb{T}^d) = \left\{ u \in L^2(\mathbb{T}^d) : \sum_{\mathbf{j} \in \mathbb{N}_0^d} \langle u, \xi_{\mathbf{j}} \rangle^2 \max\{1, |\mathbf{j}|\}^{2s} < \infty \right\}, \quad (40)$$

where throughout we consider $H^s(\mathbb{T}^d)$ equipped with the inner product

$$\langle u, v \rangle_{H^s} := \sum_{\mathbf{j} \in \mathbb{N}_0^d} \langle u, \xi_{\mathbf{j}} \rangle_{L^2} \langle v, \xi_{\mathbf{j}} \rangle_{L^2} \max\{1, |\mathbf{j}|\}^{2s}. \quad (41)$$

Fixing $s_0, t_0 \geq 0$ (to be chosen later) we let

$$\begin{aligned} \mathcal{X} &:= H^{s_0}(\mathbb{T}^d), & \psi_{\mathbf{j}} &:= \max\{1, |\mathbf{j}|\}^{-s_0} \xi_{\mathbf{j}}, \\ \mathcal{Y} &:= H^{t_0}(\mathbb{T}^d), & \eta_{\mathbf{j}} &:= \max\{1, |\mathbf{j}|\}^{-t_0} \xi_{\mathbf{j}}, \end{aligned} \quad (42)$$

so that $\Psi_{\mathcal{X}} := (\psi_j)_{j \in \mathbb{N}_0^d}$, $\Psi_{\mathcal{Y}} := (\eta_j)_{j \in \mathbb{N}_0^d}$ form ONBs of \mathcal{X} , \mathcal{Y} respectively. Next, introduce the weight sequence

$$w_j := \max\{1, |\mathbf{j}|\}^{-d} \quad \mathbf{j} \in \mathbb{N}_0^d,$$

so that $(w_j^{1+\varepsilon})_{j \in \mathbb{N}_0^d} \in \ell^1(\mathbb{N}_0^d)$ for any $\varepsilon > 0$ as required in Sec. 2.4. Then, by (40) and the definition of \mathcal{X}^s in (12), it holds for $s \geq 0$

$$\begin{aligned} \mathcal{X}^s &= \left\{ u \in H^{s_0}(\mathbb{T}^d) : \sum_{j \in \mathbb{N}_0^d} \langle u, \psi_j \rangle_{H^{s_0}}^2 w_j^{-2s} < \infty \right\} \\ &= \left\{ u \in L^2(\mathbb{T}^d) : \sum_{j \in \mathbb{N}_0^d} \langle u, \xi_j \rangle_{L^2}^2 \max\{1, |\mathbf{j}|\}^{2s_0+2sd} < \infty \right\} = H^{s_0+sd}(\mathbb{T}^d). \end{aligned}$$

Here we used that for $u = \sum_{j \in \mathbb{N}_0^d} c_j \xi_j$ holds by (41)

$$\langle u, \psi_j \rangle_{H^{s_0}} = \langle u, \xi_j \max\{1, |\mathbf{j}|\}^{-s_0} \rangle_{H^{s_0}} = c_j \max\{1, |\mathbf{j}|\}^{s_0} = \langle u, \xi_j \rangle_{L^2} \max\{1, |\mathbf{j}|\}^{s_0}.$$

By the same argument $\mathcal{Y}^t = H^{t_0+td}(\mathbb{T}^d)$ for any $t \geq 0$.

6.3 Coefficient-to-Solution surrogate approximation rates

We now give a convergence result for the approximation of the solution operator \mathcal{G} (corresponding to the PDE (38)) on a Sobolev ball. The encoder \mathcal{E} and decoder \mathcal{D} are as in (11), w.r.t. the spaces and ONBs in (42), which depend on the constants s_0 , $t_0 \geq 0$ that are still at our disposal. The parameter s_0 controls the regularity of the input space and thus determines the encoder \mathcal{E} . It will have to be chosen suitably in order to achieve possibly fast convergence. On the other hand, t_0 controls the regularity of the output space. It may be chosen freely and determines the norm in which the error is measured—smaller t_0 amounts to a weaker norm in the output space and thus yields larger convergence rates.

Proposition 2. *Assume $f \in C^\infty(\mathbb{T}^d)/\mathbb{R}$. Let $\alpha > \frac{3d}{2}$, $r > 0$, $a_{\min} > 0$ and let $\delta > 0$ (arbitrarily small). Suppose that $\bar{a} + a$ satisfies (39) for all $a \in B_r(H^\alpha(\mathbb{T}^d))$.*

Then for every $t_0 \in [0, 1]$ there exists a constant $C > 0$ and for all $N \in \mathbb{N}$ there exists a ReLU NN $\tilde{\mathbf{G}}_N$ of size $O(N)$ such that

$$\sup_{a \in B_r(H^\alpha(\mathbb{T}^d))} \|\mathcal{G}(a) - \mathcal{D} \circ \tilde{\mathbf{G}}_N \circ \mathcal{E}(a)\|_{H^{t_0}(\mathbb{T}^d)} \leq CN^{-R+\delta} \quad (43a)$$

where

$$R = \begin{cases} \frac{\alpha}{d} - \frac{3}{2} & \text{if } \alpha \in (\frac{3d}{2}, \frac{3d}{2} + 1 - t_0] \\ \frac{\alpha+1-t_0}{2d} - \frac{3}{4} & \text{if } \alpha > \frac{3d}{2} + 1 - t_0, \end{cases} \quad (43b)$$

and where \mathcal{E} , \mathcal{D} are as in (11) with the spaces/ONBs in (42) with t_0 from above and

$$s_0 = \begin{cases} \frac{d}{2} + \frac{\delta}{2} & \text{if } \alpha \in (\frac{3d}{2}, \frac{3d}{2} + 1 - t_0] \\ \frac{\alpha + t_0 - \frac{d}{2} - 1}{2} & \text{if } \alpha > \frac{3d}{2} + 1 - t_0. \end{cases}$$

Proof. Step 1. We check Assumption 1. First, recall that by the standard Sobolev embedding for all $\beta > \frac{d}{2}$

$$H^\beta(\mathbb{T}^d) \hookrightarrow C^\gamma(\mathbb{T}^d) \quad \forall \gamma \in [0, \beta - \frac{d}{2}).$$

Furthermore, classical elliptic regularity (Schauder estimates, for second order divergence-form linear elliptic equations, also with complex-valued coefficients, e.g., [3, pg. 625], [4, Sec. 2]) implies for $\beta > 0$

$$\mathcal{G} : \{a \in C^\beta(\mathbb{T}^d) : \bar{a} + a \text{ satisfies (39)}\} \rightarrow C^{1+\beta}(\mathbb{T}^d) \hookrightarrow H^{1+\beta}(\mathbb{T}^d),$$

and that $\mathcal{G}(a)$ is bounded on bounded subsets of $\{a \in C^\beta(\mathbb{T}^d) : \bar{a} + a \text{ satisfies (39)}\}$.

Thus, if

$$s_0 > \frac{d}{2}, \quad (44)$$

using that for any $\gamma \in [0, s_0 - \frac{d}{2})$ holds $H^{s_0} \hookrightarrow C^\gamma$, we find

$$\mathcal{G} : \{a \in H^{s_0} : \bar{a} + a \text{ satisfies (39)}\} \rightarrow C^{1+\gamma} \quad \forall \gamma \in [0, s_0 - \frac{d}{2}).$$

We require (44) to ensure $H^{s_0}(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$, which is necessary in order for \mathcal{G} to be well-defined, see Section 6.1. In addition,

$$C^{1+\gamma}(\mathbb{T}^d) \hookrightarrow H^{1+\gamma}(\mathbb{T}^d) = \mathcal{Y}^t$$

with $t \geq 0$ such that $t_0 + td = 1 + \gamma$, i.e. $t = \frac{1+\gamma-t_0}{d}$ ($t \geq 0$ holds since by assumption $t_0 \leq 1 \leq 1 + \gamma$). With $\mathcal{X} = H^{s_0}(\mathbb{T}^d)$ this shows

$$\mathcal{G} : \{a \in \mathcal{X} : \bar{a} + a \text{ satisfies (39)}\} \rightarrow \mathcal{Y}^t \quad \forall t \in [0, \frac{1+s_0-\frac{d}{2}-t_0}{d})$$

and for fixed t the map is bounded on bounded subsets of $\{a \in \mathcal{X} : \bar{a} + a \text{ satisfies (39)}\}$.

Next, if $s > 1$, $\tilde{C}_r^s(\mathcal{X})$ (which is equal to $C_r^s(\mathcal{X})$ by Rmk. 8) is in particular a bounded subset of $\mathcal{X} \hookrightarrow L^\infty(\mathbb{T}^d)$ (cp. Rmk. 9). Hence, for example by [55, Proposition 1.2.33 and Example 1.2.38] there exists an open complex set $O_{\mathbb{C}} \subset \mathcal{X}_{\mathbb{C}}$ containing $\tilde{C}_r^s(\mathcal{X})$ such that due to $t_0 \in [0, 1]$,

$$\mathcal{G} : O_{\mathbb{C}} \rightarrow H^1(\mathbb{T}^d, \mathbb{C}) \hookrightarrow \mathcal{Y} = H^{t_0}(\mathbb{T}^d) \quad (45)$$

is holomorphic. Furthermore, it follows from the a-priori estimate [4, Theorem 9.3], which is also valid for (38) with periodic boundary conditions, by combining the

\mathbb{T}^d -periodicity of solutions w.r. to Rex with the ‘‘hemisphere’’ a-priori bounds in [4, Theorem 9.2] on each face of \mathbb{T}^d , that

$$\mathcal{G} : \mathcal{O}_{\mathbb{C}} \rightarrow \mathcal{Y}^t \quad \forall t \in \left[0, \frac{1+s_0-\frac{d}{2}-t_0}{d}\right) \quad (46)$$

is bounded.

Step 2. We conclude the proof. According to Cor. 1, for $s > 1$ and $t \in (0, \frac{1+s_0-\frac{d}{2}-t_0}{d})$ we have with $\mathcal{X}^s = H^{s_0+sd}(\mathbb{T}^d)$, $\mathcal{Y} = H^{t_0}(\mathbb{T}^d)$ and for all $\delta > 0$ (arbitrarily small)

$$\sup_{a \in B_r(H^{s_0+sd}(\mathbb{T}^d))} \|\mathcal{G}(a) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathcal{E}(a)))\|_{H^{t_0}} \leq CN^{-\min\{s-1, t\}+\delta}.$$

Substituting $\alpha = s_0 + sd$, i.e. $s = \frac{\alpha-s_0}{d}$, and taking the maximal t this reads

$$\sup_{a \in B_r(H^\alpha(\mathbb{T}^d))} \|\mathcal{G}(a) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathcal{E}(a)))\|_{H^{t_0}} \leq CN^{-\min\{\frac{\alpha-s_0}{d}-1, \frac{1+s_0-\frac{d}{2}-t_0}{d}\}+\delta}.$$

The constraint $s > 1$ implies the constraint $\alpha > d + s_0$ on α . We are still free to choose $s_0 > \frac{d}{2}$, and wish to do so in order to maximize the resulting convergence rate. Solving

$$\frac{\alpha-s_0}{d} - 1 = \frac{1+s_0-\frac{d}{2}-t_0}{d}$$

for s_0 we have

$$s_0 = \frac{\alpha + t_0 - \frac{d}{2} - 1}{2}. \quad (47)$$

The constraint $s_0 > \frac{d}{2}$ implies the constraint $\alpha > \frac{3d}{2} + 1 - t_0$.

We therefore now distinguish between two cases. First, if $\alpha \in (\frac{3d}{2}, \frac{3d}{2} + 1 - t_0]$, then we let $s_0 := \frac{d}{2} + \varepsilon$ for some small $\varepsilon > 0$ ($\varepsilon > 0$ small enough implies in particular that $\alpha > d + s_0$). In this case we obtain, up to some arbitrarily small $\delta > 0$, the convergence rate

$$\min \left\{ \frac{\alpha - \frac{d}{2}}{d} - 1, \frac{1 + \frac{d}{2} - \frac{d}{2} - t_0}{d} \right\} = \min \left\{ \frac{\alpha}{d} - \frac{3}{2}, \frac{1-t_0}{d} \right\} = \frac{\alpha}{d} - \frac{3}{2},$$

where we used that $\alpha \leq \frac{3d}{2} + 1 - t_0$ for the last equality.

Next assume $\alpha > \frac{3d}{2} + 1 - t_0$ and define s_0 as in (47). The constraint $\alpha > d + s_0$ is then equivalent to

$$\alpha > d + \frac{\alpha + t_0 - \frac{d}{2} - 1}{2} \quad \Leftrightarrow \quad \alpha > \frac{3d}{2} + t_0 - 1,$$

which already holds since $\alpha > \frac{3d}{2} + 1 - t_0 \geq \frac{3d}{2} + t_0 - 1$ for all $t_0 \in [0, 1]$. The convergence rate amounts in this case to

$$\frac{\alpha - s_0}{d} - 1 = \frac{\alpha + 1 - t_0}{2d} - \frac{3}{4}.$$

This shows (43). \square

The above proposition is based on Cor. 1. Applying instead Thm. 1, one obtains for example that for all $s > 1$, $s_0 > \frac{d}{2}$, $t_0 \in [0, 1]$, with $\mathcal{X} = H^{s_0}(\mathbb{T}^d)$ and for $\delta > 0$ fixed but arbitrarily small (cp. Step 2 in the proof of Prop. 2)

$$\sup_{a \in C_r^s(\mathcal{X})} \|\mathcal{G}(a) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathcal{E}(a)))\|_{H^{t_0}(\mathbb{T}^d)} \leq CN^{-\min\{s-1, \frac{1+s_0-\frac{d}{2}-t_0}{d}\} + \delta}.$$

Similarly, Thm. 2 gives an improved L^2 -type error estimate, and Thm. 3 gives a convergence result for gpc operator surrogates.

7 Concluding Remarks and further developments

We established expression rate bounds for finite-parametric approximations to non-linear, holomorphic maps between scales of infinite-dimensional, separable function spaces endowed with suitable stable, affine representation systems such as frames. Our approximations are based on combining a linear input encoder with suitable, finite-parametric surrogates $\{\tilde{\mathbf{G}}_N\}_N$ of a countably-parametric map transforming coefficient sequences from the input encoder into corresponding sequences for the output decoder.

While being of independent, mathematical interest, the present results open a perspective of ‘refactoring’ key parts of widely used scientific computing methods. We mention only Schur-complement (or Dirichlet-to-Neumann) maps for elliptic PDEs with variable coefficients which constitute, in discretized form, a key component in many algorithms of scientific computation.

A further, broad range of applications for the considered operator surrogates is *efficient numerical realization of domain-to-solution maps* for elliptic PDEs. Upon pullback onto one common, canonical reference domain, physical domain shapes are encoded in variable coefficients of the transformed PDE, and the domain-to-solution map is equivalent to the coefficient-to-solution map. Such maps feature the holomorphy required for the presently developed theory (e.g. [16] for Navier-Stokes equations, [24] for nonlocal (boundary) integrodifferential operators, [28] for time-harmonic Maxwell equations). We mention [43] for a recent application to deep NNs in computational physiology.

The main results, Theorems 1 and 3, considered in detail the emulation of holomorphic maps \mathcal{G} by either NNs or by novel generalized polynomial chaos operator surrogates. The latter class of surrogate operators allows, in particular, for *efficient deterministic construction w.r. to the number of the encoded input parameters*. The presently developed technical tools also accommodate other approximation architectures for the parametric surrogate map $\tilde{\mathbf{G}}_N$ in (3), e.g. tensor-networks or multipole operators (e.g. [29]).

While the present results are limited to the case of bounded parameter ranges in the basis representations of admissible input data from the spaces \mathcal{X}^s , expression rates for inputs subject to a Gaussian measure on the input spaces \mathcal{X}^s will require admitting unbounded parameter ranges of encoded input data. Here, similar results are conceivable, but will require *ReLU DNN emulations of Wiener polynomial chaos expansions* as in [46].

Our analysis exploited the quantified holomorphy of the function space map \mathcal{G} (or its countably-parametric version \mathbf{G}) in an essential way; while at first sight, this may seem restrictive, in recent years large classes of maps of engineering interest have been identified which admit this property. We only mention [16] for the stationary Navier-Stokes equations, [28] for time-harmonic Maxwell equations and [24] for shape to boundary integral operator maps. Both, generalization error bounds and the work bounds do not incur the curse of dimensionality, which enters in straightforward application of classical approximation results.

The discussed gpc surrogate operator constructions assumed availability of noise-free evaluations of $\langle \mathcal{G}(a), \tilde{\eta}_j \rangle$ in at most N pairs of $C_r^s(\mathcal{X}) \times \tilde{\Psi}_y$. Accounting for effects of “noisy” evaluations of these functionals, e.g. through numerical discretizations, will be considered elsewhere.

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