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Neural and spectral operator surrogates: unified construction and expression rate bounds

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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 spectral 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, generalized 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

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remains 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. [58, 72, 79, 31]), 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 [53, 49, 75, 47, 9, 7] 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., [48, 39] and the references there. Versions of the *DNN universal approximation theorems for operator learning* have been established, following the pioneering work [13], recently in [76, 25, 39, 41, 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., [36] and [57] 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 [61], building on earlier results on gpc emulation rates in [6] and the references there. We also mention recent publications where operator expression rate bounds have been proved for particular en- and decoding systems, such as KL-expansions [40].

For coefficient-to-solution maps of elliptic PDEs, *on domains consisting of smooth coefficient functions*, it was shown recently in [50] 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 7 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} . Complexification is then a standard process resulting in a (canonical) extension [51].

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 [50] 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 2 and 4, 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 7 then has corresponding results for the spectral operator surrogate.

We note that alternative approaches to analyzing the generalization error of operator surrogates, such as methods from statistical learning theory (e.g. [46, 42] and the references there), deliver lower approximation rates (these results do not require holomorphy of \mathcal{G} , however).

1.3 Layout of this text

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- [44], Chebyšev- [27] and Karhunen-Loève type, as well as biorthogonal bases of spline and wavelet type (see, e.g., [73] and the references there). Examples are furnished by Sobolev and Besov spaces, and by reproducing kernel Hilbert spaces of covariance operators in statistics (e.g. [70] and [66] and the references there).

Section 3 gives a succinct statement of our main results in Theorems 2 and 4; 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 2 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 *spectral or generalized polynomial chaos operator* (“*gpc operator*”, or “*spectral 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 7 on gpc operator expression rates yields an explicit deterministic construction procedure realizing the proposed operator emulations.

Finally, in Section 7 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 real 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 summable sequences indexed over \mathbb{N} is denoted by $\ell^2(\mathbb{N})$. Complex valued, square summable sequences shall be denoted with $\ell^2(\mathbb{N}, \mathbb{C})$. The (unique, cf. e.g. [51]) complexification of a real Hilbert space \mathcal{H} is denoted by $\mathcal{H}_{\mathbb{C}}$.

2 Setting

We fix notation and introduce, following established practice in statistical learning theory, encoder and decoder operators as stipulated in [13, 41]. Throughout, \mathcal{X}, \mathcal{Y} shall denote 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 [39, 25] 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 Finite Element frames (e.g. [32]) or more general directional representation systems [29] comprising wavelet, shearlet (e.g. [28]) and curvelet 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. [70, 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 (see, e.g., [32], and the original construction due to P. Oswald in space dimension $d = 2$ [55], and subsequently in polyhedra, in [56] and the references there. A frame property in $H_0^1(D)$ of the subspace splittings furnished by the BPX iteration is also implicitly shown in [10]).

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*

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

Parseval frames are frames Ψ with ideal conditioning $\lambda_\Psi = \Lambda_\Psi = 1$.

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

$$\left\| \sum_{j \in \mathbb{N}} v_j \psi_j \right\|_{\mathcal{X}}^2 = \|F' \mathbf{v}\|_{\mathcal{X}}^2 \leq \Lambda_\Psi^2 \sum_{j \in \mathbb{N}} v_j^2 = \Lambda_\Psi^2 \|\mathbf{v}\|_{\ell_2}^2. \quad (6)$$

The *frame operator* $S := F'F : \mathcal{X} \rightarrow \mathcal{X}$ is boundedly invertible, self-adjoint and positive (e.g. [17, 33]) with $\|F'F\|_{\mathcal{X} \rightarrow \mathcal{X}} = \Lambda_\Psi^2$ and $\|(F'F)^{-1}\|_{\mathcal{X} \rightarrow \mathcal{X}} = \lambda_\Psi^{-2}$, [17, Lemma 5.1.5].

With the pseudoinverse $(F')^\dagger = F(F'F)^{-1}$ of the synthesis operator, given by

$$(F')^\dagger : \mathcal{X} \rightarrow \ell^2(\mathbb{N}) : f \mapsto \{\langle f, S^{-1} \psi_j \rangle\}_{j \in \mathbb{N}},$$

the *frame decomposition theorem* asserts that every $f \in \mathcal{X}$ can be uniquely and stably reconstructed from a corresponding sequence of frame coefficients via

$$f = F'(F')^\dagger f = \sum_{j \in \mathbb{N}} \langle f, S^{-1} \psi_j \rangle \psi_j = \sum_{j \in \mathbb{N}} \langle f, \psi_j \rangle S^{-1} \psi_j.$$

This highlights the importance of the collection $\tilde{\Psi} := S^{-1}\Psi$. It is a frame for \mathcal{X} which is referred to as the *canonical dual frame* of Ψ . Its analysis operator is $\tilde{F} := (F')^\dagger = F(F'F)^{-1}$, and its frame bounds (5) are $\lambda_{\tilde{\Psi}}^{-1}$ and $\Lambda_{\tilde{\Psi}}^{-1}$, respectively.

The frame decomposition theorem takes the form (e.g. [17, 33])

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

Whence every $v \in \mathcal{X}$ has a representation $v = \mathbf{v}^\top \Psi$ 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 equivalent to Ψ being a frame for \mathcal{X} (see, e.g., [33, Thm. 8.29 (b)]).

Remark 2. [Continuous-discrete equivalence] Given a (generally nonlinear) map $\mathcal{G} : \mathcal{X} \rightarrow \mathcal{Y}$ between separable Hilbert spaces \mathcal{X} and \mathcal{Y} over \mathbb{R} which are endowed with frames $\Psi_{\mathcal{X}}$ and $\Psi_{\mathcal{Y}}$, respectively, there exists a *coordinate map* $\mathbf{G} = \mathbf{G}(\Psi_{\mathcal{X}}, \Psi_{\mathcal{Y}}) : \ell_2(\mathbb{N}) \rightarrow \ell_2(\mathbb{N})$ such that there holds

$$\mathcal{G} = F'_{\mathcal{Y}} \circ \mathbf{G} \circ (F'_{\mathcal{X}})^\dagger = F'_{\mathcal{Y}} \circ \mathbf{G} \circ \tilde{F}_{\mathcal{X}}. \quad (9)$$

Here and throughout, in case that the representation systems $\Psi_{\mathcal{X}}$ and $\Psi_{\mathcal{Y}}$ are clear from the context, we write \mathbf{G} in place of $\mathbf{G}(\Psi_{\mathcal{X}}, \Psi_{\mathcal{Y}})$.

Remark 3. [Uniqueness of coordinate sequence] Unless Ψ is a Riesz basis (see below), representation of $v \in \mathcal{X}$ as $v = \mathbf{v}^\top \Psi$ 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 [17, 33] and the references there.

2.2.2 Riesz Bases

Riesz bases are special cases of frames which are defined as follows (e.g. [17, 33]).

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 $j \in \mathbb{N}$.

Every Riesz basis of \mathcal{X} is a frame: there exist *Riesz constants* $0 < \lambda_{\Psi} \leq \Lambda_{\Psi} < \infty$ such that

$$\forall (c_j)_{j \in \mathbb{N}} \in \ell^2(\mathbb{N}) : \quad \lambda_{\Psi}^2 \sum_{j \in \mathbb{N}} |c_j|^2 \leq \left\| \sum_{j \in \mathbb{N}} c_j \psi_j \right\|_{\mathcal{X}}^2 \leq \Lambda_{\Psi}^2 \sum_{j \in \mathbb{N}} |c_j|^2. \quad (10)$$

There holds a continuous-discrete equivalence: any $v \in \mathcal{X}$ can be *equivalently represented* by the sequence $\mathbf{c} = (c_j)_{j \in \mathbb{N}}$ of its coefficients w.r. to Ψ .

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 [17, Sec. 5] for further details and proofs.

Remark 4. Constructions of piecewise polynomial Riesz bases for Sobolev spaces in polytopal domains $D \subset \mathbb{R}^d$ are available (e.g. [24, 67] and the references there). We mention in particular [22] where locally supported wavelet bases for C^0 -Lagrange finite element spaces on regular, simplicial triangulations of polytopal domains D are constructed. The constructions in [22] provide Riesz bases in $\mathcal{X} = H^1(D)$ and $\mathcal{X} = H_0^1(D)$.

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 [33], Daubechies - type wavelets [23] and orthogonal polynomials [68]. 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. [66]). 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

$$\Psi_{\mathcal{X}} = (\psi_j)_{j \in \mathbb{N}}, \quad \tilde{\Psi}_{\mathcal{X}} = (\tilde{\psi}_j)_{j \in \mathbb{N}}, \quad \Psi_{\mathcal{Y}} = (\eta_j)_{j \in \mathbb{N}}, \quad \tilde{\Psi}_{\mathcal{Y}} = (\tilde{\eta}_j)_{j \in \mathbb{N}}. \quad (11)$$

to denote frames and their **canonical** 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 (cf. (9))

$$\mathcal{E} := \tilde{F}_{\mathcal{X}} = \begin{cases} \mathcal{X} \rightarrow \ell^2(\mathbb{N}) \\ x \mapsto (\langle x, \tilde{\psi}_j \rangle)_{j \in \mathbb{N}}, \end{cases} \quad \mathcal{D} := F'_{\mathcal{Y}} = \begin{cases} \ell^2(\mathbb{N}) \rightarrow \mathcal{Y} \\ (y_j)_{j \in \mathbb{N}} \mapsto \sum_{j \in \mathbb{N}} y_j \eta_j. \end{cases} \quad (12)$$

Remark 5. 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 (12) are boundedly invertible operators.

Remark 6. Encoders and decoders with rate-optimal performance for subsets $\mathcal{X}^s \subset \mathcal{X}$ are obtained from *n-term truncation*. In the most straightforward 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 bounded domains $D \subset \mathbb{R}^d$ with summability indices $q \in (0, 1]$ (see, e.g., [70, 71]).

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 weight 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

$$\|x\|_{\mathcal{X}^s}^2 := \sum_{j \in \mathbb{N}} \langle x, \tilde{\psi}_j \rangle^2 w_j^{-2s}, \quad \|y\|_{\mathcal{Y}^t}^2 := \sum_{j \in \mathbb{N}} \langle y, \tilde{\eta}_j \rangle^2 w_j^{-2t}. \quad (13)$$

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 $\mathcal{E} = \tilde{F}_{\mathcal{X}}$, $\mathcal{D} = F'_{\mathcal{X}}$ 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 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

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

Using that $\mathcal{D} \circ \mathcal{E}$ is the identity on \mathcal{X} (cp. (7)), we find that $\mathcal{E} \circ \mathcal{D} \circ \mathcal{E} = \mathcal{E}$ and thus $\mathcal{E} \circ \mathcal{D}$ is the identity on $\mathcal{E}(\mathcal{X})$. Hence

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.

$$\|x_n - \tilde{x}\|_{\mathcal{X}^s} = \|\mathcal{E}(x_n) - \mathcal{E}(\tilde{x})\|_{\ell_2^s} = \|\mathcal{E}(x_n) - \mathcal{E}(\mathcal{D}(\mathbf{x}))\|_{\ell_2^s} = \|\mathcal{E}(x_n) - \mathbf{x}\|_{\ell_2^s} \rightarrow 0$$

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

Remark 7. 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, [51]) 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 (12) act on weighted, complex sequence spaces.

Remark 8. 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.

Remark 9. The biorthogonal spline wavelet bases constructed in [22] are continuous, piecewise polynomial, and are stable in the Sobolev spaces $H^s(\mathbb{D})$ for $|s| \leq 3/2$. Scaling ψ_j obtained in [22] so that the Riesz basis property holds in $\mathcal{X} = L^2(\mathbb{D})$, appropriate choices of the weight sequence w_j provides in particular (13) with $0 \leq s \leq 3/2$ in $\mathcal{X}^s = H^s(\mathbb{D})$. In addition, the wavelet constructions ψ_j and $\tilde{\psi}_j$ in [22] can furnish wavelet systems with vanishing moments of any a-priori required polynomial order.

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 (11), 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 (12). With

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

and \mathbf{w} as in Section 2.4, for $s > \frac{1}{2}$, and a scaling factor $r > 0$ set

$$\sigma_r^s := \begin{cases} U \rightarrow \mathcal{X} \\ \mathbf{y} \mapsto r \sum_{j \in \mathbb{N}} w_j^s y_j \psi_j. \end{cases} \quad (14)$$

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}

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

and additionally for $s \geq 0$

$$\begin{aligned}
C_r^s(\mathcal{X}) &:= \{a \in \mathcal{X} : \mathcal{E}(a) \in \times_{j \in \mathbb{N}} [-rw_j^s, rw_j^s]\} \\
&= \left\{ a \in \mathcal{X} : \sup_{j \in \mathbb{N}} |\langle a, \tilde{\psi}_j \rangle| w_j^{-s} \leq r \right\}.
\end{aligned} \tag{15}$$

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

Remark 10. Observe $C_r^s(\mathcal{X}) \subseteq \tilde{C}_r^s(\mathcal{X})$. 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 (14) 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 frames, this does not hold in general, 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 11. 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 $s > 1$, $t > 0$, $M < \infty$ and an open set $O_{\mathbb{C}} \subseteq \mathcal{X}_{\mathbb{C}}$ containing $\tilde{C}_r^s(\mathcal{X})$ such that $\sup_{a \in O_{\mathbb{C}}} \|\mathcal{G}(a)\|_{\mathcal{Y}_{\mathbb{C}}^t} \leq M$ and $\mathcal{G} : O_{\mathbb{C}} \rightarrow \mathcal{Y}_{\mathbb{C}}$ is holomorphic.*

Remark 12. Assumption 1 is for instance satisfied by solution operators corresponding to second order elliptic PDEs. Specific examples will be discussed in full detail in Section 7 ahead.

We emphasize that in Assumption 1 the holomorphy condition is merely required w.r.t. the topology of $\mathcal{Y}_{\mathbb{C}}$ and not with respect to the stronger topology of $\mathcal{Y}_{\mathbb{C}}^t$. We will see in Lemma 3 below, that the assumed boundedness already implies holomorphy of $\mathcal{G} : O_{\mathbb{C}} \rightarrow \mathcal{Y}_{\mathbb{C}}^{t'}$ for any $t' \in [0, t)$.

3.1 Universality

We observe that, in the present setting (3), there holds a version of the universal approximation theorem. We consider admissible activation functions as in [43]:

$$\begin{aligned}
\mathcal{A} &:= \left\{ \sigma \in L_{\text{loc}}^{\infty}(\mathbb{R}) \text{ is not polynomial and the closure} \right. \\
&\quad \left. \text{of the points of discontinuity has Lebesgue measure } 0 \right\}.
\end{aligned}$$

Then there holds:

Theorem 1. *Let \mathcal{X} , \mathcal{Y} be two separable Hilbert spaces, let $\mathcal{G} : \mathcal{X} \rightarrow \mathcal{Y}$ be continuous and let $\sigma \in \mathcal{A}$.*

Then there exists a sequence of operator nets $\tilde{\mathcal{G}}_n : \mathcal{X} \rightarrow \mathcal{Y}$, $n \in \mathbb{N}$, with architecture (3) such that

$$\forall x \in \mathcal{X} : \lim_{N \rightarrow \infty} \tilde{\mathcal{G}}_N(x) = \mathcal{G}(x).$$

The convergence is uniform on every compact subset of \mathcal{X} .

The proof is given in [60, Appendix].

3.2 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 map of the form

$$\tilde{\mathbf{G}} = A_L \circ \text{ReLU} \circ A_{L-1} \cdots \circ A_1 \circ \text{ReLU} \circ A_0 \quad (16)$$

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 (16) is used to find choices of the weights and biases. Alternatively, concrete constructions of the NN weights W_j and biases b_j based on *a-priori specified samples of input-output data pairs* are sometimes proposed (e.g. [35]). 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.

$$\text{size}(\tilde{\mathbf{G}}) := \sum_{0 \leq j \leq L} \|W_j\|_0 + \|b_j\|_0 \quad (17)$$

as the *size of the NN* in (16). In other words, the “size” of the network is the number of trainable network parameters.

Remark 13. Any realization of a NN $\tilde{\mathbf{G}}$ of the form (16) represents a map from $\mathbb{R}^{n_0} \rightarrow \mathbb{R}^{n_{L+1}}$. Throughout we will also understand $\tilde{\mathbf{G}}$ as map from $\ell^2(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$: Let $\tilde{A}_0 \in \mathbb{R}^{n_1 \times \infty}$ and $\tilde{A}_L \in \mathbb{R}^{\infty \times n_L}$ be obtained from A_0 and A_L by padding the (infinitely many) entries with zeros according to

$$\tilde{A}_0 = \begin{pmatrix} (A_0)_{11} & \cdots & (A_0)_{1n_0} & 0 & \cdots \\ \vdots & \ddots & \vdots & \vdots & \cdots \\ (A_0)_{n_1 1} & \cdots & (A_0)_{n_1 n_0} & 0 & \cdots \end{pmatrix}, \quad \tilde{A}_L = \begin{pmatrix} (A_L)_{11} & \cdots & (A_L)_{1n_L} \\ \vdots & \ddots & \vdots \\ (A_L)_{n_{L+1} 1} & \cdots & (A_L)_{n_{L+1} n_L} \\ 0 & \cdots & 0 \\ \vdots & \vdots & \vdots \end{pmatrix}.$$

Formally replacing A_0, A_L by \tilde{A}_0, \tilde{A}_L in (16), $\tilde{\mathbf{G}}$ in (16) 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. (17)). The function it realizes is 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. 13.

Theorem 2. *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*

$$\sup_{a \in C_r^s(\mathcal{X})} \|\mathcal{G}(a) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathcal{E}(a)))\|_{\mathcal{Y}} \leq CN^{-\min\{s-1, t\} + \delta}. \quad (18)$$

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

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

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. (13), (15) and Rmk. 11), we trivially get the following:

Corollary 1. *Consider the setting of Theorem 2. 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*

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

Remark 14. 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 2 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 3.4 ahead.

3.3 Mean-square error for NN operator surrogates

We can improve the operator approximation rate of Theorem 2, 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. 10, the pushforward $(\sigma_r^s)_\# \mu$ of μ under σ_r^s then constitutes a measure on $C_r^s(\mathcal{X})$.

Theorem 3. *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*

$$\|\mathcal{G} - \mathcal{D} \circ \tilde{\mathbf{G}}_N \circ \mathcal{E}\|_{L^2(C_r^s(\mathcal{X}), (\sigma_r^s)_\# \mu; \mathcal{Y})} \leq CN^{-\min\{s-\frac{1}{2}, t\} + \delta}. \quad (19)$$

3.4 Worst-case error for spectral 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. 13). The advantage over the NN operator surrogate in Theorem 2 is that, while we achieve the same convergence rate, the proof is constructive, and one can explicitly compute p_N as an interpolation polynomial, based on a finite set of *judiciously chosen* (rather than random, i.i.d) input-output pairs. Hence, the ‘‘training’’ consists of an explicit and deterministic construction, rather than the minimization of a (typically non-convex) loss by stochastic optimization methods. Moreover, and as a consequence, we are able to obtain (higher-order) deterministic (‘‘worst-case’’) generalization bounds, rather than (low-order) probabilistic bounds as commonly applied within statistical learning theory.

Contrary to Section 3.3, we now allow for $\Psi_{\mathcal{X}}$ again to be a frame.

Theorem 4. *Consider the setting of Theorem 2. 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 $(a, j) \in C_r^s(\mathcal{X}) \times \mathbb{N}$.

Prior to proving these results, 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 spectral 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 2 and Theorem 3

With $s > 1$ and σ_r^s as in (14) let in the following

$$\mathbf{G} := \tilde{\mathbb{F}}_{\mathcal{Y}} \circ \mathcal{G} \circ \sigma_r^s. \quad (20)$$

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

$$u(\mathbf{y}) := (\mathcal{D} \circ \mathbf{G})(\mathbf{y}) = \mathcal{G}(\sigma_r^s(\mathbf{y})) \quad (21)$$

is well-defined for $\mathbf{y} \in U$. To prove Theorem 2 we first show that $\mathbf{G} : U \rightarrow \ell^2$ can be approximated.

4.1 Auxiliary results

We start by showing that the functions $\mathcal{G} : O \rightarrow \mathcal{Y}_{\mathbb{C}}$ in Assumption 1 are holomorphic w.r.t. the topologies of $\mathcal{Y}_{\mathbb{C}}^{t'}$ for any $t' < t$.

Lemma 3. *Let Assumption 1 hold.*

Then for every $t' \in [0, t)$, the map $\mathcal{G} : O_{\mathbb{C}} \rightarrow \mathcal{Y}_{\mathbb{C}}^{t'}$ is holomorphic.

To prove Lemma 3, use the following result:

Proposition 1. *Let X, Y, Z be three complex Banach spaces and $O \subseteq X$ open, nonempty. Let $\iota : Z \rightarrow Y$ be a bounded injective linear map. Then the following statements are equivalent:*

- (i) $\iota \circ \mathcal{G} : O \rightarrow Y$ is holomorphic and $\mathcal{G} : O \rightarrow Z$ is continuous,
- (ii) $\mathcal{G} : O \rightarrow Z$ is holomorphic.

Proof. (ii) \Rightarrow (i): Holomorphy of $\mathcal{G} : O \rightarrow Z$ implies its continuity, and the composition of the holomorphic map $\mathcal{G} : O \rightarrow Z$ with the bounded linear (thus holomorphic) map $\iota : Z \rightarrow Y$ is holomorphic (as a composition of holomorphic functions).

(i) \Rightarrow (ii): Fix a point $x \in O$ and let $r > 0$ be so small that the ball of radius $2r$ around x in X is contained in O . Additionally fix $h \in X$ with $0 < \|h\|_X \leq 1$ and $\xi \in \mathbb{C}$ with $|\xi| < r$ and consider the Bochner integral

$$\frac{1}{2\pi i} \int_{\{\zeta \in \mathbb{C} : |\zeta|=r\}} \frac{\mathcal{G}(x + \zeta h)}{\zeta - \xi} d\zeta \in Y', \quad (22)$$

which is understood w.r.t. the arclength measure on the circle $C_r := \{\zeta \in \mathbb{C} : |\zeta| = r\}$, oriented counterclockwise.

Continuity of $\mathcal{G} : O \rightarrow Z$ implies that $\zeta \mapsto \mathcal{G}(x + \zeta h) \in Z$ is measurable w.r.t. Borel σ -algebra on C_r , and that $\{\mathcal{G}(x + \zeta h) : \zeta \in C_r\} \subseteq Z$ is a compact (and thus separable) subset of Z . Hence (22) is well-defined as a Bochner integral. Using (i) the fact that bounded linear mappings may be exchanged with the Bochner integral and (ii) Cauchy's integral formula (for the holomorphic map $\iota \circ \mathcal{G} : O \rightarrow Y$) in complex Banach spaces, see [12, 13.3] or [77, Thm. 1.2.11] for this specific version, it holds

$$\begin{aligned} \iota \left(\frac{1}{2\pi i} \int_{\{\zeta \in \mathbb{C} : |\zeta|=r\}} \frac{\mathcal{G}(x + \zeta h)}{\zeta - \xi} d\zeta \right) &= \frac{1}{2\pi i} \int_{\{\zeta \in \mathbb{C} : |\zeta|=r\}} \frac{\iota \circ \mathcal{G}(x + \zeta h)}{\zeta - \xi} d\zeta \\ &= \iota \circ \mathcal{G}(x + \xi h) \end{aligned}$$

for all complex $|\xi| < r$.

Injectivity of ι yields

$$\frac{1}{2\pi i} \int_{\{\zeta \in \mathbb{C}: |\zeta|=r\}} \frac{\mathcal{G}(x + \zeta h)}{\zeta - \xi} d\zeta = \mathcal{G}(x + \xi h) \in Z.$$

Continuity of \mathcal{G} implies its local boundedness, and thus we can conclude that this function is complex differentiable for $\xi \in \mathbb{C}$ with $|\xi| < r$. This verifies so-called Gâteaux holomorphy of $\mathcal{G} : O \rightarrow Z$. Together with the continuity of this map, this implies holomorphy in the sense of complex Fréchet differentiability [12, 14.9]. \square
Proof.[of Lemma 3] Applying Prop. 1 with $X := \mathcal{X}_{\mathbb{C}}$, $Y := \mathcal{Y}_{\mathbb{C}}$ and $Z := \mathcal{Y}'_{\mathbb{C}}$, in order to show the lemma it suffices to check that $\mathcal{G} : O_{\mathbb{C}} \rightarrow \mathcal{Y}'$ is continuous, since we trivially have a continuous embedding $\iota : \mathcal{Y}'_{\mathbb{C}} \rightarrow \mathcal{Y}_{\mathbb{C}}$.

To do so fix $\varepsilon > 0$ and $x \in O_{\mathbb{C}}$. We need to show that there exists $\delta > 0$ such that $\|x - \tilde{x}\|_{\mathcal{X}_{\mathbb{C}}} < \delta$ implies $\|\mathcal{G}(x) - \mathcal{G}(\tilde{x})\|_{\mathcal{Y}'_{\mathbb{C}}} < \varepsilon$. For any $n \in \mathbb{N}$

$$\begin{aligned} \|\mathcal{G}(x) - \mathcal{G}(\tilde{x})\|_{\mathcal{Y}'_{\mathbb{C}}}^2 &= \sum_{j \in \mathbb{N}} |\langle \mathcal{G}(x) - \mathcal{G}(\tilde{x}), \tilde{\eta}_j \rangle|^2 w_j^{-2t'} \\ &\leq \sum_{j=1}^n |\langle \mathcal{G}(x) - \mathcal{G}(\tilde{x}), \tilde{\eta}_j \rangle|^2 w_j^{-2t'} + 2(\sup_{j>n} w_j^{2(t-t')}) \sum_{j>n} (|\langle \mathcal{G}(x), \tilde{\eta}_j \rangle|^2 + |\langle \mathcal{G}(\tilde{x}), \tilde{\eta}_j \rangle|^2) w_j^{-2t'} \\ &\leq \|\mathcal{G}(x) - \mathcal{G}(\tilde{x})\|_{\mathcal{Y}_{\mathbb{C}}}^2 \sum_{j=1}^n w_j^{-2t'} + 4M^2(\sup_{j>n} w_j^{2(t-t')}), \end{aligned} \quad (23)$$

where we have used that $\sum_{j \in \mathbb{N}} |\langle \mathcal{G}(a), \tilde{\eta}_j \rangle|^2 w_j^{-2t'} = \|\mathcal{G}(a)\|_{\mathcal{Y}'_{\mathbb{C}}}^2 \leq M^2$ for all $\tilde{x} \in O$ by Assumption 1. Since $(w_j)_{j \in \mathbb{N}}$ is a null-sequence, by choosing n large enough, the second term on the right-hand side of (23) is less than $\varepsilon/2$. Since $\mathcal{G} : O_{\mathbb{C}} \rightarrow \mathcal{Y}_{\mathbb{C}}$ is continuous, there exists $\delta > 0$ depending on ε and n such that $\|x - \tilde{x}\|_{\mathcal{X}_{\mathbb{C}}} < \delta$ implies the first term on the right-hand side of (23) to be less than $\varepsilon/2$. This concludes the proof. \square

It is well known, that algebraic decay of the “input” sequence $w_j^s \psi_j$ in (14) is inherited by the Legendre coefficients of the “output” $u(\mathbf{y})$, see for example [15] and the earlier works [19, 20] for the analysis for some specific choices of \mathcal{G} , and [18] for the general analysis. To provide a statement of this type, we denote by L_n the n -th Legendre polynomial normalized such that $\frac{1}{2} \int_{-1}^1 L_n(x)^2 dx = 1$. In the following \mathcal{F} stands for the set of infinite dimensional multiindices with “finite support”

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

where $|\mathbf{v}| := \sum_{j \in \mathbb{N}} v_j$. For such multiindices and $\mathbf{y} = (y_j)_{j \in \mathbb{N}} \in U = [-1, 1]^{\mathbb{N}}$ we write

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

where $\text{supp } \mathbf{v} := \{j \in \mathbb{N} : v_j \neq 0\}$ and 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., [63, Theorem 2.12], $(L_{\mathbf{v}})_{\mathbf{v} \in \mathcal{F}}$ is an orthonormal basis of $L^2(U, \mu)$. Furthermore, there holds the bound

$$\|L_{\mathbf{v}}\|_{L^\infty(U)} \leq \prod_{j \in \mathbb{N}} (1 + 2v_j)^{1/2} \quad (24)$$

for all $\mathbf{v} \in \mathcal{F}$, see [52, §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 [77, 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 $\mathbf{v} = (v_j)_{j \in \mathbb{N}} \in \mathcal{F}$ we write $\boldsymbol{\mu} \leq \mathbf{v}$ iff $\mu_j \leq v_j$ 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 5. *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 $\omega_{\mathbf{v}} := \prod_{j \in \text{supp } \mathbf{v}} (1 + 2v_j)$ 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 $\mathbf{v} \in \mathcal{F}$*

$$\omega_{\mathbf{v}}^\tau \left\| \int_U L_{\mathbf{v}}(\mathbf{y}) u(\mathbf{y}) \, d\mu(\mathbf{y}) \right\|_{\mathcal{Y}'} \leq C a_{\mathbf{v}}, \quad (25)$$

(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 $\Lambda_N := \{\mathbf{v}_i : i \leq N\} \subseteq \mathcal{F}$ is downward closed for each $N \in \mathbb{N}$, and additionally*

$$m(\Lambda_N) := \sup_{\mathbf{v} \in \Lambda_N} |\mathbf{v}| = O(\log(|\Lambda_N|)), \quad d(\Lambda_N) := \sup_{\mathbf{v} \in \Lambda_N} |\text{supp } \mathbf{v}| = o(\log(|\Lambda_N|)) \quad (26)$$

as $N \rightarrow \infty$,

(iii) *there exist $T > 1$ and $t > 0$ such that with*

$$\boldsymbol{\rho} = (\rho_j)_{j \in \mathbb{N}} \quad \text{where} \quad \rho_j := \max\{T, t w_j^{s(p-1)}\} \quad (27)$$

and $e_{\mathbf{v}} := \boldsymbol{\rho}^{\mathbf{v}}$ it holds $(a_{\mathbf{v}} e_{\mathbf{v}})_{\mathbf{v} \in \mathcal{F}} \in \ell^1(\mathcal{F})$ and $(e_{\mathbf{v}}^{-1})_{\mathbf{v} \in \mathcal{F}} \in \ell^{p/(1-p)}$,

(iv) *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 $\sum_{j \in \mathbb{N}} \|w_j^s \psi_j\|_{\mathcal{X}}^p \leq \Lambda_{\boldsymbol{\Psi}}^{p/2} \sum_{j \in \mathbb{N}} w_j^{sp} < \infty$, where we used that $\|\psi_j\|_{\mathcal{X}} \leq \Lambda_{\boldsymbol{\Psi}}^{1/2}$ by (6). By Lemma 3 the map $\mathcal{G} : \mathcal{O}_{\mathbb{C}} \rightarrow \mathcal{Y}'_{\mathbb{C}}$ is holomorphic and uni-

formly 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_C . Thus $u(\mathbf{y}) := \mathcal{G}(\sigma_r^s(\mathbf{y}))$ satisfies [77, Assumption 1.3.7].

Now [77, 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 [77, Theorem 2.2.10 (iii)] and [77, Lemma 1.4.15]. We apply [77, Theorem 2.2.10 (iii)] here with the set \mathfrak{J} occurring in [77, Theorem 2.2.10 (iii)] chosen as $\mathfrak{J} = \mathbb{N}_0$. Item (iii) then holds by [77, Theorem 2.2.10 (iii)]. Finally (iv) holds by [77, Corollary 2.2.12]. \square

To approximate the bounded function $u : U \rightarrow \mathcal{Y}$ in (21), we first expand it in the frame $(\eta_j L_{\mathbf{v}}(\mathbf{y}))_{j, \mathbf{v}}$ of $L^2(U, \mu; \mathcal{Y})$:

$$u(\mathbf{y}) = \mathcal{G}(\sigma_r^s(\mathbf{y})) = \sum_{j \in \mathbb{N}} \sum_{\mathbf{v} \in \mathcal{F}} c_{\mathbf{v}, j} \eta_j L_{\mathbf{v}}(\mathbf{y}) \quad (28a)$$

with coefficients

$$c_{\mathbf{v}, j} := \int_U L_{\mathbf{v}}(\mathbf{y}) \langle \mathcal{G}(\sigma_r^s(\mathbf{y})), \tilde{\eta}_j \rangle d\mu(\mathbf{y}) \quad (28b)$$

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

Proposition 2. *Consider the setting of Theorem 5. 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

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

Together with (25) this gives the statement. \square

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

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

In addition,

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

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 15. The bounds in the above lemma are optimal as can be checked.

4.2 Proof in a particular case

We prove a particular case of Theorem 2, with fixed parameter range $y_j \in [-1, 1]$.

Theorem 6. *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

$$\sup_{\mathbf{y} \in U} \|\mathcal{G}(\sigma_r^s(\mathbf{y})) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathbf{y}))\|_{\mathcal{Y}} \leq CN^{-\min\{s-1, t\} + \delta} \quad (29)$$

and

$$\|\mathcal{G}(\sigma_r^s(\mathbf{y})) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathbf{y}))\|_{L^2(U, \mathcal{Y})} \leq CN^{-\min\{s-\frac{1}{2}, t\} + \delta}. \quad (30)$$

Proof. Let $(a_{\mathbf{v}})_{\mathbf{v} \in \mathcal{F}}$ and the enumeration $(\mathbf{v}_i)_{i \in \mathbb{N}}$ be as in Theorem 5 (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 5. By [54, 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 (26) one has the bound

$$\text{size}((\tilde{L}_{\mathbf{v}})_{\mathbf{v} \in \Lambda_N}) = O(N \log(N)^4 \log(1/\gamma)) \quad (31)$$

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 (31) is $O(N \log(N)^5)$.

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

$$\omega_{\mathbf{v}_i}^{1/2} \left(\sum_{j \in \mathbb{N}} w_j^{-2t'} c_{\mathbf{v}_i, j}^2 \right)^{1/2} \lesssim a_{\mathbf{v}_i} \lesssim i^{-s+\frac{\delta}{2}}. \quad (32a)$$

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

$$w_j^{t'} \lesssim j^{-t+\frac{\delta}{2}}. \quad (32b)$$

We now show (29) and (30) separately.

- (i) Due to (32) 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

$$\sum_{i \in \mathbb{N}} \omega_{\mathbf{v}_i}^{1/2} \left(\sum_{j > m_i} c_{\mathbf{v}_i, j}^2 \right)^{1/2} \leq N^{-\min\{s-1, t\} + \delta}. \quad (33)$$

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

$$\tilde{g}_j(\mathbf{y}) := \sum_{\{i \in \mathbb{N} : m_i \geq j\}} \tilde{L}_{\mathbf{v}_i}(\mathbf{y}) c_{\mathbf{v}_i, j}. \quad (34)$$

Then by (28) 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 (24) and (33) 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 (29).

The size of $\tilde{\mathbf{G}}_N = (\tilde{g}_j)_{j \in \mathbb{N}}$ in (34) 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 (32) 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

$$\sum_{i \in \mathbb{N}} \sum_{j > m_i} c_{\mathbf{v}_i, j}^2 \leq N^{-\min\{s-\frac{1}{2}, t\} + \delta}. \quad (35)$$

The rest of the calculation is similar as in the first case. Let \tilde{g}_j be as in (34). Then by (28) and because $(L_{\mathbf{v}}(\mathbf{y}) \eta_j)_{\mathbf{v}, j}$ is a frame of $L^2(U, \mu; \mathcal{Y})$

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

where $\Lambda_{\mathcal{Y}}$ denotes again the upper frame constant in (5) for the frame $\boldsymbol{\Psi}_{\mathcal{Y}} = (\eta_j)_{j \in \mathbb{N}}$. By (35) 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 (30).

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

4.3 Proof of Theorem 2 in the general case

We obtain Theorem 2 from Theorem 6 by a scaling argument, via the weight sequences which characterize the admissible input data.

Introduce the scaling

$$S = \times_{j \in \mathbb{N}} [-rw_j^s, rw_j^s] \rightarrow U : (x_j)_{j \in \mathbb{N}} \mapsto \left(\frac{x_j}{rw_j^s} \right)_{j \in \mathbb{N}}, \quad (36)$$

where $U = [-1, 1]^{\mathbb{N}}$. Then (cp. (12) and (15))

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

Let $\tilde{\mathbf{G}}_N : \ell^2(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$ be as in Theorem 6. Since $\boldsymbol{\sigma}_r^s : U \rightarrow \tilde{C}_r^s(\mathcal{X})$ is surjective and $\tilde{C}_r^s(\mathcal{X}) \supseteq C_r^s(\mathcal{X})$ (see Rmk. 10), (29) in Theorem 6 implies with $\hat{\mathbf{G}}_N := \tilde{\mathbf{G}}_N \circ S$

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

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 6 (cp. Rmk. 13 and (16)).

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 (18). The calculation for (19) is similar.

4.4 Proof of Theorem 3 in the general case

The argument is similar as in Sec. 4.3. Let S be as in (36). Since $\Psi_{\mathcal{X}}$ is assumed to be a Riesz basis, by Rmk. 10 it holds (cp. (14) and (36))

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

With $\tilde{\mathbf{G}}_N$ as in Thm. 6 and $\hat{\mathbf{G}}_N := \tilde{\mathbf{G}}_N \circ S$ we find with (30)

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

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. Further, for the case of uniform approximation we will prove the same convergence rate as in Theorem 2. 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. [14]) 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 $\mathbf{y} = (y_j)_{j \in \mathbb{N}} \in U$

$$(I_{\mathbf{v}}u)(\mathbf{y}) = \sum_{\{\boldsymbol{\mu} \in \mathcal{F} : \boldsymbol{\mu} \leq \mathbf{v}\}} u((\chi_{\mu_j})_{j \in \mathbb{N}}) \prod_{j \in \mathbb{N}} \prod_{\substack{i=0 \\ i \neq \mu_j}}^{v_j} \frac{y_j - \chi_i}{\chi_{\mu_j} - \chi_i}, \quad (37)$$

where $\mathbf{v} \leq \boldsymbol{\mu}$ is understood as $\mu_j \leq v_j$ for all $j \in \mathbb{N}$. The sum in (37) is over $\prod_{j \in \mathbb{N}} (1 + v_j)$ indices, which is finite since $\mathbf{v} \in \mathcal{F}$. We emphasize 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

$$L((\chi_j)_{j=0}^n) \leq (1+n)^\tau \quad \forall n \in \mathbb{N}_0 \quad (38)$$

for some fixed $\tau > 0$. One popular example for such a sequence are the so-called Leja points, see [16] 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

$$I_\Lambda := \sum_{\mathbf{v} \in \Lambda} \zeta_{\Lambda, \mathbf{v}} I_{\mathbf{v}}, \quad \zeta_{\Lambda, \mathbf{v}} := \sum_{\{\mathbf{e} \in \{0,1\}^{\mathbb{N}} : \mathbf{v} + \mathbf{e} \in \Lambda\}} (-1)^{|\mathbf{e}|}. \quad (39)$$

Remark 16. 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 [77, Lemma 1.3.3], [14].

Lemma 5. *Let Λ be finite and downward closed. Then with τ as in (38) 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 6 for NNs, for Smolyak interpolation p_N of the components of the parametric map \mathbf{G} :

Theorem 7. *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 (38) 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

$$\sup_{\mathbf{y} \in U} \|\mathcal{G}(\sigma_r^s(\mathbf{y})) - \mathcal{D}(p_N(\mathbf{y}))\|_{\mathcal{Y}} \leq CN^{-\min\{s-1, t\} + \delta}. \quad (40)$$

Remark 17. 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 (21)).

Before giving the proof of the theorem, we first show a variant of Lemma 4 required for the proof.

Lemma 6. *Let $\alpha > 1$, $\beta > 0$ and assume given three sequences $(a_i)_{i \in \mathbb{N}}$, $(d_j)_{j \in \mathbb{N}}$, $(e_k)_{k \in \mathbb{N}} \subset (0, \infty)^{\mathbb{N}}$ with $\sum_{i \in \mathbb{N}} a_i e_i < \infty$ and $d_j \lesssim j^{-\beta}$, $e_k^{-1} \lesssim k^{1-\alpha}$, for all $i, k \in \mathbb{N}$. Assume additionally that $(d_j)_{j \in \mathbb{N}}$, $(e_k)_{k \in \mathbb{N}}$ are monotonically decreasing. Suppose that there exists $C < \infty$ such that the sequence $(c_{i,j})_{j, i \in \mathbb{N}}$ satisfies*

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

Fix $\delta > 0$. Then 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

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

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,

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

and for $i > n$ we have $(\sum_{j > m_i} c_{i,j}^2)^{1/2} = (\sum_{j \geq 1} c_{i,j}^2)^{1/2} \lesssim a_i$. Note that for $n \in \mathbb{N}$ due to the monotonicity of $(e_k)_{k \in \mathbb{N}}$ and because $\sum_{i \in \mathbb{N}} a_i e_i < \infty$

$$\sum_{i > n} a_i = \sum_{i > n} a_i e_i e_i^{-1} \lesssim e_n^{-1} \lesssim n^{1-\alpha}.$$

Similarly,

$$\sum_{i \leq n} m_i^{-\beta} a_i = \sum_{i \leq n} m_i^{-\beta} a_i e_i e_i^{-1} \lesssim \max_{1 \leq i \leq n} m_i^{-\beta} e_i^{-1} \lesssim \max_{1 \leq i \leq n} \left(\frac{n}{i} \right)^{1-\alpha} i^{1-\alpha} = n^{1-\alpha}.$$

Thus

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

In addition,

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

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 $M(n) \sim N$. \square

Proof. [Proof of Theorem 7] Fix $p \in (\frac{1}{s}, 1]$ such that $\frac{1}{p} \geq s - \delta/2$. Consider Theorem 5 (with “ τ ” being $\frac{3}{2} + \tau$ for the value in (38)), and let $(a_{\mathbf{v}})_{\mathbf{v} \in \mathcal{F}} \in \ell^p(\mathcal{F})$ and $(e_{\mathbf{v}})_{\mathbf{v} \in \mathcal{F}}$ be as in this theorem. Moreover, let $(\mathbf{v}_i)_{i \in \mathbb{N}}$ be an arbitrary enumeration such that

$(e_{\mathbf{v}_i}^{-1})_{i \in \mathbb{N}}$ is monotonically decreasing. According to Theorem 5 (iii) it holds in particular

$$\sum_{i \in \mathbb{N}} a_{\mathbf{v}_i} e_{\mathbf{v}_i} < \infty \quad (41a)$$

and $(e_{\mathbf{v}}^{-1})_{\mathbf{v} \in \mathcal{F}} \in \ell^{p/(1-p)}(\mathcal{F})$. Due to $ie_{\mathbf{v}_i}^{-p/(1-p)} \leq \sum_{j \in \mathbb{N}} e_{\mathbf{v}_j}^{-p/(1-p)} < \infty$ this implies

$$e_{\mathbf{v}_i}^{-1} \lesssim i^{-\frac{1-p}{p}} \leq i^{1-s+\frac{\delta}{2}}. \quad (41b)$$

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

$$\omega_{\mathbf{v}_i}^{3/2+\tau} \left(\sum_{j \in \mathbb{N}} w_j^{-2t'} c_{\mathbf{v}_i, j}^2 \right)^{1/2} \lesssim a_{\mathbf{v}_i} \lesssim i^{-s+\frac{\delta}{2}}. \quad (41c)$$

In addition, 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

$$w'_j \lesssim j^{-t+\frac{\delta}{2}}. \quad (41d)$$

Due to (41) with $\alpha := s - \delta/2$ and $\beta := t - \delta/2$, by Lemma 6 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

$$\sum_{i \in \mathbb{N}} \omega_{\mathbf{v}_i}^{3/2+\tau} \left(\sum_{j > m_i} c_{\mathbf{v}_i, j}^2 \right)^{1/2} \leq N^{-\min\{s-1, t\}+\delta}. \quad (42)$$

Now define for $j \leq N$

$$\Lambda_{N, j} := \{\mathbf{v}_i : m_i \geq j\} = \{\mathbf{v}_i : i \leq \max\{r : m_r \geq j\}\}, \quad (43)$$

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 5. In addition,

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

With (28) 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 $p_N(\mathbf{y}) = (I_{\Lambda_{N, j}} \langle u, \eta_j \rangle)_{j=1}^N$

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

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 (24) 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 (42) 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 4 is now a direct consequence of Theorem 7; specifically the statement of Theorem 4 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 2.

6 Implementation of spectral operator surrogates

As mentioned above, sparse-grid interpolation is deterministic, and the proof of Theorem 7 is constructive. Thus the polynomial surrogate in Theorem 7 can be explicitly computed. For the convenience of the reader we summarize the procedure, and sketch out the algorithm in the following. In particular, this provides a “training algorithm” for the determination of surrogates. Its practicality and performance remains to be investigated, which we leave for future work.

The proof of Theorem 7 proceeds in three steps: For fixed $N \in \mathbb{N}$

- (i) Determine the sets $\Lambda_{N,j} \subseteq \mathcal{F}$ for $j = 1, \dots, N$.
- (ii) For $\mathbf{y} \in [-1, 1]^{\mathbb{N}}$ let

$$f_j(\mathbf{y}) := \left\langle \mathcal{G} \left(\sum_{j \in \mathbb{N}} y_j \psi_j \right), \tilde{\eta}_j \right\rangle \quad (44)$$

and compute the interpolants

$$p_{N,j}(\mathbf{y}) := I_{\Lambda_{N,j}}[f_j](\mathbf{y}) \quad (45)$$

using (37) and (39) for all $j = 1, \dots, N$.

(iii) Compute the operator surrogate

$$\mathcal{D} \circ p_N \circ \mathcal{E}(a) = \sum_{j=1}^N \eta_j p_{N,j}(\mathcal{E}(a)).$$

While the interpolation polynomials $p_{N,j}$ in (45) formally are functions of $\mathbf{y} \in [-1, 1]^{\mathbb{N}}$, due to each multiindex $\mathbf{v} \in \Lambda_{N,j}$ having finite support, in practice these are polynomials depending only on the finitely many variables $\{y_j : \exists \mathbf{v} \in \Lambda_{N,j} \text{ s.t. } v_j \neq 0\}$. Hence they are computable.

The critical step is the determination of the index sets $\Lambda_{N,j}$ in (i). These sets are constructed in the proofs of Lemma 6 and Theorem 7. Simplifying a bit by ignoring logarithmic terms and the (positive but arbitrarily small) constant $\delta > 0$, the procedure reads: For fixed $N \in \mathbb{N}$

(i) Set $m_{N,j} := (n(N)/j)^{(s-1)/t}$, $j = 1, \dots, N$, where

$$n(N) := \begin{cases} N^{\frac{t}{s-1}} & \text{if } s-1 > t \\ N & \text{otherwise.} \end{cases}$$

(ii) With $T > 1$, $t > 0$ as in Theorem 5, define

$$e_{\mathbf{v}} := \prod_{j \in \text{supp } \mathbf{v}} \rho_j^{v_j} \quad \text{where} \quad \rho_j := \max\{T, t w_j^{s(1-p)}\}. \quad (46)$$

where an empty product equals 1.

(iii) Determine an enumeration $(\mathbf{v}_i)_{i \in \mathbb{N}}$ of \mathcal{F} such that $(e_{\mathbf{v}_i}^{-1})_{i \in \mathbb{N}}$ is monotonically decreasing.

(iv) For $j = 1, \dots, N$ let (as in (43))

$$\Lambda_{N,j} = \{\mathbf{v}_i : i \leq \max\{r : m_{N,r} \geq j\}\} \simeq \{\mathbf{v}_i : i \leq n(N)j^{t/(1-s)}\}.$$

Again, all steps are straightforward, except for (iii). There exist different algorithms (recursive and non-recursive) capable of determining $\mathbf{v}_1, \dots, \mathbf{v}_N$ in linear complexity. We refer to [8, Alg. 4.13], [77, Alg. 2] and [74, Alg. 6].

Finally, we emphasize that the constants $T > 1$ and $t > 0$ in (46) are unknown. In practice they may be set to 1, or determined by trial and error. While the precise tuning of the constants can make a difference in the performance, different constructions seem to yield asymptotically similar results, as long as the correct behaviour with regards to the importance of each dimension is captured. We refer for instance to the numerical experiments in [78, Sec. 5.4] and [77, Chapter 5].

7 Examples

7.1 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.

7.1.1 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

$$-\nabla \cdot ((\bar{a} + a)\nabla u) = f \text{ on } \mathbb{T}^d \quad \text{and} \quad \int_{\mathbb{T}^d} u(x) \, dx = 0 \quad (47)$$

in a weak sense. Assuming

$$\operatorname{ess\,inf}_{x \in \mathbb{T}^d} (\bar{a}(x) + a(x)) > a_{\min}, \quad (48)$$

for some constant $a_{\min} > 0$, it follows by the Lax-Milgram Lemma that (47) 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 $\{a \in L^\infty(\mathbb{T}^d) : (48) \text{ holds}\} \rightarrow H^1(\mathbb{T}^d)/\mathbb{R} \hookrightarrow H^1(\mathbb{T}^d)$.

7.1.2 \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 $\mathbf{j} \in \mathbb{N}_0^d$

$$\xi_{\mathbf{j}}(x_1, \dots, x_d) := \prod_{k=1}^d \xi_{j_k}(x_k). \quad (49)$$

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

$$H^s(\mathbb{T}^d) = \left\{ u \in L^2(\mathbb{T}^d) : \sum_{\mathbf{j} \in \mathbb{N}_0^d} \langle u, \xi_{\mathbf{j}} \rangle^2 \max\{1, |\mathbf{j}|\}^{2s} < \infty \right\}, \quad (50)$$

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

$$\langle u, v \rangle_{H^s} := \sum_{\mathbf{j} \in \mathbb{N}_0^d} \langle u, \xi_{\mathbf{j}} \rangle_{L^2} \langle v, \xi_{\mathbf{j}} \rangle_{L^2} \max\{1, |\mathbf{j}|\}^{2s}. \quad (51)$$

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

$$\begin{aligned} \mathcal{X} &:= H^{s_0}(\mathbb{T}^d), & \psi_{\mathbf{j}} &:= \max\{1, |\mathbf{j}|\}^{-s_0} \xi_{\mathbf{j}}, \\ \mathcal{Y} &:= H^{t_0}(\mathbb{T}^d), & \eta_{\mathbf{j}} &:= \max\{1, |\mathbf{j}|\}^{-t_0} \xi_{\mathbf{j}}, \end{aligned} \quad (52)$$

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

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

so that $(w_{\mathbf{j}}^{1+\varepsilon})_{\mathbf{j} \in \mathbb{N}_0^d} \in \ell^1(\mathbb{N}_0^d)$ for any $\varepsilon > 0$ as required in Sec. 2.4. Then, by (50) and the definition of \mathcal{X}^s in (13), it holds for $s \geq 0$

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

Here we used that for $u = \sum_{\mathbf{j} \in \mathbb{N}_0} c_{\mathbf{j}} \xi_{\mathbf{j}}$ holds by (51)

$$\langle u, \psi_{\mathbf{j}} \rangle_{H^{s_0}} = \langle u, \xi_{\mathbf{j}} \max\{1, |\mathbf{j}|\}^{-s_0} \rangle_{H^{s_0}} = c_{\mathbf{j}} \max\{1, |\mathbf{j}|\}^{s_0} = \langle u, \xi_{\mathbf{j}} \rangle_{L^2} \max\{1, |\mathbf{j}|\}^{s_0}.$$

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

7.1.3 Coefficient-to-solution surrogate rates

We now give a convergence result for the approximation of the solution operator \mathcal{G} (corresponding to the PDE (47)) on a Sobolev ball. The encoder \mathcal{E} and decoder \mathcal{D} are as in (12), w.r.t. the spaces and ONBs in (52), 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 3. *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 (48) 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 \mathbf{G}_N of size $O(N)$ such that

$$\sup_{a \in B_r(H^\alpha(\mathbb{T}^d))} \|\mathcal{G}(a) - \mathcal{D} \circ \tilde{\mathbf{G}}_N \circ \mathcal{E}(a)\|_{H^{t_0}(\mathbb{T}^d)} \leq CN^{-R+\delta} \quad (53a)$$

where

$$R = \begin{cases} \frac{\alpha}{d} - \frac{3}{2} & \text{if } \alpha \in (\frac{3d}{2}, \frac{3d}{2} + 1 - t_0] \\ \frac{\alpha + 1 - t_0}{2d} - \frac{3}{4} & \text{if } \alpha > \frac{3d}{2} + 1 - t_0, \end{cases} \quad (53b)$$

and where \mathcal{E} , \mathcal{D} are as in (12) with the spaces/ONBs in (52) 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 verify Assumption 1. By classical elliptic regularity (Schauder estimates, for second order divergence-form linear elliptic equations, also with complex-valued coefficients, e.g., [3, pg. 625], [5, Sec. 2]) it holds for all $\gamma > 0$

$$\mathcal{G} : \{a \in C^\gamma(\mathbb{T}^d) : \bar{a} + a \text{ satisfies (48)}\} \rightarrow C^{1+\gamma}(\mathbb{T}^d) \hookrightarrow H^{1+\gamma}(\mathbb{T}^d),$$

and that $\mathcal{G}(a)$ is bounded on bounded subsets of $\{a \in C^\gamma(\mathbb{T}^d) : \bar{a} + a \text{ satisfies (48)}\}$. Thus, if

$$s_0 > \frac{d}{2}, \quad (54)$$

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

$$\mathcal{G} : \{a \in H^{s_0} : \bar{a} + a \text{ satisfies (48)}\} \rightarrow C^{1+\gamma} \quad \forall \gamma \in [0, s_0 - \frac{d}{2}).$$

We require (54) 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 7.1.1. 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

$$\mathcal{G} : \{a \in \mathcal{X} : \bar{a} + a \text{ satisfies (48)}\} \rightarrow \mathcal{Y}^t \quad \forall t \in [0, \frac{1+s_0-\frac{d}{2}-t_0}{d})$$

and for fixed t the map is bounded on bounded subsets of $\{a \in \mathcal{X} : \bar{a} + a \text{ satisfies (48)}\}$.

Next, if $s > 1$, $\tilde{\mathcal{C}}_r^s(\mathcal{X})$ (which is equal to $C_r^s(\mathcal{X})$ by Rmk. 10) is in particular a bounded subset of $\mathcal{X} \hookrightarrow L^\infty(\mathbb{T}^d)$ (cp. Rmk. 11). Hence, for example by [77, Proposition 1.2.33 and Example 1.2.38] there exists an open complex set $O_{\mathbb{C}} \subset \mathcal{X}_{\mathbb{C}}$ containing $\tilde{\mathcal{C}}_r^s(\mathcal{X})$ such that due to $t_0 \in [0, 1]$,

$$\mathcal{G} : O_{\mathbb{C}} \rightarrow H^1(\mathbb{T}^d, \mathbb{C}) \hookrightarrow \mathcal{Y} = H^{t_0}(\mathbb{T}^d) \quad (55)$$

is holomorphic. Furthermore, it follows from the a-priori estimate [5, Theorem 9.3], which is also valid for (47) with periodic boundary conditions, by combining the \mathbb{T}^d -periodicity of solutions w.r. to Rex with the ‘‘hemisphere’’ a-priori bounds in [5, Theorem 9.2] on each face of \mathbb{T}^d , that

$$\mathcal{G} : \mathcal{O}_{\mathbb{C}} \rightarrow \mathcal{Y}^t \quad \forall t \in \left[0, \frac{1+s_0-\frac{d}{2}-t_0}{d}\right) \quad (56)$$

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

$$s_0 = \frac{\alpha + t_0 - \frac{d}{2} - 1}{2}. \quad (57)$$

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 (57). 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 (53). \square

The above proposition is based on Cor. 1. Applying instead Thm. 2, 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. 3)

$$\sup_{a \in C_1^s(\mathcal{X})} \|\mathcal{G}(a) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathcal{E}(a)))\|_{H^{t_0}(\mathbb{T}^d)} \leq CN^{-\min\{s-1, \frac{1+s_0-\frac{d}{2}-t_0}{d}\} + \delta}.$$

Similarly, Thm. 3 gives an improved L^2 -type error estimate, and Thm. 4 gives a convergence rate bound for spectral operator surrogates.

7.2 Diffusion equation on a polygonal domain

Denote in the following by $D \subset \mathbb{T}^2 \simeq [0, 1]^2$ a convex polygonal domain with positive distance from the boundary $\partial[0, 1]^2$ of the unit cube.

7.2.1 Operator \mathcal{G}

Similar to Section 7.1.1, given a nominal coefficient $\bar{a} \in L^\infty(\mathbb{T}^2)$, a diffusion coefficient $a \in L^\infty(\mathbb{T}^2)$, and a source $f \in H^{-1}(D)$, we wish to find $u \in H^1(D)$ such that

$$-\nabla \cdot ((\bar{a} + a)\nabla u) = f \text{ on } D \quad \text{and} \quad u|_{\partial D} \equiv 0 \quad (58)$$

in a weak sense. Assuming

$$\operatorname{ess\,inf}_{x \in D} (\bar{a}(x) + a(x)) > a_{\min}, \quad (59)$$

for some constant $a_{\min} > 0$, it follows by the Lax-Milgram Lemma that (47) has a unique solution $u \in H_0^1(D)$ that we denote by $\mathcal{G}(a) := u$. Thus \mathcal{G} is a well-defined map from $\{a \in L^\infty(\mathbb{T}^2) : (59) \text{ holds}\} \rightarrow H_0^1(D) \hookrightarrow H^1(D)$.

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

For the input space, we use the same representation as in Section 7.1.2. That is, for some $s_0 \geq 0$ (to be chosen later) we let with (49) for all $\mathbf{j} \in \mathbb{N}_0^2$

$$\mathcal{X} := H^{s_0}(\mathbb{T}^2), \quad \psi_{\mathbf{j}} := \max\{1, |\mathbf{j}|\}^{-s_0} \xi_{\mathbf{j}}, \quad (60)$$

so that $\Psi_{\mathcal{X}} := (\psi_{\mathbf{j}})_{\mathbf{j} \in \mathbb{N}_0^2}$ forms an ONB of \mathcal{X} . With the weight sequence

$$w_{\mathbf{j}}^{\mathcal{X}} := \max\{1, |\mathbf{j}|\}^{-d} \quad \mathbf{j} \in \mathbb{N}_0^2,$$

this then amounts to

$$\mathcal{X}^s = H^{s_0+2s}(\mathbb{T}^2)$$

as explained in Section 7.1.2.

For the output space, we cannot resort to Fourier representations of the solution u of (58), since the underlying domain is not the torus. Therefore we employ a frame representation. Specifically, the authors in [24] provide an explicit construction of functions $\hat{\eta}_{n,j}$, $j \in J_n$, $n \in \mathbb{N}$, for certain index sets $J_n \subseteq \mathbb{N}$; their cardinality is bounded according to

$$|J_n| \lesssim 9^n \quad \forall n \in \mathbb{N}, \quad (61)$$

as a consequence of the particular basis construction in [24], which is based on the successive subdivision of quadrilaterals into nine sub-quadrilaterals (see [24, Section 2]). For all $t \in (0, 3/2)$, it is shown in [24] that the sequence $(3^{-tn} \hat{\eta}_{n,j})_{n,j}$ constitutes a Riesz basis of $H^{1+t}(D)$. In particular, every element of H^{1+t} can be expanded (uniquely) in terms of the $\hat{\eta}_{n,j}$ and

$$\left\| \sum_{n,j} c_{n,j} \hat{\eta}_{n,j} \right\|_{H^{1+t}(D)}^2 \simeq \sum_{n,j} 3^{2tn} c_{n,j}^2. \quad (62)$$

For details see [24], and in particular the top of page 389 in that reference.

Introducing the weight sequence

$$w_{n,j}^{\mathcal{Y}} := 3^{-2n} \quad j \in J_n, n \in \mathbb{N},$$

we note that for any $\varepsilon > 0$ due to (61)

$$\sum_{n,j} (w_{n,j}^{\mathcal{Y}})^{1+\varepsilon} = \sum_{n \in \mathbb{N}} \sum_{j \in J_n} 3^{-2n(1+\varepsilon)} \leq \sum_{n \in \mathbb{N}} 3^{-2n(1+\varepsilon)+2n} = \sum_{n \in \mathbb{N}} 3^{-2\varepsilon n} < \infty$$

as required.

We fix in the following $\delta > 0$ and let

$$\eta_{n,j} := \hat{\eta}_{n,j} (w_{n,j}^{\mathcal{Y}})^{\delta/2} \quad (63)$$

and

$$\mathcal{Y} = \left\{ \sum_{n,j} c_{n,j} \eta_{n,j} : \left\| \sum_{n,j} c_{n,j} \eta_{n,j} \right\|_{\mathcal{Y}}^2 := \sum_{n,j} c_{n,j}^2 < \infty \right\}.$$

Due to (62) it then holds

$$\begin{aligned} \mathcal{Y} &= \left\{ \sum_{n,j} c_{n,j} (w_{n,j}^{\mathcal{Y}})^{\delta/2} \hat{\eta}_{n,j} : \sum_{n,j} c_{n,j}^2 < \infty \right\} \\ &= \left\{ \sum_{n,j} d_{n,j} \hat{\eta}_{n,j} : \sum_{n,j} d_{n,j}^2 (w_{n,j}^{\mathcal{Y}})^{-\delta} < \infty \right\} = H^{1+\delta}(D). \end{aligned} \quad (64)$$

Similarly, for $t \in (0, 3/4 - \delta/2)$ we have due to (62)

$$\begin{aligned} \mathcal{Y}^t &= \left\{ \sum_{n,j} c_{n,j} \eta_{n,j} : \sum_{n,j} c_{n,j}^2 (w_{n,j}^{\mathcal{Y}})^{-2t} < \infty \right\} \\ &= \left\{ \sum_{n,j} d_{n,j} \hat{\eta}_{n,j} : \sum_{n,j} d_{n,j}^2 (w_{n,j}^{\mathcal{Y}})^{-2t-\delta} < \infty \right\} = H^{1+2t+\delta}(D). \end{aligned} \quad (65)$$

7.2.3 Coefficient-to-solution surrogate rates

Analogous to Proposition 3, we now discuss a convergence result for the approximation of the solution operator \mathcal{G} (corresponding to the PDE (58) on the convex polygonal domain $D \subseteq [0, 1]^2$), for all diffusion coefficients in a Sobolev ball. The encoder \mathcal{E} is as in (12), w.r.t. the space and orthonormal bases in (60). Here $s_0 \geq 0$ is still at our disposal. The decoder \mathcal{D} is also as in (12), with respect to the Riesz basis $(\eta_{n,j})_{n,j}$ of \mathcal{Y} .

The next theorem gives essentially the same convergence rates as Proposition 3, with two restrictions:

- (i) Since D is (convex) polygonal, the solution $\mathcal{G}(a) = u$ of (58) belongs in general at best to $H^2(D)$, so unlike for the PDE in Section 7.1 posed on the torus, we cannot get arbitrarily high algebraic operator emulation rates. Therefore we assume $\alpha \leq 5$ in the following.
- (ii) Since the Riesz basis from Section 7.2.2 is *not* stable in H^{t_0} for $t_0 \in [0, 1]$, we only measure the error in $\mathcal{Y} \hookrightarrow H^1(D)$, cp. (64).

Proposition 4. *Assume $f \in C^\infty(D)$. Let $\alpha \in (3, 5]$, $r > 0$, $a_{\min} > 0$ and let $\delta > 0$ (arbitrarily small). Suppose that $\bar{a} + a$ satisfies (48) for all $a \in B_r(H^\alpha(D))$.*

Then 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

$$\sup_{a \in B_r(H^\alpha(\mathbb{T}^2))} \|\mathcal{G}(a) - \mathcal{D} \circ \tilde{\mathbf{G}}_N \circ \mathcal{E}(a)\|_{H^1(D)} \leq CN^{-R+\delta} \quad (66a)$$

where the expression rate R is given by

$$R = \frac{\alpha - 3}{4}, \quad (66b)$$

and the encoder \mathcal{E} is as in (12) and (60) with $s_0 = \frac{\alpha-1}{2}$, and the decoder \mathcal{D} is as in (12) and (63).

Proof. Step 1. We verify Assumption 1. The argument is analogous to Step 1 of the proof of Prop. 3.

By [69, Lemma 5.2] (see also [30, Theorem 9.1.12]) for all $\bar{\gamma}, \gamma \in (0, 1]$ such that $\bar{\gamma} > \gamma$

$$\mathcal{G} : \{a \in C^{\bar{\gamma}}(\mathbb{T}^2) : \bar{a} + a \text{ satisfies (59)}\} \rightarrow H^{1+\gamma}(\mathbb{T}^2),$$

and $\mathcal{G}(a)$ is bounded on bounded subsets of $\{a \in C^{\bar{\gamma}}(\mathbb{T}^2) : \bar{a} + a \text{ satisfies (59)}\}$.

Thus, if

$$s_0 \in (1, 2], \quad (67)$$

using that for any $\bar{\gamma} \in [0, s_0 - 1)$ holds $H^{s_0}(\mathbb{T}^2) \hookrightarrow C^{\bar{\gamma}}(\mathbb{T}^2)$, we find

$$\mathcal{G} : \{a \in H^{s_0}(\mathbb{T}^2) : \bar{a} + a \text{ satisfies (48)}\} \rightarrow H^{1+\gamma}(D) \quad \forall \gamma \in [0, s_0 - 1).$$

In addition, for $\gamma \in (\delta, 1]$ by (65)

$$H^{1+\gamma}(D) = \mathcal{Y}^{t-\delta/2}$$

with $t = \gamma/2$. With $\mathcal{X} = H^{s_0}(\mathbb{T}^2)$ this shows for $s_0 \in (1, 2]$

$$\mathcal{G} : \{a \in \mathcal{X} : \bar{a} + a \text{ satisfies (59)}\} \rightarrow \mathcal{Y}^{t-\delta/2} \quad \forall t \in \left(\frac{\delta}{2}, \frac{s_0-1}{2}\right)$$

and for fixed t the map is bounded on bounded subsets of $\{a \in \mathcal{X} : \bar{a} + a \text{ satisfies (59)}\}$.

Next, if $s > 1$, $\tilde{C}_r^s(\mathcal{X})$ (which is equal to $C_r^s(\mathcal{X})$ by Rmk. 10) is in particular a bounded subset of $\mathcal{X} \hookrightarrow L^\infty(\mathbb{T}^2)$ (cp. Rmk. 11). Hence by [77, 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

$$\mathcal{G} : O_{\mathbb{C}} \rightarrow H^1(D, \mathbb{C})$$

is holomorphic. Furthermore, it follows from the a-priori estimates in [4, Chap. III] that

$$\mathcal{G} : O_{\mathbb{C}} \rightarrow \mathcal{Y}^{t-\delta/2} \quad \forall t \in \left(\frac{\delta}{2}, \frac{s_0-1}{2}\right) \quad (68)$$

is bounded.

Step 2. We conclude the proof. According to Cor. 1, (64) and (68), for $s > 1$ and $t \in (\frac{\delta}{2}, \frac{s_0-1}{2})$ we have with $\mathcal{X}^s = H^{s_0+2s}(\mathbb{T}^2)$

$$\begin{aligned} \sup_{a \in B_r(H^{s_0+2s}(\mathbb{T}^2))} \|\mathcal{G}(a) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathcal{E}(a)))\|_{H^1(D)} &\leq \sup_{a \in B_r(H^{s_0+2s}(\mathbb{T}^2))} \|\mathcal{G}(a) - \mathcal{D}(\tilde{\mathbf{G}}_N(\mathcal{E}(a)))\|_{\mathcal{Y}} \\ &\leq CN^{-\min\{s-1, t-\delta/2\}+\delta/2} \\ &\leq CN^{-\min\{s-1, t\}+\delta}. \end{aligned}$$

Substituting $\alpha = s_0 + 2s$, i.e. $s = \frac{\alpha-s_0}{2}$, and taking the maximal t in (68) this reads

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

We are still free to choose $s_0 \in (1, 2]$, and wish to do so in order to maximize the resulting convergence rate. Solving

$$\frac{\alpha - s_0}{2} - 1 = \frac{s_0 - 1}{2}$$

for s_0 we have

$$s_0 = \frac{\alpha - 1}{2}.$$

The constraint (67) on s_0 implies the constraint $\alpha \in (3, 5]$. The constraint $s > 1$ implies the constraint $\alpha > s_0 + 2$ which is automatically satisfied with this choice of s_0 . The convergence rate then amounts to

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

This shows (66). □

8 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 and parabolic 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. [21] for Navier-Stokes equations, [34] for nonlocal (boundary) integrodifferential operators, [37] for time-harmonic Maxwell equations). We mention [59] for a recent application to deep NNs in computational physiology.

The main results, Theorems 2 and 4, considered in detail the emulation of holomorphic maps \mathcal{G} by either ReLU activated 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*.

As observed in [61, Prop. 3.7], the presently proved approximation rates by strict ReLU NNs can also be expected for other neural architectures: non-ReLU activations satisfying the ‘usual’ assumptions will also suffice. As shown in [65] strict ReLU operator expression rate bounds as shown herein will imply the same rates for so-called spiking neural networks, which are prototypical neuromorphic computing models.

The presently developed technical tools also accommodate other approximation architectures for the high-dimensional, parametric surrogate map $\tilde{\mathbf{G}}_N$ in (3), e.g. tensor-networks or multipole operators (e.g. [38]).

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 [62], [26].

The surrogates \mathcal{G}_N in (3) were based on *linear en- and decoders*. Significant quantitative improvements are achievable by *nonlinear encoding and decoding*. For example, transformer-based emulators \mathcal{E} as proposed e.g. in [45, 11] or manifold-decoders \mathcal{D} such as NOMAD in [64].

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 [21] for the stationary Navier-Stokes equations, [37] for time-harmonic Maxwell equations and [34] 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 noiseless evaluations of $\langle \mathcal{G}(a), \tilde{\eta}_j \rangle$ in at most N pairs of input-output ‘snapshots’ in $C_r^s(\mathcal{X}) \times \tilde{\Psi}_\mathcal{Y}$. Accounting for effects of ‘noisy’ evaluations of these functionals, e.g. through numerical discretizations, will be considered elsewhere.

Declarations

Conflict of interest Authors declare no competing interests.

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