

De Rham compatible Deep Neural Networks

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Abstract

We construct several classes of neural networks with ReLU and BiSU (Binary Step Unit) activations, which exactly emulate the lowest order Finite Element (FE) spaces on regular, simplicial partitions of polygonal and polyhedral domains $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. For continuous, piecewise linear (CPwL) functions, our constructions generalize previous results in that arbitrary, regular simplicial partitions of Ω are admitted, also in arbitrary dimension $d \geq 2$.

Vector-valued elements emulated include the classical Raviart-Thomas and the first family of Nédélec edge elements on triangles and tetrahedra. Neural Networks emulating these FE spaces are required in the correct approximation of boundary value problems of electromagnetism in nonconvex polyhedra $\Omega \subset \mathbb{R}^3$, thereby constituting an essential ingredient in the application of e.g. the methodology of “physics-informed NNs” or “deep Ritz methods” to electromagnetic field simulation via deep learning techniques. They satisfy exact (De Rham) sequence properties, and also spawn discrete boundary complexes on $\partial\Omega$ which satisfy exact sequence properties for the surface divergence and curl operators div_r and curl_r , respectively, thereby enabling “neural boundary elements” for computational electromagnetism.

We indicate generalizations of our constructions to higher-order compatible spaces and other, non-compatible classes of discretizations in particular the Crouzeix-Raviart elements and Hybridized, Higher Order (HHO) methods.

Key words: De Rham Complex, Finite Elements, Neural Networks

Subject Classification: 41A05, 68Q32, 26B40, 65N30

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1 Introduction

Recent years have seen the emergence of Deep Neural Network (DNN) based methods for the numerical approximation of solutions to partial differential equations (PDEs for short). In one class of proposed methods, DNNs serve as *approximation architectures* in a suitable, weak form of the PDE of interest. In [14], for elliptic, self-adjoint PDEs the variational principle associated to the PDE is computationally minimized over suitable DNNs, so that the energy functional of the physical system of interest gives rise to a consistent loss function for the training of the DNN. Numerical solutions obtained from training the approximating DNN in this way correspond to approximate variational solutions of the PDE under consideration.

The recently promoted “physics-informed NNs” (PiNNs), e.g. [24, 27] and references there, insert DNN approximations with suitably smooth activations (e.g. softmax or tanh) as approximation architecture into the strong form of the governing PDE. Approximate solutions are obtained by numerical minimization of loss functions obtained by discretely enforcing smallness of the residual at collocation points in the spatio-temporal domain. While empirically successful in a large number of test cases, also DNN based approximations are subject to the fundamental paradigm that “stability and consistency implies convergence”. A key factor of recent successful DNN deployment in numerical PDE solution is their excellent approximation properties, in particular on high-dimensional state- and parameter-spaces, e.g. [23, 20, 26] and the references there. High smoothness of DNNs with smooth activations may, however, preclude convergence of so-called “deep Ritz” approaches where loss functions in DNN training are derived from energies in variational principles [14], even for linear, deterministic and well posed PDEs.

1.1 Previous work

The connection between DNNs with Rectified Linear Unit (ReLU for short) activation and continuous piecewise linear (CPwL for short) spline approximation spaces has been known for some time: *nodal discretizations* based on CPwL Finite Element Methods (FEM) can be emulated by ReLU NNs (e.g. as introduced in [3] and [18]). When applied to, for example, weak formulations of the Maxwell equations, they are known to converge, generally, only for convex polygons or polyhedra: if Ω admits re-entrant corners or edges, the $H^1(\Omega)$ fields in X_N , the space of electric fields u in Ω with square integrable curl and divergence, satisfying the perfect conductor boundary condition $u \times n = 0$ on the boundary $\partial\Omega$, are closed in X_N *without being*

dense, see, e.g., [10, 12]. Since any discrete conforming space based on a standard nodal finite element method is contained in $H^1(\Omega)$, nodal FEM generally converges to a wrong solution as the meshwidth tends to zero (respectively as the width of the corresponding NN tends to infinity) in this situation [11]. Similar issues will arise for PiNN numerical approximations of low-regularity solutions for $H^0(\text{curl}, \Omega)$ -based PDEs such as the time-harmonic Maxwell equations. They will persist also for DNN surrogates with more regular activation functions such as ReLU^k and sigmoidal or softmax activations.

A second, broad class of variational models, where continuous, nodal FEM in approximation of minimizers of energy functionals are known to incur problems, arises for “deep Ritz” type approaches as in [14] applied to certain nonconvex energy functionals in the calculus of variations. Here, the so-called “Lavrentiev gap” incurred by CPwL approximation architectures is known to be a fundamental obstruction to obtain convergent families of discrete minimizers. Again, relaxing continuity below H^1 -conformity is known to remedy this issue; see, e.g. [5] and the discussion and references there. Accordingly, in the present paper we present CR-Net, a DNN emulation of the Crouzeix–Raviart element, on general regular, simplicial partitions which, when used in a deep Ritz method style approach for variational problems, affords convergent sequences of DNN approximations of minimizers. CR-Net will also afford advantages in image segmentation (e.g. [8] and the references there).

The ability of PiNNs to represent accurately geometric or physical invariances, in the PDE context e.g. $H^0(\text{curl}, \Omega)$ -conformity and divergence-preservation, see [29], has proved crucial for the wide deployment of the “PiNN” [24] and the “deep Ritz” [14] neural network based simulation methodologies in computational science and engineering.

1.2 Contributions

To leverage the methodology of PiNNs and e.g. the variational Ritz method for computational electromagnetics, computational magneto-hydrodynamics etc., *structure-preserving DNNs* must be adopted. We provide here, therefore, *De Rham complex compatible DNN emulations* of the standard, lowest order FE spaces on regular, simplicial triangulations of polytopal domains Ω in two and three space dimensions.

Specifically, let us assume that $\Omega \subset \mathbb{R}^3$ is a simply connected Lipschitz domain with connected boundary $\partial\Omega$. Then, it is well-known that the following sequence is exact (e.g. [16, Proposition 16.14]):

$$\mathbb{R} \xrightarrow{i} H^1(\Omega) \xrightarrow{\text{grad}} H^0(\text{curl}, \Omega) \xrightarrow{\text{curl}} H^0(\text{div}, \Omega) \xrightarrow{\text{div}} L^2(\Omega) \xrightarrow{o} \{0\}. \quad (1.1)$$

Here, the tag i denotes ‘injection’ and the tag o denotes the zero operator.

Finite dimensional subspaces preserving this structure are usually required to fit into a *Discrete De Rham complex* (e.g. [16, Proposition 16.15])

$$\mathbb{R} \xrightarrow{i} S_1(\mathcal{T}, \Omega) \xrightarrow{\text{grad}} N_0(\mathcal{T}, \Omega) \xrightarrow{\text{curl}} \text{RT}_0(\mathcal{T}, \Omega) \xrightarrow{\text{div}} S_0(\mathcal{T}, \Omega) \xrightarrow{o} \{0\}. \quad (1.2)$$

Here, for a given triangulation \mathcal{T} of a domain Ω , $S_1(\mathcal{T}, \Omega)$ stands for the class of continuous piecewise linear functions, $S_0(\mathcal{T}, \Omega)$ stands for the class of piecewise constant functions, and $\text{RT}_0(\mathcal{T}, \Omega)$, $N_0(\mathcal{T}, \Omega)$ are the lowest order Raviart–Thomas and Nédélec spaces respectively (see Section 3.2 and Section 3.3 for precise definitions). The design of DNNs which emulate *exactly*, on arbitrary regular, simplicial partitions of polytopal domains $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, the FE spaces $S_1(\mathcal{T}, \Omega)$, $N_0(\mathcal{T}, \Omega)$, $\text{RT}_0(\mathcal{T}, \Omega)$ is the purpose of the present paper. We provide constructions of DNNs based on a combination of ReLU and BiSU (Binary Step Unit) activations, which emulate the classical, lowest-order FE spaces in the De Rham complex on a regular, simplicial partition \mathcal{T} of Ω . We underline that our construction of NNs which emulate, in particular, the classical “Courant Finite Elements” $S_1(\mathcal{T}, \Omega)$, as well as $S_0(\mathcal{T}, \Omega)$ and $\text{RT}_0(\mathcal{T}, \Omega)$ apply

on polytopal domains Ω of any dimension $d \geq 2$. For the practically relevant space $S_1(\mathcal{T}, \Omega)$, we provide DNN constructions based on ReLU activation only, which work in arbitrary, finite dimension $d \geq 2$ (the univariate case $d = 1$ being trivial).

Our constructions accommodate general, regular simplicial partitions \mathcal{T} of Ω . In particular, apart from regularity of the simplicial partition \mathcal{T} of Ω , no further constraints of geometric nature are imposed on \mathcal{T} . Our results therefore unify and generalize earlier ones such as in [18], which covered only CPwL FE spaces on particular triangulations of Ω .

1.3 Layout

The structure of this paper is as follows. In Section 2, we recapitulate notation and basic definitions for the NNs which we consider. We also review a basic NN calculus that shall be used subsequently in order to derive several properties of the proposed NN architectures.

Sections 3 and 4 contain the core material of the paper: in Section 3, using ReLU and BiSU activations, we provide explicit constructions of emulations for all bases of the FE spaces considered in this paper, without geometric conditions on the triangulations \mathcal{T} of Ω . In Section 4 we show that for the special case of the emulation of CPwL functions, networks employing solely ReLU activations are sufficient.

In Section 5 we discuss the implications of our results for function approximation by NNs in the respective Sobolev spaces. Section 6 provides a construction of NN emulations for compatible spaces on the boundary $\Gamma = \partial\Omega$ of the polytopal domains. These spaces are required in the deep neural network approximation of boundary integral equations in electromagnetics, among others, as discussed in [7, 6] and the references there. Finally, in Section 7 we present conclusions and explain how our analysis may be extended to higher order polynomial spaces and to certain Finite Element families which are non-compatible with (1.1).

2 Neural network definitions

To accommodate for both continuous components and discontinuous components in the functions we want to emulate, we consider neural networks where several different activation functions are used throughout the network. We define neural networks as a collection of parameters and for each position in the network (also called neuron or unit) we specify the activation function used. Associated to such a neural network is a function, called realization, which is the iterated composition of affine transformations defined in terms of the parameters and non-linear activation functions.

Definition 2.1 For $d, L \in \mathbb{N}$, a neural network Φ with input dimension $d \geq 1$ and number of layers $L \geq 1$, comprises a finite collection of activation functions $\varrho = \{\varrho_\ell\}_{\ell=1}^L$ and a finite sequence of matrix-vector tuples, i.e.

$$\Phi = ((A_1, b_1, \varrho_1), (A_2, b_2, \varrho_2), \dots, (A_L, b_L, \varrho_L)).$$

For $N_0 := d$ and numbers of neurons $N_1, \dots, N_L \in \mathbb{N}$ per layer, for all $\ell = 1, \dots, L$ it holds that $A_\ell \in \mathbb{R}^{N_\ell \times N_{\ell-1}}$ and $b_\ell \in \mathbb{R}^{N_\ell}$, and that ϱ_ℓ is a list of length N_ℓ of activation functions $(\varrho_\ell)_i : \mathbb{R} \rightarrow \mathbb{R}$, $i = 1, \dots, N_\ell$, acting on node i in layer ℓ .

The realization of $\Phi : \mathbb{R}^{N_0} \rightarrow \mathbb{R}^{N_L}$ as a map is the function

$$R(\Phi) : \mathbb{R}^d \rightarrow \mathbb{R}^{N_L} : x \rightarrow x_L,$$

where

$$\begin{aligned} x_0 &:= x, \\ x_\ell &:= \varrho_\ell(A_\ell x_{\ell-1} + b_\ell), \quad \text{for } \ell = 1, \dots, L-1, \\ x_L &:= A_L x_{L-1} + b_L. \end{aligned}$$

Here, for $\ell = 1, \dots, L-1$, the list of activation functions ϱ_ℓ of length N_ℓ is effected componentwise: for $y = (y_1, \dots, y_{N_\ell}) \in \mathbb{R}^{N_\ell}$ we denote $\varrho_\ell(y) = ((\varrho_\ell)_1(y_1), \dots, (\varrho_\ell)_{N_\ell}(y_{N_\ell}))$. I.e., $(\varrho_\ell)_i$ is the activation function applied in position i of layer ℓ .

We call the layers indexed by $\ell = 1, \dots, L-1$ hidden layers, in those layers activation functions are applied. No activation is applied in the last layer of the NN. For consistency of notation, we define $\varrho_L := \text{Id}_{\mathbb{R}^{N_L}}$.

We refer to $L(\Phi) := L$ as the depth of Φ . For $\ell = 1, \dots, L$ we denote by $M_\ell(\Phi) := \|A_\ell\|_0 + \|b_\ell\|_0$ the size of layer ℓ , which is the number of nonzero components in the weight matrix A_ℓ and the bias vector b_ℓ , and call $M(\Phi) := \sum_{\ell=1}^L M_\ell(\Phi)$ the size of Φ . Moreover, we call d and N_L the input dimension and the output dimension, and denote by $M_{\text{in}}(\Phi) := M_1(\Phi)$ and $M_{\text{out}}(\Phi) := M_L(\Phi)$ the size of the first and the last layer, respectively.

Our networks will use two different activation functions. Firstly, we use the *Rectified Linear Unit (ReLU)* activation

$$\rho(x) = \max\{0, x\}.$$

Networks which only contain ReLU activations realize continuous, piecewise linear functions. By *ReLU NNs* we refer to NNs which only have ReLU activations, including networks of depth 1, which do not have hidden layers and realize affine transformations. Secondly, for the emulation of discontinuous functions, we in addition use the *Binary Step Unit (BiSU)* activation

$$\sigma(x) = \begin{cases} 0 & \text{if } x \leq 0, \\ 1 & \text{if } x > 0, \end{cases} \quad (2.1)$$

which is also called *Heaviside* function. *BiSU NNs* are defined analogously to ReLU NNs. Alternatively, the BiSU can be defined to equal $\frac{1}{2}$ in $x = 0$. That function, which we denote by $\tilde{\sigma}$, can be written as an affine combination of activation functions σ : $2\tilde{\sigma}(x) = \sigma(x) + 1 - \sigma(-x)$ for all $x \in \mathbb{R}$. Hence, for every NN with $\tilde{\sigma}$ as activation function, there exists a network with σ -activations instead, with proportional depth and size.

In the following sections, we will construct NNs from smaller networks using a ReLU-based *calculus of NNs*, which we now recall from [23]. The results cited from [23] were derived for NNs which only use the ReLU activation function, but they also hold for networks with multiple activation functions without modification.

Proposition 2.2 (Parallelization of NNs [23, Definition 2.7]) *For $d, L \in \mathbb{N}$ let $\Phi^1 = ((A_1^{(1)}, b_1^{(1)}, \varrho_1^{(1)}), \dots, (A_L^{(1)}, b_L^{(1)}, \varrho_L^{(1)}))$ and $\Phi^2 = ((A_1^{(2)}, b_1^{(2)}, \varrho_1^{(2)}), \dots, (A_L^{(2)}, b_L^{(2)}, \varrho_L^{(2)}))$ be two NNs with input dimension d and depth L . Let the parallelization $P(\Phi^1, \Phi^2)$ of Φ^1 and Φ^2 be defined by*

$$\begin{aligned} P(\Phi^1, \Phi^2) &:= ((A_1, b_1, \varrho_1), \dots, (A_L, b_L, \varrho_L)), \\ A_1 &= \begin{pmatrix} A_1^{(1)} \\ A_1^{(2)} \end{pmatrix}, \quad A_\ell = \begin{pmatrix} A_\ell^{(1)} & 0 \\ 0 & A_\ell^{(2)} \end{pmatrix}, & \text{for } \ell = 2, \dots, L, \\ b_\ell &= \begin{pmatrix} b_\ell^{(1)} \\ b_\ell^{(2)} \end{pmatrix}, \quad \varrho_\ell = \begin{pmatrix} \varrho_\ell^{(1)} \\ \varrho_\ell^{(2)} \end{pmatrix}, & \text{for } \ell = 1, \dots, L. \end{aligned}$$

Then,

$$\begin{aligned} R(P(\Phi^1, \Phi^2))(x) &= (R(\Phi^1)(x), R(\Phi^2)(x)), \quad \text{for all } x \in \mathbb{R}^d, \\ L(P(\Phi^1, \Phi^2)) &= L, \quad M(P(\Phi^1, \Phi^2)) = M(\Phi^1) + M(\Phi^2). \end{aligned}$$

The parallelization of more than two NNs is handled by repeated application of Proposition 2.2.

Proposition 2.3 (Sum of NNs) For $d, N, L \in \mathbb{N}$ let $\Phi^1 = \left((A_1^{(1)}, b_1^{(1)}, \varrho_1^{(1)}), \dots, (A_L^{(1)}, b_L^{(1)}, \varrho_L^{(1)}) \right)$ and $\Phi^2 = \left((A_1^{(2)}, b_1^{(2)}, \varrho_1^{(2)}), \dots, (A_L^{(2)}, b_L^{(2)}, \varrho_L^{(2)}) \right)$ be two NNs with input dimension d , output dimension N and depth L . Let the sum $\Phi^1 + \Phi^2$ of Φ^1 and Φ^2 be defined by

$$\begin{aligned} \Phi^1 + \Phi^2 &:= ((A_1, b_1, \varrho_1), \dots, (A_L, b_L, \varrho_L)), \\ A_1 &= \begin{pmatrix} A_1^{(1)} \\ A_1^{(2)} \end{pmatrix}, \quad b_1 = \begin{pmatrix} b_1^{(1)} \\ b_1^{(2)} \end{pmatrix}, \quad \varrho_1 = \begin{pmatrix} \varrho_1^{(1)} \\ \varrho_1^{(2)} \end{pmatrix}, \\ A_\ell &= \begin{pmatrix} A_\ell^{(1)} & 0 \\ 0 & A_\ell^{(2)} \end{pmatrix}, \quad b_\ell = \begin{pmatrix} b_\ell^{(1)} \\ b_\ell^{(2)} \end{pmatrix}, \quad \varrho_\ell = \begin{pmatrix} \varrho_\ell^{(1)} \\ \varrho_\ell^{(2)} \end{pmatrix}, \quad \text{for } \ell = 2, \dots, L-1. \\ A_L &= \begin{pmatrix} A_L^{(1)} & A_L^{(2)} \end{pmatrix}, \quad b_L = b_L^{(1)} + b_L^{(2)}, \quad \varrho_L = \text{Id}_{\mathbb{R}^N}. \end{aligned}$$

Then,

$$\begin{aligned} \text{R}(\Phi^1 + \Phi^2)(x) &= \text{R}(\Phi^1)(x) + \text{R}(\Phi^2)(x), \quad \text{for all } x \in \mathbb{R}^d, \\ L(\Phi^1 + \Phi^2) &= L, \quad M(\Phi^1 + \Phi^2) \leq M(\Phi^1) + M(\Phi^2). \end{aligned}$$

Next, we define the concatenation of two NNs, which realizes exactly the composition of the realizations of the two networks. It uses the fact that we allow the ReLU activation.

Proposition 2.4 (Sparse Concatenation of NNs [23, Remark 2.6]) For $L^{(1)}, L^{(2)} \in \mathbb{N}$, let $\Phi^1 = \left((A_1^{(1)}, b_1^{(1)}, \varrho_1^{(1)}), \dots, (A_{L^{(1)}}^{(1)}, b_{L^{(1)}}^{(1)}, \varrho_{L^{(1)}}^{(1)}) \right)$ and $\Phi^2 = \left((A_1^{(2)}, b_1^{(2)}, \varrho_1^{(2)}), \dots, (A_{L^{(2)}}^{(2)}, b_{L^{(2)}}^{(2)}, \varrho_{L^{(2)}}^{(2)}) \right)$ be two NNs with depths $L^{(1)}$ and $L^{(2)}$, respectively, such that $N_{L^{(2)}}^{(2)} = N_0^{(1)}$, i.e. the output dimension of Φ^2 equals the input dimension of Φ^1 . Let the sparse concatenation $\Phi^1 \odot \Phi^2$ of Φ^1 and Φ^2 be a NN of depth $L := L^{(1)} + L^{(2)}$ defined by

$$\begin{aligned} \Phi^1 \odot \Phi^2 &:= ((A_1, b_1, \varrho_1), \dots, (A_L, b_L, \varrho_L)), \\ (A_\ell, b_\ell, \varrho_\ell) &= (A_\ell^{(2)}, b_\ell^{(2)}, \varrho_\ell^{(2)}), \quad \text{for } \ell = 1, \dots, L^{(2)} - 1, \\ A_{L^{(2)}} &= \begin{pmatrix} A_{L^{(2)}}^{(2)} \\ -A_{L^{(2)}}^{(2)} \end{pmatrix}, \quad b_{L^{(2)}} = \begin{pmatrix} b_{L^{(2)}}^{(2)} \\ -b_{L^{(2)}}^{(2)} \end{pmatrix}, \quad \varrho_{L^{(2)}} = \begin{pmatrix} \rho \\ \vdots \\ \rho \end{pmatrix}, \\ A_{L^{(2)}+1} &= \begin{pmatrix} A_1^{(1)} & -A_1^{(1)} \end{pmatrix}, \quad b_{L^{(2)}+1} = b_1^{(1)}, \quad \varrho_{L^{(2)}+1} = \varrho_1^{(1)}, \\ (A_\ell, b_\ell, \varrho_\ell) &= (A_{\ell-L^{(2)}}^{(1)}, b_{\ell-L^{(2)}}^{(1)}, \varrho_{\ell-L^{(2)}}^{(1)}), \quad \text{for } \ell = L^{(2)} + 2, \dots, L^{(1)} + L^{(2)}. \end{aligned}$$

Then, it holds that

$$\begin{aligned} \text{R}(\Phi^1 \odot \Phi^2) &= \text{R}(\Phi^1) \circ \text{R}(\Phi^2), \quad L(\Phi^1 \odot \Phi^2) = L^{(1)} + L^{(2)}, \\ M(\Phi^1 \odot \Phi^2) &\leq M(\Phi^1) + M_{\text{in}}(\Phi^1) + M_{\text{out}}(\Phi^2) + M(\Phi^2) \leq 2M(\Phi^1) + 2M(\Phi^2). \end{aligned}$$

Proposition 2.2 only applies to networks of equal depth. To parallelize two networks of unequal depth, the shallowest can be concatenated with a network that emulates the identity using Proposition 2.4. One example of ReLU NNs that emulate the identity are provided by the following proposition.

Proposition 2.5 (ReLU NN emulation of $\text{Id}_{\mathbb{R}^d}$ [23, Remark 2.4]) For all $d, L \in \mathbb{N}$, there exists a ReLU NN $\Phi_{d,L}^{\text{Id}}$ with input dimension d , output dimension d and depth L which satisfies $\text{R}(\Phi_{d,L}^{\text{Id}}) = \text{Id}_{\mathbb{R}^d}$, $L(\Phi_{d,L}^{\text{Id}}) = L$ and $M(\Phi_{d,L}^{\text{Id}}) \leq 2dL$.

To emulate exactly shape functions of lowest order, conforming FEM in the function spaces introduced in Section 3, we will need ReLU NNs which emulate the minimum or maximum of $d \in \mathbb{N}$ inputs. These are provided in Lemma 2.6. We also need to multiply values from a bounded interval $[-\kappa, \kappa]$ for $\kappa > 0$ by values from the discrete set $\{0, 1\}$, which is the range of the BiSU defined in (2.1). A ReLU NN which emulates such multiplications exactly is constructed in the proof of Proposition 2.8 below.

Lemma 2.6 (ReLU NN emulation of min and max, [18, Proof Theorem 3.1]) *For all $d \in \mathbb{N}$, there exist ReLU NNs Φ_d^{\max} and Φ_d^{\min} which satisfy*

$$\begin{aligned} \mathbb{R}(\Phi_d^{\max})(x) &= \max\{x_1, \dots, x_d\}, & \text{for all } x \in \mathbb{R}^d, \\ \mathbb{R}(\Phi_d^{\min})(x) &= \min\{x_1, \dots, x_d\}, & \text{for all } x \in \mathbb{R}^d, \\ L(\Phi_d^{\max}) &= L(\Phi_d^{\min}) \leq 2 + \log_2(d), & M(\Phi_d^{\max}) = M(\Phi_d^{\min}) \leq Cd. \end{aligned}$$

Here, the constant $C > 0$ is independent of d and of the NN sizes and depths.

Remark 2.7 *The network Φ_d^{\max} is obtained by repeated applications of Φ_2^{\max} , which itself can for instance be constructed as*

$$\Phi_2^{\max} := \left(\left(\left(\begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \rho \\ \rho \end{pmatrix} \right), \left(\begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix}, 0, \text{Id}_{\mathbb{R}} \right) \right).$$

We point out that this construction of Φ_2^{\max} leads to a slightly more efficient representation of Φ_d^{\max} than the one given in [18, Theorem 3.1], as it requires less neurons, weights and biases. However, this will merely improve the constant C in Lemma 2.6, but not the stated asymptotic d -dependence of $L(\Phi_2^{\max})$ and $M(\Phi_2^{\max})$.

The d -dependence can be completely avoided by admitting recurrent neural nets (RNNs), i.e., RNNs can express the maximum of d inputs with a network of size, depth and width $O(1)$. We shortly sketch the idea: An RNN allows for information to flow backwards, i.e., we can take the output of Φ_2^{\max} in time step t as one of its inputs at time step $t+1$. With the initialization $\tilde{x}_0 := x_1$, this leads to the iteration

$$\tilde{x}_t = \Phi_2^{\max}(\tilde{x}_{t-1}, x_t),$$

where the network receives in step t the input x_t . Then the network's output \tilde{x}_n in step n equals $\max\{x_1, \dots, x_n\}$.

The whole remark applies verbatim to min networks.

The following proposition provides the exact ReLU NN emulation of products of elements from a bounded interval $[-\kappa, \kappa]$ for $\kappa > 0$ by elements from the discrete set $\{0, 1\}$. The network depth and size are independent of κ .

Proposition 2.8 *For all $d \in \mathbb{N}$ and $\kappa > 0$ there exists a ReLU NN $\Phi_{d,\kappa}^\times$*

$$\begin{aligned} \mathbb{R}(\Phi_{d,\kappa}^\times)(x_1, \dots, x_d, y) &= xy = (x_1 y, \dots, x_d y)^\top, & \text{for all } x \in [-\kappa, \kappa]^d \text{ and } y \in \{0, 1\}, \\ L(\Phi_{d,\kappa}^\times) &\leq 2, & M(\Phi_{d,\kappa}^\times) \leq 12d. \end{aligned}$$

Proof. This proof is given in two steps. In Step 1, we define a function of x, y that computes the desired output for $d = 1$. In Step 2, we describe a NN which exactly emulates that function d times and estimate its depth and size.

Step 1. For $x, y \in \mathbb{R}$ let

$$f(x, y) := \frac{1}{2} (\rho(x+y) + \rho(-x-y) - \rho(x-y) - \rho(-x+y)).$$

where the first $2k$ elements of A equal -1 and the last $N - k$ equal 1 .

Then, for all $x \in \mathbb{R}^d$

$$\mathbf{R}(\Phi_{\Omega}^{\mathbb{1}})(x) = \begin{cases} 1 & \text{if } x \in \Omega, \\ 0 & \text{otherwise,} \end{cases} \quad L(\Phi_{\Omega}^{\mathbb{1}}) = 3, \quad M(\Phi_{\Omega}^{\mathbb{1}}) \leq (d+2)(N+k) + 2.$$

Proof. From

$$1 - \sigma(y) - \sigma(-y) = \begin{cases} 1 & \text{if } y = 0, \\ 0 & \text{otherwise,} \end{cases} \quad \text{for all } y \in \mathbb{R},$$

it follows that for all $x \in \mathbb{R}^d$

$$\begin{aligned} \mathbf{R}(\Phi_{\Omega}^{\mathbb{1}})(x) &= \sigma \left(\sum_{i=1}^k (1 - \sigma(A_i x + b_i) - \sigma(-A_i x - b_i)) + \sum_{i=k+1}^N \sigma(A_i x + b_i) - (N - \frac{1}{4}) \right) \\ &= \begin{cases} 1 & \text{if } x \in \Omega, \\ 0 & \text{otherwise,} \end{cases} \\ L(\Phi_{\Omega}^{\mathbb{1}}) &= 3, \quad M(\Phi_{\Omega}^{\mathbb{1}}) \leq ((N+k)d + (N+k)) + ((N+k) + 1) + 1 = (d+2)(N+k) + 2. \end{aligned}$$

□

3 NN emulation of lowest order conforming Finite Element shape functions

Consider a bounded polytopal domain $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N} \setminus \{1\}$. For $k \in \{0, \dots, d\}$ we define a k -simplex T by $T = \text{conv}(\{a_0, \dots, a_k\}) \subset \mathbb{R}^d$, for some $a_0, \dots, a_k \in \mathbb{R}^d$ which do not all lie in one affine subspace of dimension $k - 1$, and where

$$\text{conv}(Y) := \left\{ x = \sum_{y \in Y} \lambda_y y : \lambda_y > 0 \text{ and } \sum_{y \in Y} \lambda_y = 1 \right\}$$

denotes the open convex hull. We consider a simplicial mesh \mathcal{T} on Ω of d -simplices, which satisfies that $\bar{\Omega} = \bigcup_{T \in \mathcal{T}} \bar{T}$ and $T \cap T' = \emptyset$, for all $T \neq T'$. We assume that \mathcal{T} is a *regular* partition, i.e. for all distinct $T, T' \in \mathcal{T}$ it holds that $\bar{T} \cap \bar{T}'$ is the closure of a k -subsimplex of T for some $k \in \{0, \dots, d-1\}$, i.e. there exist $a_0, \dots, a_d \in \Omega$ such that $T = \text{conv}(\{a_0, \dots, a_d\})$ and $\bar{T} \cap \bar{T}' = \text{conv}(\{a_0, \dots, a_k\})$.

Moreover, we define the *shape-regularity constant* $C_{\text{sh}} := C_{\text{sh}}(\mathcal{T})$ of a mesh \mathcal{T} by $C_{\text{sh}} := \max_{T \in \mathcal{T}} \frac{h_T}{r_T} > 0$ where $h_T := \text{diam}(T)$ and r_T is the radius of the largest ball contained in \bar{T} .

Let \mathcal{V} be the set of vertices of \mathcal{T} . We also let \mathcal{F}, \mathcal{E} be the sets of $(d-1)$ - and 1 -simplices of \mathcal{T} , whose elements are called *faces* and *edges*, respectively, that is

$$\begin{aligned} \mathcal{F} &:= \{f \subset \bar{\Omega} : \exists T = \text{conv}(\{a_0, \dots, a_d\}) \in \mathcal{T}, \exists i \in \{0, \dots, d\} \text{ with } f = \text{conv}(\{a_0, \dots, a_d\} \setminus \{a_i\})\}, \\ \mathcal{E} &:= \{e \subset \bar{\Omega} : \exists T = \text{conv}(\{a_0, \dots, a_d\}) \in \mathcal{T}, \exists i, j \in \{0, \dots, d\}, i \neq j, \text{ with } e = \text{conv}(\{a_i, a_j\})\}. \end{aligned}$$

We denote the *skeleton* by $\partial\mathcal{T} := \bigcup_{T \in \mathcal{T}} \partial T$.

Below, we will present neural network emulations of the lowest order conforming FEM spaces for $H^1(\Omega), H^0(\text{curl}, \Omega), H^0(\text{div}, \Omega)$ and $L^2(\Omega)$. These finite-dimensional spaces appear naturally in discretizations of the the De Rham complex and will be defined in (3.27), (3.22), (3.6) and (3.3) below. For each type of shape function, we explicitly define a network which emulates that shape function exactly. Global approximations can be obtained by taking a linear

combination of these shape functions using Proposition 2.3, (scalar multiples of shape functions are obtained by scaling all weights and biases of the output layer).

For shape functions which are discontinuous after extending them to Ω by the value zero outside their domain of definition, we use Lemma 2.9 based on BiSU activation to emulate indicator functions of (parts of) their domain of definition. We then use Proposition 2.8 based on ReLU activation to multiply a continuous, piecewise linear function, which is equal to the shape function on part of Ω , by the indicator function of that part of the domain.

The following lemma provides NN emulations of possibly discontinuous, piecewise linear functions, and will be used in the following sections.

Lemma 3.1 (Emulation of piecewise linear functions) *For $d, s, k \in \mathbb{N}$ let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz polytope and \mathcal{T} be a regular, simplicial partition of Ω with $s = \#\mathcal{T}$ elements, $\mathcal{T} = \{T_i\}_{i=1, \dots, s}$. Let $u : \Omega \rightarrow \mathbb{R}^k$ be a function which for all $i = 1, \dots, s$ satisfies $u|_{T_i} \in [\mathbb{P}_1]^k$ and $u|_{T_i}(x) = A^{(i)}x + b^{(i)}$, $x \in T_i$.*

Then

$$\Phi_u^{PwL} := \sum_{i=1}^s \Phi_{k, \kappa}^\times \odot \text{P} \left(\Phi_{k, 2}^{\text{Id}} \odot \left(\left(A^{(i)}, b^{(i)}, \text{Id}_{\mathbb{R}^k} \right) \right), \Phi_{T_i}^1 \right) \quad (3.1)$$

satisfies $u(x) = \text{R}(\Phi_u^{PwL})(x)$ for a.e. $x \in \Omega$, for any

$$\kappa \geq \max_{i=1, \dots, s} \sup_{x \in T_i} \|A^{(i)}x + b^{(i)}\|_\infty. \quad (3.2)$$

Moreover, if $\|A^{(i)}\|_0 + \|b^{(i)}\|_0 \leq m$ for all $i = 1, \dots, s$, then

$$L(\Phi_u^{PwL}) = 5, \quad M(\Phi_u^{PwL}) \leq Cs(k + m + d^2).$$

Proof. Firstly, we observe that indeed $u(x) = \text{R}(\Phi_u^{PwL})(x)$ for a.e. $x \in \Omega$.

Secondly, we estimate

$$\begin{aligned} L(\Phi_u^{PwL}) &= L(\Phi_{k, \kappa}^\times) + L(\Phi_{T_i}^1) = 5, \\ M(\Phi_u^{PwL}) &\leq s \left(2M(\Phi_{k, \kappa}^\times) + 2M \left(\text{P} \left(\Phi_{k, 2}^{\text{Id}} \odot \left(\left(A^{(i)}, b^{(i)}, \text{Id}_{\mathbb{R}^k} \right) \right), \Phi_{T_i}^1 \right) \right) \right) \\ &\leq s \left(2M(\Phi_{k, \kappa}^\times) + 4M(\Phi_{k, 2}^{\text{Id}}) + 4M \left(\left(\left(A^{(i)}, b^{(i)}, \text{Id}_{\mathbb{R}^k} \right) \right) \right) + 2M(\Phi_{T_i}^1) \right) \\ &\leq s(Ck + Ck + Cm + Cd^2) \leq Cs(k + m + d^2). \end{aligned}$$

□

3.1 Piecewise constants S_0

The lowest order approximation space for $L^2(\Omega)$ is the finite dimensional subspace

$$S_0(\mathcal{T}, \Omega) := \{v \in L^2(\Omega) : v|_T \equiv c_T \in \mathbb{R}, \forall T \in \mathcal{T}\} \subset L^2(\Omega). \quad (3.3)$$

A basis is given by $\{\theta_T^S\}_{T \in \mathcal{T}}$, whose elements are indicator functions $\theta_T^S := \mathbb{1}_T$ and can be expressed by applying Lemma 2.9 with $N = d+1$ and $k = 0$: for all $T = \text{conv}(\{a_0, \dots, a_d\}) \in \mathcal{T}$, we define $(A_i, b_i) \in \mathbb{R}^{1 \times (d+1)}$, $i = 1, \dots, d+1$ by the relations

$$(A_i, b_i) \begin{pmatrix} (a_0)_1 & & (a_d)_1 \\ & \ddots & \\ (a_0)_d & & (a_d)_d \\ 1 & \dots & 1 \end{pmatrix} = e_i^\top, \quad \text{for all } i = 1, \dots, d+1, \quad (3.4)$$

where $(e_i)_j = \delta_{ij}$, so that $T = \bigcap_{i=1, \dots, d+1} \{x \in \mathbb{R}^d : A_i x + b_i > 0\}$. Then there exists $C > 0$ such that

$$\theta_T^S = \text{R}(\Phi_T^1), \quad L(\Phi_T^1) = 3, \quad M(\Phi_T^1) \leq (d+2)(d+1) + 2 \leq Cd^2. \quad (3.5)$$

3.2 Raviart-Thomas elements RT_0

Define the vector-valued polynomial space $\text{RT}_0 = (\mathbb{P}_0)^d \oplus x\mathbb{P}_0$ and, for all $f \in \mathcal{F}$, let n_f denote a unit normal to the face f . The *Raviart-Thomas finite element space of lowest order* is (e.g. [16, Section 14.1])

$$\text{RT}_0(\mathcal{T}, \Omega) := \{v \in (L^1(\Omega))^d : v|_T \in \text{RT}_0 \ \forall T \in \mathcal{T} \text{ and } [v \cdot n_f]_f = 0 \ \forall f \in \mathcal{F}\} \subset H^0(\text{div}, \Omega). \quad (3.6)$$

This space has one degree of freedom per face $f \in \mathcal{F}$.

For $f \subset \partial\Omega$, we define $\theta_f^{RT}(x) := \frac{|f|}{d|T|}(x - a)\mathbb{1}_T$, where $f \subset \bar{T}$, $T \in \mathcal{T}$ and a is the only vertex of T that does not belong to \bar{f} .¹ For interior faces $f \subset \Omega$ we construct θ_f^{RT} by assembling local shape functions of the neighboring simplices T_1, T_2 with $\bar{f} = \bar{T}_1 \cap \bar{T}_2$, [16, Equation (14.3)]

$$\theta_f^{RT}(x) := \begin{cases} \frac{|f|}{d|T_1|}(x - a_1) & \text{if } x \in T_1, \\ -\frac{|f|}{d|T_2|}(x - a_2) & \text{if } x \in T_2, \\ 0 & \text{if } x \notin \bar{T}_1 \cap \bar{T}_2, \end{cases} \quad (3.7)$$

where a_1, a_2 are the the only vertices of T_1, T_2 , respectively, not belonging to \bar{f} . The functions $\{\theta_f^{RT}\}_{f \in \mathcal{F}}$ form a basis of $\text{RT}_0(\mathcal{T}, \Omega)$ (see, e.g., [16, Proposition 14.1]).

Proposition 3.2 *Given $f \in \mathcal{F}$, $f \subset \partial\Omega$, let $T \in \mathcal{T}$ be the simplex adjacent to f and $a := (\mathcal{V} \cap \bar{T}) \setminus \bar{f} \in \mathbb{R}^d$.*

Then

$$\Phi_f^{RT} := \Phi_{d,\kappa}^\times \odot \text{P} \left(\Phi_{d,2}^{\text{Id}} \odot \left(\left(\frac{|f|}{d|T|} \text{Id}_{d \times d}, -\frac{|f|}{d|T|} a, \text{Id}_{\mathbb{R}^d} \right) \right), \Phi_T^{\mathbb{1}} \right) \quad (3.8)$$

satisfies $\theta_f^{RT}(x) = \text{R}(\Phi_f^{RT})(x)$ for a.e. $x \in \Omega$, for any

$$\kappa \geq \sup_{x \in T} \frac{|f|}{d|T|} \|x - a\|_\infty. \quad (3.9)$$

Given $f \in \mathcal{F}$, $f \subset \Omega$, let T_1, T_2 be the simplices adjacent to f and let $a_i := (\mathcal{V} \cap \bar{T}_i) \setminus \bar{f} \in \mathbb{R}^d$, $i = 1, 2$. Then

$$\Phi_f^{RT} := \sum_{i=1,2} (-1)^{i-1} \Phi_{d,\kappa}^\times \odot \text{P} \left(\Phi_{d,2}^{\text{Id}} \odot \left(\left(\frac{|f|}{d|T_i|} \text{Id}_{d \times d}, -\frac{|f|}{d|T_i|} a_i, \text{Id}_{\mathbb{R}^d} \right) \right), \Phi_{T_i}^{\mathbb{1}} \right) \quad (3.10)$$

satisfies $\theta_f^{RT}(x) = \text{R}(\Phi_f^{RT})(x)$ for a.e. $x \in \Omega$, for any

$$\kappa \geq \max_{i=1,2} \sup_{x \in T_i} \frac{|f|}{d|T_i|} \|x - a_i\|_\infty. \quad (3.11)$$

In addition, there exists an absolute constant $C > 0$ such that for all $f \in \mathcal{F}$

$$L(\Phi_f^{RT}) = 5, \quad M(\Phi_f^{RT}) \leq Cd^2.$$

Remark 3.3 *We note that the right-hand sides of (3.9) and (3.11) are bounded from above by a constant which only depends on the shape regularity constant C_{sh} .*

Proof of Proposition 3.2. Firstly, we observe that indeed $\theta_f^{RT}(x) = \text{R}(\Phi_f^{RT})(x)$ for all $x \in \Omega \setminus \partial\mathcal{T}$, where $\partial\mathcal{T} := \bigcup_{T \in \mathcal{T}} \partial T$.

Secondly, we apply Lemma 3.1 with $k = d$ and $m = 2d$, and with $s = 1$ in (3.8) and $s = 2$ in (3.10). \square

¹ We use a different normalization of the shape functions than in [16, Section 14.1]. This has no consequences for the analysis that follows.

Alternatively, we can build the same shape functions by enforcing strongly, via ReLU activation, continuity of the component normal to f , as imposed in (3.6). We select the unit normal vector n_f to f pointing towards T_2 and an orthonormal system $\{t_1, \dots, t_{d-1}\}$ spanning the hyperplane tangent to f . Then, we decompose

$$\theta_f^{RT}(x) = (\theta_f^{RT}(x) \cdot n_f)n_f + \sum_{j=1}^{d-1} (\theta_f^{RT}(x) \cdot t_j)t_j. \quad (3.12)$$

Thus, it suffices to compute separately $\theta_f^{RT}(x) \cdot n_f$ and $\theta_f^{RT}(x) \cdot t_j$ and take the linear combination (3.12) in the last layer.

Proposition 3.4 *Given $f \in \mathcal{F}$, $f \subset \partial\Omega$, let $T \in \mathcal{T}$ be the simplex adjacent to f . Then there exist $A_{n_f} \in \mathbb{R}^{1 \times d}$, $b_{n_f} \in \mathbb{R}$ such that*

$$\Phi_f^{RT,n} := \Phi_{1,1}^\times \odot \text{P} \left(\Phi_{1,2}^{\text{Id}} \odot ((A_{n_f}, b_{n_f}, \text{Id}_{\mathbb{R}})), \Phi_T^1 + \Phi_f^1 \right) \quad (3.13)$$

satisfies $\theta_f^{RT}(x) \cdot n_f = \text{R} \left(\Phi_f^{RT,n} \right) (x)$ for a.e. $x \in \Omega$ and every $x \in f$. Also, there exist $A_{t_j} \in \mathbb{R}^{1 \times d}$, $b_{t_j} \in \mathbb{R}$, $j = 1, \dots, d-1$ such that

$$\Phi_f^{RT,t_j} := \Phi_{1,\kappa}^\times \odot \text{P} \left(\Phi_{1,2}^{\text{Id}} \odot ((A_{t_j}, b_{t_j}, \text{Id}_{\mathbb{R}})), \Phi_T^1 \right) \quad (3.14)$$

satisfies $\theta_f^{RT}(x) \cdot t_j = \text{R} \left(\Phi_f^{RT,t_j} \right) (x)$ for a.e. $x \in \Omega$, where

$$\kappa \geq \max_{j=1, \dots, d-1} \sup_{x \in T} \|A_{t_j}x + b_{t_j}\|_\infty. \quad (3.15)$$

Given $f \in \mathcal{F}$, $f \subset \Omega$, let T_1, T_2 be the simplices adjacent to f . Then there exist $A_{n_f}^{(i)} \in \mathbb{R}^{1 \times d}$, $b_{n_f}^{(i)} \in \mathbb{R}$, $i = 1, 2$ such that

$$\Phi_f^{RT,n} := \Phi_{1,1}^\times \odot \text{P} \left(\Phi_2^{\min} \odot \left(\left(\begin{pmatrix} A_{n_f}^{(1)} \\ A_{n_f}^{(2)} \end{pmatrix}, \begin{pmatrix} b_{n_f}^{(1)} \\ b_{n_f}^{(2)} \end{pmatrix}, \text{Id}_{\mathbb{R}^2} \right) \right), \Phi_{T_1}^1 + \Phi_f^1 + \Phi_{T_2}^1 \right) \quad (3.16)$$

satisfies $\theta_f^{RT}(x) \cdot n_f = \text{R} \left(\Phi_f^{RT,n} \right) (x)$ for a.e. $x \in \Omega$ and every $x \in f$. There also exist $A_{t_j}^{(i)} \in \mathbb{R}^{1 \times d}$, $b_{t_j}^{(i)} \in \mathbb{R}$, $i = 1, 2$, $j = 1, \dots, d-1$ such that

$$\Phi_f^{RT,t_j} := \sum_{i=1,2} \Phi_{1,\kappa}^\times \odot \text{P} \left(\Phi_{1,2}^{\text{Id}} \odot \left((A_{t_j}^{(i)}, b_{t_j}^{(i)}, \text{Id}_{\mathbb{R}}) \right), \Phi_{T_i}^1 \right) \quad (3.17)$$

satisfies $\theta_f^{RT}(x) \cdot t_j = \text{R} \left(\Phi_f^{RT,t_j} \right) (x)$ for a.e. $x \in \Omega$, where

$$\kappa \geq \max_{j=1, \dots, d-1} \sup_{x \in T_i} \left| A_{t_j}^{(i)}x + b_{t_j}^{(i)} \right|. \quad (3.18)$$

In addition, there exists a constant $C > 0$ such that

$$\begin{aligned} L(\Phi_f^{RT,n}) &= 5, & L(\Phi_f^{RT,t_j}) &= 5, \\ M(\Phi_f^{RT,n}) &\leq Cd^2, & M(\Phi_f^{RT,t_j}) &\leq Cd^2. \end{aligned}$$

Proof. Below, we prove the result for $f \subset \Omega$. The case $f \subset \partial\Omega$ follows analogously.

Observe that we can write $T_i = \text{conv}(\{a_i, p_1, \dots, p_d\})$ where $\{p_1, \dots, p_d\} := \mathcal{V} \cap \bar{f}$. The point values $\theta_f^{RT}(p_i) \cdot n_f = 1, \forall i = 1, \dots, d$ are well-defined by continuity of $\theta_f^{RT} \cdot n_f$ across f . Therefore, we can take $A_{n_f}^{(i)} \in \mathbb{R}^{1 \times d}, b_{n_f}^{(i)} \in \mathbb{R}, i = 1, 2$ to be the matrices and vectors solving

$$(A_{n_f}^{(i)}, b_{n_f}^{(i)}) \begin{pmatrix} (a_i)_1 & (p_1)_1 & & (p_d)_1 \\ \vdots & & \ddots & \\ (a_i)_d & (p_1)_d & \dots & (p_d)_d \\ 1 & 1 & \dots & 1 \end{pmatrix} = (0, 1, \dots, 1), \quad (3.19)$$

where $(0, 1, \dots, 1) = (-1)^{i-1} \frac{|f|}{d|T_i|} (0, (p_1 - a_i) \cdot n_f, \dots, (p_d - a_i) \cdot n_f)$. With this choice, since $(\theta_f^{RT}(x) \cdot n_f) \in [0, 1]$ for $x \in T_1 \cup T_2 \cup f$, it holds that $\theta_f^{RT}(x) \cdot n_f = \mathbf{R}(\Phi_f^{RT, n})(x)$ for a.e. $x \in \Omega$ and every $x \in f$. On the other hand, the discontinuous tangential component can be assembled element by element, as in Proposition 3.2: matrices and vectors $(A_{t_j}^{(i)}, b_{t_j}^{(i)}) \in \mathbb{R}^{1 \times (d+1)}, i = 1, 2$ and $j = 1, \dots, d-1$ which only depend on T_i and t_j can be computed as in (3.19), but with different right-hand sides, namely $(-1)^{i-1} \frac{|f|}{d|T_i|} (0, (p_1 - a_i) \cdot t_j, \dots, (p_d - a_i) \cdot t_j) \in \mathbb{R}^{1 \times d+1}$.

Finally, we estimate the network depth and size. For $d = 2$, as in Remark 2.7 let

$$\Phi_2^{\min} := \left(\left(\begin{pmatrix} -1 & 1 \\ 0 & 1 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \rho \\ \rho \\ \rho \end{pmatrix} \right), ((-1 \ 1 \ -1), 0, \text{Id}_{\mathbb{R}}) \right)$$

$$L(\Phi_2^{\min}) = 2, \quad M(\Phi_2^{\min}) = 7.$$

In particular, we use that $L(\Phi_2^{\min}) + 1 = L(\Phi_{T_1}^{\frac{1}{2}} + \Phi_f^{\frac{1}{2}} + \Phi_{T_2}^{\frac{1}{2}}) = 3$, i.e. in (3.16) both components in the parallelization have equal depth. Also, because the networks defined in Equations (3.13) and (3.14) have smaller sizes than those defined in (3.16) and (3.17), we will only estimate the sizes of the latter. In the bound on the size of $\Phi_{T_1}^{\frac{1}{2}} + \Phi_f^{\frac{1}{2}} + \Phi_{T_2}^{\frac{1}{2}}$ in (3.16), we use for T_1, T_2 Lemma 2.9 with $N = d + 1$ and $k = 0$, whereas for f we use Lemma 2.9 with $N = d + 1$ and $k = 1$. The size of the network in (3.17) is estimated using Lemma 3.1 with $k = 1, m = d + 1$ and $s = 2$.

$$L(\Phi_f^{RT, n}) = L(\Phi_{1,1}^{\times}) + L(\Phi_{T_1}^{\frac{1}{2}} + \Phi_f^{\frac{1}{2}} + \Phi_{T_2}^{\frac{1}{2}}) = 5,$$

$$M(\Phi_f^{RT, n}) \leq 2M(\Phi_{1,1}^{\times}) + 2M \left(\mathbf{P} \left(\Phi_2^{\min} \odot \left(\left(\begin{pmatrix} A_{n_f}^{(1)} \\ A_{n_f}^{(2)} \end{pmatrix}, \begin{pmatrix} b_{n_f}^{(1)} \\ b_{n_f}^{(2)} \end{pmatrix}, \text{Id}_{\mathbb{R}^2} \right) \right), \Phi_{T_1}^{\frac{1}{2}} + \Phi_f^{\frac{1}{2}} + \Phi_{T_2}^{\frac{1}{2}} \right) \right)$$

$$\leq 2M(\Phi_{1,1}^{\times}) + 4M(\Phi_2^{\min}) + 4M \left(\left(\left(\begin{pmatrix} A_{n_f}^{(1)} \\ A_{n_f}^{(2)} \end{pmatrix}, \begin{pmatrix} b_{n_f}^{(1)} \\ b_{n_f}^{(2)} \end{pmatrix}, \text{Id}_{\mathbb{R}^2} \right) \right) \right)$$

$$+ 2M(\Phi_{T_1}^{\frac{1}{2}}) + 2M(\Phi_f^{\frac{1}{2}}) + 2M(\Phi_{T_2}^{\frac{1}{2}})$$

$$\leq C(C + C + Cd + Cd^2 + Cd^2 + Cd^2) \leq Cd^2.$$

□

Remark 3.5 *The right-hand sides of Equations (3.15) and (3.18) are bounded from above by a constant which only depends on the shape regularity constant C_{sh} of the mesh \mathcal{T} .*

Corollary 3.6 *The network*

$$\Phi_f^{RT, *} := ((n_f, 0, \text{Id}_{\mathbb{R}^d}) \odot \Phi_f^{RT, n} + \sum_{j=1}^{d-1} ((t_j, 0, \text{Id}_{\mathbb{R}^d}) \odot \Phi_f^{RT, t_j}) \quad (3.20)$$

satisfies $\theta_f^{RT}(x) = \mathbf{R}(\Phi_f^{RT,*})(x)$ for a.e. $x \in \Omega$ and $(\theta_f^{RT}(x) \cdot n_f)n_f = \mathbf{R}(\Phi_f^{RT,*})(x)$ for all $x \in f$. In addition, it holds that

$$L(\Phi_f^{RT,*}) = 6, \quad M(\Phi_f^{RT,*}) \leq Cd^3.$$

Proof. We estimate the network size and depth as follows:

$$\begin{aligned} L(\Phi_f^{RT,*}) &= 6, \\ M(\Phi_f^{RT,*}) &\leq 2M((n_f, 0, \text{Id}_{\mathbb{R}^d})) + 2M(\Phi_f^{RT,n}) \\ &\quad + \sum_{j=1}^{d-1} \left(2M((t_j, 0, \text{Id}_{\mathbb{R}^d})) + 2M(\Phi_f^{RT,t_j}) \right) \leq Cd^3. \end{aligned}$$

□

3.3 Nédélec elements \mathbb{N}_0

In this section we restrict ourselves to the space dimension $d \in \{2, 3\}$. For $d = 2$, the two-dimensional curl is defined as $\text{curl} v = (-\partial_1 v_2, \partial_2 v_1)$ and we can relate the Nédélec basis functions to the Raviart-Thomas basis. In fact, one can verify that, for an edge $f \in \mathcal{E} = \mathcal{F}$ (which is also a face), the finite element basis $\{\theta_f^{NE}\}_{f \in \mathcal{F}}$ for \mathbb{N}_0 satisfies

$$\theta_f^{NE} \cdot t_f = \theta_f^{RT} \cdot n_f, \quad \text{and} \quad \theta_f^{NE} \cdot n_f = -\theta_f^{RT} \cdot t_f, \quad (3.21)$$

where $n_f := ((n_f)_1, (n_f)_2)$ is a unit normal vector to f as in (3.12) and $t_f = (-(n_f)_2, (n_f)_1)$ is a unit vector tangent to f . Hence, a NN emulation for θ_f^{NE} can be derived from Proposition 3.2 or Corollary 3.6.

We now focus on the case $d = 3$. Define $\mathbb{NE}_0 = (\mathbb{P}_0)^3 \oplus x \times (\mathbb{P}_0)^3$ and for all $f \in \mathcal{F}$, let n_f denote a unit vector normal to the face f . Then the Nédélec finite element space of lowest order [16, Section 15.1] reads

$$\mathbb{N}_0(\mathcal{T}, \Omega) := \{v \in (L^1(\Omega))^3 : v|_T \in \mathbb{NE}_0 \ \forall T \in \mathcal{T} \text{ and } [v \times n_f]_f = 0 \ \forall f \in \mathcal{F}\} \subset H^0(\text{curl}, \Omega). \quad (3.22)$$

This space has one degree of freedom per edge $e \in \mathcal{E}$.

A basis $\{\theta_e^{NE}\}_{e \in \mathcal{E}}$ for $\mathbb{N}_0(\mathcal{T}, \Omega)$ can be constructed by assembling local shape functions of all simplices $T_1, \dots, T_{s(e)}$, $s(e) \in \mathbb{N}$ sharing an edge e . We fix $e \in \mathcal{E}$ and a unit vector t_e tangent to e , and denote the midpoint of e by m_e . We denote by $\tilde{e}(i)$ the only edge of T_i that does not share a vertex with e , and let $t_{\tilde{e}(i)}$ be a unit vector tangent to $\tilde{e}(i)$, directed in such a way that $t_e \cdot [(m_e - m_{\tilde{e}(i)}) \times t_{\tilde{e}(i)}] > 0$. Then,

$$\theta_e^{NE}(x) := \begin{cases} \frac{(x - m_{\tilde{e}(i)}) \times t_{\tilde{e}(i)}}{t_e \cdot [(m_e - m_{\tilde{e}(i)}) \times t_{\tilde{e}(i)}]} & \text{if } x \in T_i, i = 1, \dots, s(e), \\ 0 & \text{if } x \notin \bigcup_{i=1, \dots, s(e)} T_i. \end{cases} \quad (3.23)$$

Note that

$$\mathfrak{s}(\mathcal{E}) := \max_{e \in \mathcal{E}} s(e) \quad (3.24)$$

is bounded from above by a constant only dependent on the shape regularity constant C_{sh} of \mathcal{T} .

Proposition 3.7 *Given $e \in \mathcal{E}$, let $A_e^{(i)} \in \mathbb{R}^{3 \times 3}$, $b_e^{(i)} \in \mathbb{R}^3$ be such that for $i = 1, \dots, s(e)$*

$$A_e^{(i)} x := \frac{x \times t_{\tilde{e}(i)}}{t_e \cdot [(m_e - m_{\tilde{e}(i)}) \times t_{\tilde{e}(i)}]} \quad \forall x \in \mathbb{R}^3, \quad b_e^{(i)} := -\frac{m_{\tilde{e}(i)} \times t_{\tilde{e}(i)}}{t_e \cdot [(m_e - m_{\tilde{e}(i)}) \times t_{\tilde{e}(i)}]},$$

Then

$$\Phi_e^{NE} := \sum_{i=1}^{s(e)} \Phi_{3,\kappa}^\times \odot \mathbf{P} \left(\Phi_{3,2}^{\text{Id}} \odot \left((A_e^{(i)}, b_e^{(i)}, \text{Id}_{\mathbb{R}^3}) \right), \Phi_{T_i}^1 \right) \quad (3.25)$$

satisfies $\theta_e^{NE}(x) = \mathbf{R}(\Phi_e^{NE})(x)$ for a.e. $x \in \Omega$, for any κ such that

$$\kappa \geq \max_{i=1,\dots,s(e)} \sup_{x \in \bar{T}_i} \frac{\|(x - m_{\bar{e}(i)}) \times t_{\bar{e}(i)}\|_\infty}{t_e \cdot [(m_e - m_{\bar{e}(i)}) \times t_{\bar{e}(i)}]}. \quad (3.26)$$

Moreover,

$$L(\Phi_e^{NE}) = 5, \quad M(\Phi_e^{NE}) \leq C_5(\mathcal{E}).$$

Proof. Firstly, we observe that indeed $\theta_e^{NE}(x) = \mathbf{R}(\Phi_e^{NE})(x)$ for all $x \in \Omega \setminus \partial\mathcal{T}$. Secondly, we use Lemma 3.1 with $k = d = 3$, $m = d^2 + d = 12$ and $s = s(e)$. \square

3.4 CPwL elements S_1

In this section, we provide a construction based on element-by-element assembly of the shape functions, similar to that in the previous sections, using both ReLU and BiSU activations. Let

$$S_1(\mathcal{T}, \Omega) := \{v \in H^1(\Omega) : v|_T \in \mathbb{P}_1, \forall T \in \mathcal{T}\} \subset H^1(\Omega) \quad (3.27)$$

be the FE space of continuous piecewise linear functions on \mathcal{T} . A basis $\{\theta_p^{PL}\}_{p \in \mathcal{V}}$ of this space is uniquely defined by the relations $\theta_{p_i}^{PL}(p_j) = \delta_{ij}$, for $p_i, p_j \in \mathcal{V}$. Define $n(p) := |\{T \in \mathcal{T} : p \in \bar{T}\}| \in \mathbb{N}$. Note that

$$\mathbf{n}(\mathcal{V}) := \max_{p \in \mathcal{V}} n(p) \quad (3.28)$$

is bounded from above by a constant only dependent on the shape regularity constant C_{sh} of \mathcal{T} . The following proposition is analogous to Propositions 3.2 and 3.7.

Proposition 3.8 *Given $p \in \mathcal{V}$, let $T_1, \dots, T_{n(p)} \in \mathcal{T}$, $n(p) \in \mathbb{N}$ be the simplices adjacent to p . Let $A_p^{(i)} \in \mathbb{R}^{1 \times d}$, $b_p^{(i)} \in \mathbb{R}^1$ for $i = 1, \dots, n(p)$ be such that*

$$(A_p^{(i)}, b_p^{(i)}) \begin{pmatrix} p_1 & (a_{i,1})_1 & & (a_{i,d})_1 \\ \vdots & & \ddots & \\ p_d & (a_{i,1})_d & & (a_{i,d})_d \\ 1 & 1 & \dots & 1 \end{pmatrix} = (1, 0, \dots, 0),$$

where the points $a_{i,j} \in \mathbb{R}^d$ are such that $T_i = \text{conv}(p, a_{i,1}, \dots, a_{i,d})$. Then

$$\Phi_p^{PL} := \sum_{i=1}^{n(p)} \Phi_{1,1}^\times \odot \mathbf{P} \left(\Phi_{1,2}^{\text{Id}} \odot (A_p^{(i)}, b_p^{(i)}, \text{Id}_{\mathbb{R}}), \Phi_{T_i}^1 \right) \quad (3.29)$$

satisfies $\theta_p^{PL}(x) = \mathbf{R}(\Phi_p^{PL})(x)$ for a.e. $x \in \Omega$. Moreover,

$$L(\Phi_p^{PL}) = 5, \quad M(\Phi_p^{PL}) \leq C \mathbf{n}(\mathcal{V}) d^2.$$

Proof. Observing that $\theta_p^{PL}(x) = \mathbf{R}(\Phi_p^{PL})(x)$ for all $x \in \Omega \setminus \partial\mathcal{T}$, we use Lemma 3.1 with $k = 1$, $m = d + 1$ and $s = n(p)$ to estimate the NN size. \square

4 CPwL elements using ReLU NNs

For continuous shape functions which vanish on the boundary of their domain of definition, one can use the ReLU activation function alone, as shown in [18] for a class of meshes with convex patches. The purpose of this section is to extend the results from [18] to more general, shape-regular simplicial meshes. In the sequel, for a vertex $p \in \mathcal{V}$ we write

$$\omega(p) := \bigcup_{i=1, \dots, n(p)} \bar{T}_i, \quad (4.1)$$

where $T_1, \dots, T_{n(p)} \in \mathcal{T}$ denote the simplices adjacent to p . We call $\omega(p)$ a *patch*. One key assumption in [18] was that $\omega(p)$ is convex for all vertices $p \in \mathcal{V}$.

Removing this assumption is the main topic of the Section 4.2. We remark that the construction given in Section 3.4 also does not require convexity of the patches and, since no minimum is computed, the depth of the network is independent of the input dimension d and the maximum number of elements meeting in one point $n(\mathcal{V})$. However, in this section we avoid the use of BiSU activations, which is unnatural for continuous functions in $S_1(\mathcal{T}, \Omega)$.

4.1 Meshes with convex patches

Under the assumption of convexity of patches, the hat basis functions $\{\theta_p^{PL}\}_{p \in \mathcal{V}} \subset S_1(\mathcal{T}, \Omega)$ satisfy [18, Lemma 3.1]

$$\theta_p^{PL}(x) = \max \left\{ 0, \min_{i=1, \dots, n(p)} A_p^{(i)} x + b_p^{(i)} \right\}, \quad (4.2)$$

with $A_p^{(i)} \in \mathbb{R}^{1 \times d}$, $b_p^{(i)} \in \mathbb{R}^1$ such that $A_p^{(i)} x + b_p^{(i)} = \theta_p^{PL}|_{T_i}(x)$ for all $T_i \subset \omega(p)$, $i = 1, \dots, n(p)$.

We now recall the emulation of the shape functions from [18], and show the dependence of the constants on d . We remark that the d -dependence was not studied in [18].

Proposition 4.1 ([18, Theorem 3.1]) *Consider $p \in \mathcal{V}$ for which $\omega(p)$ is convex and let $T_1, \dots, T_{n(p)} \in \mathcal{T}$, $n(p) \in \mathbb{N}$ be the simplices adjacent to p . Let $(A_p^{(i)}, b_p^{(i)}) \in \mathbb{R}^{d+1, 1}$, $i = 1, \dots, n(p)$ be as in (4.2).*

Then

$$\Phi_p^{CPL} := \left((1, 0, \rho), (1, 0, \text{Id}_{\mathbb{R}}) \right) \odot \Phi_{n(p)}^{\min} \odot \left(\left(\left(\begin{array}{c} A_p^{(1)} \\ \vdots \\ A_p^{(n(p))} \end{array} \right), \left(\begin{array}{c} b_p^{(1)} \\ \vdots \\ b_p^{(n(p))} \end{array} \right), \text{Id}_{\mathbb{R}^{n(p)}} \right) \right)$$

satisfies $R(\Phi_p^{CPL})(x) = \theta_p^{PL}(x)$ for all $x \in \Omega$ and

$$L(\Phi_p^{CPL}) = 5 + \log_2(n(p)), \quad M(\Phi_p^{CPL}) \leq Cdn(p).$$

Proof. The network depth and size can be bounded as

$$\begin{aligned}
L(\Phi_p^{CPL}) &= L\left(\left((1, 0, \rho), (1, 0, \text{Id}_{\mathbb{R}})\right)\right) + L(\Phi_{n(p)}^{\min}) \\
&\quad + L\left(\left(\left(\left(\left(A_p^{(1)}\right), \left(b_p^{(1)}\right), \text{Id}_{\mathbb{R}^{n(p)}}\right)\right), \left(\left(A_p^{(n(p))}\right), \left(b_p^{(n(p))}\right), \text{Id}_{\mathbb{R}^{n(p)}}\right)\right)\right) \\
&\leq 2 + (2 + \log_2(n(p))) + 1 \leq 5 + \log_2(n(p)), \\
M(\Phi_p^{CPL}) &\leq CM\left(\left((1, 0, \rho), (1, 0, \text{Id}_{\mathbb{R}})\right)\right) + CM(\Phi_{n(p)}^{\min}) \\
&\quad + CM\left(\left(\left(\left(\left(A_p^{(1)}\right), \left(b_p^{(1)}\right), \text{Id}_{\mathbb{R}^{n(p)}}\right)\right), \left(\left(A_p^{(n(p))}\right), \left(b_p^{(n(p))}\right), \text{Id}_{\mathbb{R}^{n(p)}}\right)\right)\right) \\
&\leq C(2 + n(p) + n(p)(d + 1)) \leq Cdn(p).
\end{aligned}$$

□

The preceding result can be used to construct emulations of shape functions on non-convex patches which only use the ReLU activation.

4.2 Meshes including non-convex patches

We now extend the result from Sec. 4.1 to the case of non-convex patches, i.e. we show that ReLU NNs can emulate CPwL functions on arbitrary simplicial meshes in $d \in \mathbb{N}$ dimensions. Our proof strategy is to write a non-convex patch as a suitable union of convex ones, and thereby reduce the problem to the convex case.

Lemma 4.2 *For $d \in \mathbb{N}$, let $T = \text{conv}(\{a_0, \dots, a_d\})$ be a simplex and $\delta > 0$. Define $q := a_0 + \delta \sum_{i=1}^d (a_0 - a_i)$. Then $T_\delta := \text{conv}(\{q, a_1, \dots, a_d\})$ is a simplex and $a_0 \in T_\delta$.*

Proof. Without loss of generality, $a_0 = 0$. To show that T_δ is a simplex, it suffices to verify $a_0 = 0 \in T_\delta$, as it then follows that $T \subset T_\delta$, i.e. T_δ has nonempty interior and is thus a simplex. By definition,

$$T_\delta = \left\{ \alpha_0 \left(\delta \sum_{i=1}^d -a_i \right) + \sum_{i=1}^d \alpha_i a_i : \sum_{i=0}^d \alpha_i = 1 \text{ and } \alpha_i > 0 \right\}.$$

Therefore, $a_0 \in T_\delta$ is equivalent to

$$\alpha_0 \delta \sum_{i=1}^d a_i = \sum_{i=1}^d \alpha_i a_i,$$

which holds if and only if $\alpha_0 \delta = \alpha_i$ for all $i = 1, \dots, d$. A viable choice satisfying $\sum_{i=0}^d \alpha_i = 1$ and $\alpha_i > 0$ is $\alpha_0 = (1 + d\delta)^{-1}$ and $\alpha_i = \delta(1 + d\delta)^{-1}$ for all $i = 1, \dots, d$, and thus $a_0 \in T_\delta$. □

Proposition 4.3 *Given a simplex $T = \text{conv}(\{a_0, \dots, a_d\})$ and a point $p \in T$, let*

$$T_i := \text{conv}(\{p, a_0, \dots, a_d\} \setminus \{a_i\}) \quad \text{for all } i \in \{0, \dots, d\}.$$

Then

$$\overline{\bigcup_{i \in \{0, \dots, d\}} T_i} = \overline{T} \tag{4.3}$$

and this is a patch.

Proof. Let $p \in T$, i.e.

$$p = \sum_{i=0}^d \alpha_i a_i, \quad \alpha_i > 0 \text{ and } \sum_{i=0}^d \alpha_i = 1.$$

First we show that T_0 is a simplex, which by symmetry implies that T_i is a simplex for all $i \in \{0, \dots, d\}$. It suffices to check that $p - a_1 \notin \text{span}\{a_2 - a_1, \dots, a_d - a_1\}$, since then $\{p - a_1, a_2 - a_1, \dots, a_d - a_1\}$ is a set of linearly independent vectors. This is true since $\{a_0 - a_1, a_2 - a_1, \dots, a_d - a_1\}$ are linearly independent vectors, $\alpha_1 = 1 - \sum_{i \neq 1} \alpha_i$ and thus

$$p - a_1 = \sum_{i \neq 1} \alpha_i (a_i - a_1),$$

with $\alpha_0 > 0$ does not belong to $\text{span}\{a_2 - a_1, \dots, a_d - a_1\}$. Furthermore, $\bigcup_{i \in \{0, \dots, d\}} \overline{T_i} \subset \overline{T}$ follows by the fact that $p \in T$ implies $T_i \subset T$ for all $i \in \{0, \dots, d\}$.

Next we show $\bigcup_{i \in \{0, \dots, d\}} \overline{T_i} \supset \overline{T}$. Fix $\bar{p} := \sum_{j=0}^d \gamma_j a_j$ with $\gamma_j \geq 0$ satisfying $\sum_{j=0}^d \gamma_j = 1$, i.e. \bar{p} is an arbitrary point in \overline{T} . We wish to show that $\bar{p} \in \overline{T_i}$ for some $i \in \{0, \dots, d\}$, i.e.

$$\sum_{j=0}^d \gamma_j a_j = \sum_{j \neq i} \beta_j a_j + \beta_i \sum_{j=0}^d \alpha_j a_j \quad \text{for some } \beta_j \geq 0, \quad \sum_{j=0}^d \beta_j = 1.$$

This is equivalent to

$$\sum_{j=0}^d (\gamma_j - \beta_i \alpha_j) a_j = \sum_{j \neq i} \beta_j a_j. \quad (4.4)$$

We now show that there exist $(\beta_j)_{j=0}^d$ for which this holds. Let

$$i \in \operatorname{argmin}_{j \in \{0, \dots, d\}} \frac{\gamma_j}{\alpha_j}, \quad (4.5)$$

which is well-defined because $\gamma_j \geq 0$ and $\alpha_j > 0$ for all $j \in \{0, \dots, d\}$. Since $\sum_{j=0}^d \alpha_j = 1 = \sum_{j=0}^d \gamma_j$, for i in (4.5) it must hold $\frac{\gamma_i}{\alpha_i} \leq 1$. Equation (4.4) holds if $\gamma_i - \beta_i \alpha_i = 0$ and $\gamma_j - \beta_i \alpha_j = \beta_j$ for all $j \neq i$. The former is satisfied for $\beta_i = \frac{\gamma_i}{\alpha_i} \in [0, 1]$ and the latter is satisfied if $\beta_j = \gamma_j - \beta_i \alpha_j$, which implies $\beta_j = \alpha_j (\frac{\gamma_j}{\alpha_j} - \frac{\gamma_i}{\alpha_i}) \geq 0$ and $\beta_j = \alpha_j (\frac{\gamma_j}{\alpha_j} - \frac{\gamma_i}{\alpha_i}) \leq \gamma_j \leq 1$. It is left to show that $\sum_{j=0}^d \beta_j = 1$. We have

$$\sum_{j \neq i} \beta_j + \beta_i = \sum_{j \neq i} \alpha_j \left(\frac{\gamma_j}{\alpha_j} - \frac{\gamma_i}{\alpha_i} \right) + \frac{\gamma_i}{\alpha_i} = \sum_{j \neq i} \gamma_j + \frac{\gamma_i}{\alpha_i} \left(1 - \sum_{j \neq i} \alpha_j \right) = \sum_{j \neq i} \gamma_j + \frac{\gamma_i}{\alpha_i} \alpha_i = 1.$$

We found $i \in \{0, \dots, d\}$ and $(\beta_j)_{j=0}^d$ for which (4.4) holds. Thus $\bar{p} \in \overline{T_i}$, and $\bigcup_{i \in \{0, \dots, d\}} \overline{T_i} \supset \overline{T}$.

It is left to show that for all $m \neq n \in \{0, \dots, d\}$ the intersection of $\overline{T_m}$ and $\overline{T_n}$ is the closure of a sub-simplex of both. Consider

$$\overline{T_m} = \left\{ \sum_{j \neq m} \beta_j a_j + \beta_m p : \sum_{j=0}^d \beta_j = 1 \text{ and } \beta_j \geq 0 \right\},$$

$$\overline{T_n} = \left\{ \sum_{j \neq n} \beta_j a_j + \beta_n p : \sum_{j=0}^d \beta_j = 1 \text{ and } \beta_j \geq 0 \right\}.$$

Then

$$\overline{T_m} \cap \overline{T_n} = \left\{ \sum_{j \neq m, n}^d \beta_j a_j + \beta p : \beta + \sum_{j \neq m, n}^d \beta_j = 1 \text{ and } \beta, \beta_j \geq 0 \right\},$$

which, by definition, is the closure of a sub-simplex of both $\overline{T_m}$ and $\overline{T_n}$. \square

For a set $S \subset \mathbb{R}^d$, in the following we call $x \in S$ a *star point* of S iff for all $y \in S \setminus \{x\}$ holds $\text{conv}(\{x, y\}) \subset S$.

Lemma 4.4 *Let $p \in \mathcal{V} \cap \text{int } \Omega$ and let $T_1, \dots, T_{n(p)} \in \mathcal{T}$ be the simplices adjacent to p . For each $j = 1, \dots, n(p)$, we denote by P_{T_j} the hyperplane passing through all vertices of T_j except p . Then, any $x \in \text{int } \omega(p)$ that is on the same side of the hyperplane P_{T_j} as p for all $j = 1, \dots, n(p)$ is a star point for the patch $\omega(p)$.*

Proof. We divide the claim in two steps:

Step 1. We claim that $\partial\omega(p) \subset \bigcup_{j=1}^{n(p)} P_{T_j}$ for all $p \in \mathcal{V} \cap \text{int } \Omega$. Define a regular partition \mathcal{T}' of \mathbb{R}^d that extends \mathcal{T} , i.e. such that $\mathcal{T} \subset \mathcal{T}'$. For every point z on $\partial\omega(p)$, z is on the boundary of an element $T \subset \omega(p)$ and of an element $T' \subset \mathbb{R}^d \setminus \omega(p)$, $T, T' \in \mathcal{T}'$. By regularity of \mathcal{T}' , $\overline{T} \cap \overline{T'}$ is the closure of a subsimplex f of both \overline{T} and $\overline{T'}$. Because T is a simplex with p as one of its vertices, if z is not in P_T , then f touches p , which implies that $T' \subset \omega(p)$ and gives a contradiction.

Step 2. Assume that $x \in \text{int } \omega(p)$ is not a star point of $\omega(p)$. Then there exists $q \in \omega(p)$ and $t \in [0, 1]$ such that $tx + (1-t)q \notin \omega(p)$. Therefore, there exist $\underline{t}, \bar{t} \in [0, 1]$ satisfying $\underline{t} < \bar{t}$, and $T \in \mathcal{T}$, $T \subset \omega(p)$, such that, using Step 1, $\bar{t}x + (1-\bar{t})q \in P_T$ and $sx + (1-s)q \in T$, $\forall s \in (\underline{t}, \bar{t})$. Since p and T lie on the same side of P_T , $sx + (1-s)q$ lies on the other side of P_T than p for all $s \in (\bar{t}, 1]$. For $s = 1$, this implies that x is on the other side of the hyperplane P_T than p . Thus if $x \in \text{int } \omega(p)$ is not a star point, it lies on the other side of at least one hyperplane P_{T_j} than p . Therefore, if a point $x \in \text{int } \omega(p)$ is on the same side of P_{T_j} as p for all $j = 1, \dots, n(p)$, then x is a star point for $\omega(p)$, by contradiction. \square

Remark 4.5 *The converse implication of Lemma 4.4 holds as well: the set of all star points of the patch $\omega(p)$ coincides with the intersection $\bigcap_{j=1}^{n(p)} \overline{H_j}$ of all closed half-spaces $\overline{H_j}$, where $H_j \subset \mathbb{R}^d$ is defined as the set of all points that lie on the same side of P_{T_j} as p .*

In the following, denote by $B_\epsilon(p) \subset \mathbb{R}^d$ the ball of radius $\epsilon > 0$ centered at $p \in \mathbb{R}^d$, with respect to the Euclidean norm.

Lemma 4.6 *For all $p \in \mathcal{V} \cap \text{int } \Omega$, there exists $\epsilon > 0$ such that $B_\epsilon(p) \subset \omega(p)$ and such that every $x \in B_\epsilon(p)$ is a star point of $\omega(p)$.*

Proof. For $j = 1, \dots, n(p)$ denote by $H_j \subset \mathbb{R}^d$ the open half-space containing all points that lie on the same side of P_{T_j} as p . Then $\bigcap_{j=1}^{n(p)} H_j$ is open, contains p and is a subset of the set of all star-points of $\omega(p)$ by Lemma 4.4. \square

Lemma 4.7 *Given $p \in \mathcal{V} \cap \text{int } \Omega$, let $T_1, \dots, T_{n(p)} \in \mathcal{T}$ be the simplices adjacent to p . For all $j = 1, \dots, n(p)$, let $a_0 := p$ and $a_1, \dots, a_d \in \mathbb{R}^d$ be such that $T_j = \text{conv}(\{a_0, \dots, a_d\})$ and let $q_j := p + \delta_j \sum_{i=1}^d (p - a_i)$ for some sufficiently small $\delta_j > 0$. With*

$$\tilde{T}_{ij} := \begin{cases} \text{conv}(\{q_j, a_0, \dots, a_d\} \setminus \{a_i\}) & \text{if } i \in \{1, \dots, d\} \\ T_j & \text{if } i = 0, \end{cases}$$

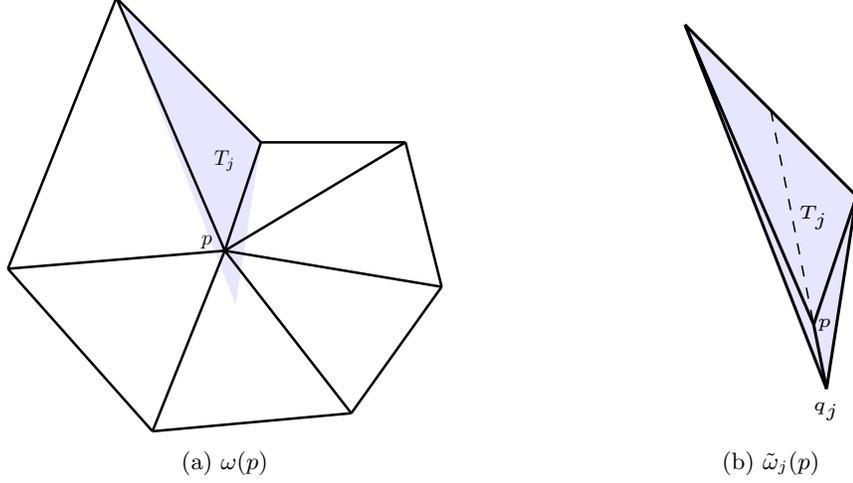


Figure 4.1: The patches $\omega(p)$ and (shaded) $\tilde{\omega}_j(p) \subset \omega(p)$ in Lemma 4.7.

set

$$\tilde{\omega}_j(p) := \bigcup_{i=0}^d \overline{\tilde{T}_{ij}}.$$

Then $\tilde{\omega}_j(p)$ is convex and $\overline{\tilde{T}_j} \subset \tilde{\omega}_j(p) \subset \omega(p)$. The sets $\{\tilde{T}_{ij}\}_{i=0,\dots,d}$ form a regular partition of $\tilde{\omega}_j(p)$.

Proof. For $\epsilon > 0$ as in Lemma 4.6, let $\delta_j > 0$ in the definition of q_j be such that $\|q_j - p\|_2 = \frac{\epsilon}{2}$. Then $q_j \in B_\epsilon(p) \subset \omega(p)$ is a star point of $\omega(p)$ by Lemma 4.6. Therefore, $\tilde{T}_{ij} \subset \omega(p)$ for all $i = 1, \dots, d$, and thus $\tilde{\omega}_j(p) \subset \omega(p)$. It also holds that $\overline{\tilde{T}_j} = \overline{\tilde{T}_{0j}} \subset \tilde{\omega}_j(p)$. After observing that $\text{int } \tilde{\omega}_j(p) = (\tilde{T}_j)_{\delta_j}$ in the notation of Lemma 4.2, Lemma 4.2 shows that $\tilde{\omega}_j(p)$ is a simplex and thus convex. The sets $\{\tilde{T}_{ij}\}_{i=0,\dots,d}$ form a regular partition of $\tilde{\omega}_j(p)$ by Lemma 4.3 (q_j, a_1, \dots, a_d, p in the notation of this proof correspond to a_0, \dots, a_d, p in the notation of the lemma). \square

Corollary 4.8 Let $\tilde{\omega}_j(p)$ be as in Lemma 4.7, then

$$\omega(p) = \bigcup_{j=1}^{n(p)} \tilde{\omega}_j(p).$$

Proof. Using $\overline{\tilde{T}_j} \subset \tilde{\omega}_j(p) \subset \omega(p)$ for all $j = 1, \dots, n(p)$ we have

$$\omega(p) = \bigcup_{j=1}^{n(p)} \overline{\tilde{T}_j} \subset \bigcup_{j=1}^{n(p)} \tilde{\omega}_j(p) \subset \omega(p).$$

\square

Corollary 4.9 In the notation of Lemma 4.7, for $p \in \mathcal{V} \cap \text{int } \Omega$ and $j = 1, \dots, n(p)$, let $\tilde{\theta}_{p,j}^{PL} \in C^0(\Omega)$ be the function defined by $\tilde{\theta}_{p,j}^{PL}(p) = 1$ and $\tilde{\theta}_{p,j}^{PL}(q) = 0$ for all other vertices q of $\tilde{\omega}_j(p)$, such that $\tilde{\theta}_{p,j}^{PL}|_{\tilde{T}_{ij}} \in \mathbb{P}_1$ for all $i = 0, \dots, d$, and $\tilde{\theta}_{p,j}^{PL}|_{\Omega \setminus \tilde{\omega}_j(p)} = 0$.

For all $p \in \mathcal{V} \cap \text{int } \Omega$ and $j = 1, \dots, n(p)$, these functions can be written as

$$\tilde{\theta}_{p,j}^{PL}(x) = \max \left\{ 0, \min_{i=0, \dots, d} \tilde{A}_p^{(i,j)} x + \tilde{b}_p^{(i,j)} \right\}, \quad x \in \Omega,$$

where each $x \mapsto \tilde{A}_p^{(i,j)} x + \tilde{b}_p^{(i,j)}$ is a globally linear function fulfilling $(\tilde{A}_p^{(i,j)} x + \tilde{b}_p^{(i,j)})|_{\tilde{T}_{ij}} = \tilde{\theta}_{p,j}^{PL}|_{\tilde{T}_{ij}}$.

Proof. Since $\tilde{\omega}_j(p)$ is a convex patch, the statement follows by Prop. 4.1 (which corresponds to [18, Theorem 3.1]). The function $x \mapsto \tilde{A}_p^{(i,j)} x + \tilde{b}_p^{(i,j)}$ in our notation corresponds to g_k in the notation of [18], and $\tilde{\theta}_{p,j}^{PL}$ corresponds to ϕ_i . \square

Lemma 4.10 For all $p \in \mathcal{V}$, $j, k = 1, \dots, n(p)$ and $i = 0, \dots, d$, let $x \mapsto \tilde{A}_p^{(i,j)} x + \tilde{b}_p^{(i,j)}$ be as defined in Corollary 4.9 and let $x \mapsto A_p^{(k)} x + b_p^{(k)}$ be the function defined by $(A_p^{(k)} x + b_p^{(k)})|_{T_k} = \theta_p^{PL}|_{T_k}$. Then,

$$0 \leq \tilde{A}_p^{(i,j)} x + \tilde{b}_p^{(i,j)} \leq A_p^{(k)} x + b_p^{(k)}, \quad \forall x \in T_k \cap \tilde{T}_{ij},$$

for all $j, k = 1, \dots, n(p)$ and $i = 0, \dots, d$.

Proof. First consider $p \in \mathcal{V} \cap \text{int } \Omega$, such that $p \in \text{int } \omega(p)$. For all $j, k \in \{1, \dots, n(p)\}$ and $i \in \{0, \dots, d\}$, we first note that $\tilde{A}_p^{(i,j)} p + \tilde{b}_p^{(i,j)} = A_p^{(k)} p + b_p^{(k)} = 1$ as well as $\tilde{A}_p^{(i,j)} y + \tilde{b}_p^{(i,j)} = 0$ for all y on the face of \tilde{T}_{ij} opposite to p . Similarly, $A_p^{(k)} y + b_p^{(k)} = 0$ for all y on the face of T_k opposite to p . Next, let $x \in T_k \cap \tilde{T}_{ij}$ in case this set is nonempty. Let L be the halfline starting in p through x . Note that $p \in \text{int } \tilde{\omega}_j(p) \subset \text{int } \omega(p)$ is a star point of both $\tilde{\omega}_j(p)$ and $\omega(p)$. It follows from $\tilde{\omega}_j(p) \subset \omega(p)$ that the intersection point $y_1 \in L \cap \partial \tilde{\omega}_j(p)$ is closer to p than (or equal to) the intersection point $y_2 \in L \cap \partial \omega(p)$. Because $y \mapsto \tilde{A}_p^{(i,j)} y + \tilde{b}_p^{(i,j)}$ linearly interpolates between the value 1 in p and 0 in y_1 , and $y \mapsto A_p^{(k)} y + b_p^{(k)}$ linearly interpolates between 1 in p and 0 in y_2 , it follows that $\tilde{A}_p^{(i,j)} y + \tilde{b}_p^{(i,j)} \leq A_p^{(k)} y + b_p^{(k)}$ for all points y between p and y_1 , which includes x . Finally, the first inequality in the lemma follows from Corollary 4.9.

For $p \in \mathcal{V} \cap \partial \Omega$, we can apply the argument above after extending \mathcal{T} to a regular, simplicial partition of all of \mathbb{R}^d , of which only the elements touching p are relevant. \square

Theorem 4.11 For all $p \in \mathcal{V}$, let $T_1, \dots, T_{n(p)} \in \mathcal{T}$, $n(p) \in \mathbb{N}$ be the simplices adjacent to p . Then, for all $p \in \mathcal{V}$ and all $x \in \omega(p)$

$$\theta_p^{PL}(x) = \max_{j=1, \dots, n(p)} \tilde{\theta}_{p,j}^{PL}(x) = \max_{j=1, \dots, n(p)} \max \left\{ 0, \min_{i \in \{0, \dots, d\}} \tilde{A}_p^{(i,j)} x + \tilde{b}_p^{(i,j)} \right\}, \quad (4.6)$$

where each $x \mapsto \tilde{A}_p^{(i,j)} x + \tilde{b}_p^{(i,j)}$ is a globally linear function fulfilling $(\tilde{A}_p^{(i,j)} x + \tilde{b}_p^{(i,j)})|_{\tilde{T}_{ij}} = \tilde{\theta}_{p,j}^{PL}|_{\tilde{T}_{ij}}$ for \tilde{T}_{ij} defined in Lemma 4.7 and $\tilde{\theta}_{p,j}^{PL}$ defined in Corollary 4.9.

Proof. For all $j = 1, \dots, n(p)$, applying Lemma 4.10 for all $i = 0, \dots, d$ and all $k = 1, \dots, n(p)$ shows that $0 \leq \tilde{\theta}_{p,j}^{PL}(x) \leq \theta_p^{PL}(x)$ for all $x \in \tilde{\omega}_j(p)$. Together with $\tilde{\theta}_{p,j}^{PL}(x) = 0$ for all $x \in \Omega \setminus \tilde{\omega}_j(p)$, this shows that $0 \leq \tilde{\theta}_{p,j}^{PL}(x) \leq \theta_p^{PL}(x)$ for all $x \in \Omega$. To finish the proof, recall that for all $j = 1, \dots, n(p)$ and $x \in T_j$

$$\theta_p^{PL}(x) = A_p^{(j)} x + b_p^{(j)} = \tilde{A}_p^{(0,j)} x + \tilde{b}_p^{(0,j)} = \tilde{\theta}_{p,j}^{PL}(x).$$

The first and the last equality hold by definition, and the second holds because both functions are linear and equal the value 1 in p and 0 in the other vertices of T_j . \square

Theorem 4.12 For all $p \in \mathcal{V}$ let $T_1, \dots, T_{n(p)} \in \mathcal{T}$, $n(p) \in \mathbb{N}$ be the simplices adjacent to p . For $\tilde{\theta}_{p,j}^{PL}$, $j = 1, \dots, n(p)$ defined in Corollary 4.9, let $\tilde{\Phi}_{p,j}^{CPL}$, $j = 1, \dots, n(p)$ be the NNs from Proposition 4.1 satisfying $R(\tilde{\Phi}_{p,j}^{CPL}) = \tilde{\theta}_{p,j}^{PL}$ on Ω .

Then

$$\Phi_p^{CPL} := \Phi_{n(p)}^{\max} \odot P(\tilde{\Phi}_{p,1}^{CPL}, \dots, \tilde{\Phi}_{p,n(p)}^{CPL}) \quad (4.7)$$

satisfies $R(\Phi_p^{CPL})(x) = \theta_p^{PL}(x)$ for all $x \in \Omega$ and

$$L(\Phi_p^{CPL}) \leq 7 + \log_2(n(p)) + \log_2(d+1), \quad M(\Phi_p^{CPL}) \leq Cd^2n(p).$$

Proof. Because $\tilde{\omega}_j(p) = \cup_{i=0}^d \tilde{T}_{ij}$ is a regular partition of the convex set $\tilde{\omega}_j(p)$ by Lemma 4.7, we can apply Proposition 4.1 and it follows that for all $j = 1, \dots, n(p)$

$$L(\tilde{\Phi}_{p,j}^{CPL}) \leq 5 + \log_2(d+1), \quad M(\tilde{\Phi}_{p,j}^{CPL}) \leq Cd(d+1) \leq Cd^2$$

The fact that $R(\Phi_p^{CPL})(x) = \theta_p^{PL}(x)$ for all $x \in \Omega$ follows from Theorem 4.11, and the network depth and size are bounded as follows:

$$\begin{aligned} L(\Phi_p^{CPL}) &= L(\Phi_{n(p)}^{\max}) + L(\tilde{\Phi}_{p,1}^{CPL}) \leq 2 + \log_2(n(p)) + 5 + \log_2(d+1), \\ M(\Phi_p^{CPL}) &\leq 2M(\Phi_{n(p)}^{\max}) + 2 \sum_{j=1}^{n(p)} M(\tilde{\Phi}_{p,j}^{CPL}) \leq Cn(p) + n(p)Cd^2 \leq Cd^2n(p). \end{aligned}$$

□

5 Approximation results

Since we defined explicit constructions of shape functions for all finite elements in the discrete De Rham complex of the lowest polynomial order (1.2), we now lift known approximation results for finite elements to obtain constructive NN approximations of arbitrary functions in the Sobolev spaces belonging to the De Rham complex (1.1).

We apply the previous results to shape-regular families of meshes $\{\mathcal{T}_h\}_{h>0}$ in dimension $d = 2, 3$. For $V = H^1(\Omega)$, $H^0(\text{curl}, \Omega)$ for $d = 3$, $H^0(\text{div}, \Omega)$ or $L^2(\Omega)$, define the template for the respective smoothness spaces $V^\bullet \subset V$ as follows

$$\begin{aligned} V &= H^1(\Omega) \longleftrightarrow V^\bullet = H^2(\Omega), \\ \text{for } d = 3: \quad V &= H^0(\text{curl}, \Omega) \longleftrightarrow V^\bullet = H^1(\text{curl}, \Omega) := \{v \in [H^1(\Omega)]^d : \text{curl } v \in [H^1(\Omega)]^d\}, \\ V &= H^0(\text{div}, \Omega) \longleftrightarrow V^\bullet = H^1(\text{div}, \Omega) := \{v \in [H^1(\Omega)]^d : \text{div } v \in H^1(\Omega)\}, \\ V &= L^2(\Omega) \longleftrightarrow V^\bullet = H^1(\Omega). \end{aligned} \quad (5.1)$$

Then we get the following result.

Theorem 5.1 Given a bounded, simply connected polytopal Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, assume that $V \in \{H^1(\Omega), H^0(\text{curl}, \Omega), H^0(\text{div}, \Omega), L^2(\Omega)\}$, that V^\bullet is as in (5.1) and that $d = 3$ if $V = H^0(\text{curl}, \Omega)$. Then there exists a constant $C > 0$ such that, for all $h > 0$, a NN Φ_h can be constructed satisfying

$$\|v - R(\Phi_h)\|_V \leq Ch\|v\|_{V^\bullet} \quad \forall v \in V^\bullet, \quad (5.2)$$

and

$$L(\Phi_h) \leq 6, \quad M(\Phi_h) \leq Ch^{-d}.$$

Proof. Let $\{\mathcal{T}_h\}_{h>0}$ be a family of quasi-uniform meshes on Ω with mesh-width $h > 0$ and shape regularity constant $C_{\text{sh}} > 0$ independent of h . Define $V_h \in \{S_1(\mathcal{T}_h, \Omega), N_0(\mathcal{T}_h, \Omega), \text{RT}_0(\mathcal{T}_h, \Omega), S_0(\mathcal{T}_h, \Omega)\}$ corresponding to (in this order) $V \in \{H^1(\Omega), H^0(\text{curl}, \Omega), H^0(\text{div}, \Omega), L^2(\Omega)\}$. Then

$$\forall v_h \in V_h : \quad v_h(x) = \sum_{i=1}^{\dim(V_h)} \underline{v}_i \theta_i(x), \quad (5.3)$$

where $\theta_i, i = 1, \dots, \dim(V_h)$ are the shape functions for V_h and $\underline{v} \in \mathbb{R}^{\dim(V_h)}$. Therefore, due to Equation (3.5) and Propositions 3.2, 3.7, 3.8, for all $v_h \in V_h$, we get an explicit construction of a NN Φ_h such that $v_h(x) = \text{R}(\Phi_h)(x)$ for a.e. $x \in \Omega$. In particular,

$$\|v - \text{R}(\Phi_h)\|_V = \|v - v_h\|_V.$$

For $v \in V^\bullet$, we can apply the approximation results e.g. [16, Theorem 11.13] for $V = H^1(\Omega)$, [1, Equations (5.7) and (5.8)] for $V = H^0(\text{curl}, \Omega)$ in case $d = 3$, [16, Theorem 16.4] for $V = H^0(\text{div}, \Omega)$ and Poincaré's inequality for $V = L^2(\Omega)$. More precisely, there exist interpolation operators $\mathcal{I}_h: V^\bullet \rightarrow V_h$ such that for a constant C only dependent on d, C_{sh}

$$\inf_{v_h \in V_h} \|v - v_h\|_V \leq \|v - \mathcal{I}_h v\|_V \leq Ch \|v\|_{V^\bullet}. \quad (5.4)$$

The upper bound on $L(\Phi_h)$ follows from the corresponding bounds in (3.5) and Propositions 3.2, 3.7, 3.8, adding one extra layer to evaluate the linear combination (5.3). In addition, the size $M(\Phi_h)$ depends on d, C_{sh} and, to evaluate (5.3), grows linearly with respect to $\dim(V_h) \sim h^{-d}$ as $h \downarrow 0$. \square

Remark 5.2 *The choice of interpolation operators $\mathcal{I}_h: V^\bullet \rightarrow V_h$ in Theorem 5.1 is made to have the approximation property (5.4). However, other interpolation or quasi-interpolation operators in V_h can be equally emulated with NNs. In [15, Corollary 5.3], the authors give a particular definition of quasi-interpolation for $V_h \in \{S_1(\mathcal{T}_h, \Omega), N_0(\mathcal{T}_h, \Omega), \text{RT}_0(\mathcal{T}_h, \Omega)\}$, requiring minimal regularity of the function v , that yields*

$$\|v - \text{R}(\Phi_h)\|_{L^p(\Omega)} \leq Ch^r |v|_{W^{r,p}(\Omega)} \quad \forall v \in [W^{r,p}(\Omega)]^{d_L}, \quad (5.5)$$

for any $p \in [1, \infty]$, $r \in \{0, 1\}$ or any $p \in [1, \infty], r \in (0, 1)$, where $d_L = d$ if $V_h = \text{RT}_0(\mathcal{T}_h, \Omega)$ or $V_h = N_0(\mathcal{T}_h, \Omega)$ and $d_L = 1$ otherwise.

6 Neural emulation of trace spaces

In the previous sections, we have developed ReLU NN emulations of the lowest order, De Rham compatible Finite Elements on cellular complexes in the bounded Lipschitz polyhedral domains $\Omega \subset \mathbb{R}^3$. In certain applications, however, corresponding boundary complexes are required; we mention only variational boundary integral equations which arise in computational electromagnetism (e.g. [7, 6] and the references there). We approximate traces on the boundary $\Gamma = \partial\Omega$, which is a finite union of plane sides, with the network constructions developed in Sections 4.1, 3.2 and 3.1 for $d = 2$. As has been emphasized e.g. in [6] trace spaces of the spaces occurring in the De Rham complex satisfy exact sequence properties derived from the compatibility of the corresponding sequences in Ω .

We recall the trace operators (e.g. from [6, Definition 2.1]):

$$\gamma_0 : H^1(\Omega) \rightarrow H^{1/2}(\Gamma) : \quad \gamma_0(u)(x_0) = \lim_{x \rightarrow x_0} u(x), \quad (6.1a)$$

$$\check{\gamma}_0 : H^0(\text{curl}, \Omega) \rightarrow H^{-1/2}(\text{curl}_\Gamma, \Gamma) : \quad \check{\gamma}_0(u)(x_0) = \lim_{x \rightarrow x_0} u(x) - (u(x) \cdot n_{x_0})n_{x_0}, \quad (6.1b)$$

$$\gamma_t : H^0(\text{curl}, \Omega) \rightarrow H_\times^{-1/2}(\text{div}_\Gamma, \Gamma) : \quad \gamma_t(u)(x_0) = \lim_{x \rightarrow x_0} u(x) \times n_{x_0}, \quad (6.1c)$$

$$\gamma_n : H^0(\text{div}, \Omega) \rightarrow H^{-1/2}(\Gamma) : \quad \gamma_n(u)(x_0) = \lim_{x \rightarrow x_0} u(x) \cdot n_{x_0}, \quad (6.1d)$$

for almost all $x_0 \in \Gamma$, where we use x to denote points in Ω , and where n_{x_0} denotes the outward unit normal to Γ in x_0 . These trace operators render the diagram in Figure 6.1 commutative (e.g. [6]).

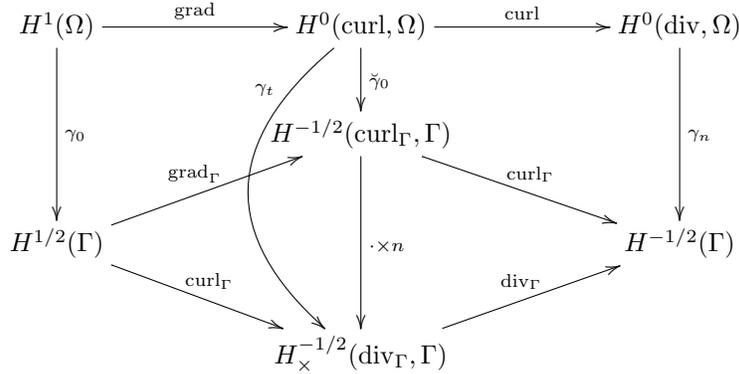


Figure 6.1: Boundary complex

Given a regular simplicial partition \mathcal{T} of Ω , for each face f of Ω , the set $\mathcal{T}_f = \{\text{int}(f \cap \bar{T}) : T \in \mathcal{T}\}$ is a regular, simplicial triangulation of f (where the interior $\text{int}(\dots)$ is defined with respect to the subspace topology on the face f). Discretizations of the trace spaces can be defined as the traces in the sense of (6.1) of the finite element spaces on Ω (see [17, Section 1.6]). The corresponding diagram for the lowest order conforming FEM spaces also commutes (Figure 6.2).

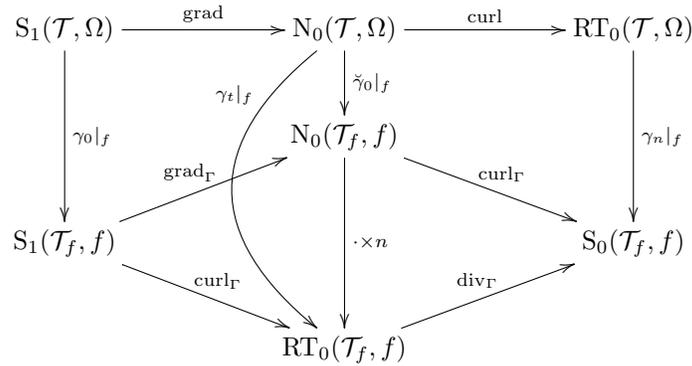


Figure 6.2: Discrete boundary complex

Upon parametrizing the faces of Ω by a polygon in \mathbb{R}^2 , we can construct NN approximations of the traces on f . We parametrize each face f by an affine bijection $F_f : D_f \rightarrow f$ for some

polygon $D_f \subset \mathbb{R}^2$, which can be partitioned by $\mathcal{T}_{D_f} := \{F_f^{-1}(T) : T \in \mathcal{T}_f\}$. Functions in $S_1(\mathcal{T}_f, f)$, $\text{RT}_0(\mathcal{T}_f, f)$ and $S_0(\mathcal{T}_f, f)$ can be pulled back to D_f . In particular,

$$\{u \circ F_f : u \in S_1(\mathcal{T}_f, f)\} = S_1(\mathcal{T}_{D_f}, D_f), \quad \{u \circ F_f : u \in S_0(\mathcal{T}_f, f)\} = S_0(\mathcal{T}_{D_f}, D_f).$$

NN emulations of these spaces have already been provided in Sections 4.1 and 3.1. The spaces $\text{RT}_0(\mathcal{T}_f, f)$ and $\text{RT}_0(\mathcal{T}_{D_f}, D_f)$ are related by the Piola transform. For J denoting the Jacobian of F_f ,

$$\{\det(J)J^{-1}(u \circ F_f) : u \in \text{RT}_0(\mathcal{T}_f, f)\} = \text{RT}_0(\mathcal{T}_{D_f}, D_f).$$

Thus, for $u \in \text{RT}_0(\mathcal{T}_f, f)$, a network that emulates $u \circ F_f : D_f \rightarrow \mathbb{R}^3$ is given by $\det(J^{-1})J\Phi$, for a NN Φ from Section 3.2 emulating $\det(J)J^{-1}(u \circ F_f) \in \text{RT}_0(\mathcal{T}_{D_f}, D_f)$. Here, ReLU activations imply that the affine transformation $\det(J^{-1})J$ can be emulated exactly either by applying this transformation to the weights and biases of the output layer of Φ , or by concatenating Φ with a ReLU NN of depth one. In both cases, the network size is increased by at most Cd^2 (with $C > 0$ independent of d and \mathcal{T}), and the network depth is increased by 0 respectively 1.

The shape functions of $N_0(\mathcal{T}_f, f)$ equal those of $\text{RT}_0(\mathcal{T}_f, f)$ up to a rotation. As explained in Section 3.3, we can use results from Section 3.2 for the NN emulation of the $N_0(\mathcal{T}_{D_f}, D_f)$ shape functions. Therefore, for $u \in N_0(\mathcal{T}_f, f)$, a network that emulates $u \circ F_f : D_f \rightarrow \mathbb{R}^3$ is given by $\det(J^{-1})J\mathcal{R}(\Phi)$, for a NN Φ from Section 3.2 emulating $\det(J)J^{-1}(u \circ F_f) \in N_0(\mathcal{T}_{D_f}, D_f)$.

The results of this section can be summarized as follows:

Proposition 6.1 *Assume given a bounded polytopal domain $\Omega \subset \mathbb{R}^3$ with Lipschitz boundary $\Gamma = \partial\Omega$. For a regular, simplicial partition \mathcal{T} on Ω , and for a side $f \subset \Gamma$ of Ω , consider the regular, simplicial partition $\mathcal{T}_f = \{\text{int}(f \cap \bar{T}) : T \in \mathcal{T}\}$ of f . Let $F_f : D_f \rightarrow f$ be a bijective affine parametrization of f for some polygonal parameter domain $D_f \subset \mathbb{R}^2$ partitioned by $\mathcal{T}_{D_f} := \{F_f^{-1}(T) : T \in \mathcal{T}_f\}$. In the following, C only depends on the shape regularity constant of the mesh \mathcal{T}_f . Then:*

- (i) *For all $T \in \mathcal{T}_f$, there exists a DNN Φ of depth 3 and size at most 14, with only σ as activation function, such that $\mathcal{R}(\Phi) = \theta_T^S \circ F_f$ a.e. in D_f .*
- (ii) *For all edges $e \subset \bar{f}$, there exist DNNs Φ, Φ' of depth 5 and size at most C , with ρ and σ as activation function, such that $\mathcal{R}(\Phi) = \theta_e^{RT} \circ F_f$ a.e. in D_f and $\mathcal{R}(\Phi') = \theta_e^{NE} \circ F_f$ a.e. in D_f . If $e \subset f$, there also exist networks Φ, Φ' of depth 6 which in addition satisfy that the normal respectively tangential component is continuous across e .*
- (iii) *For all nodes $p \in \bar{f}$, there exists a DNN Φ of depth C and size at most C , with ρ as activation function, such that $\mathcal{R}(\Phi) = \theta_p^{PL} \circ F_f$ everywhere in D_f .*

7 Extensions and conclusions

We conclude this paper by indicating some extensions of the main results, as well as further possible directions of research.

7.1 Higher order polynomial spaces

For $p \in \mathbb{N}$ and $d \geq 2$ denote in the following by $\mathbb{P}_p(\mathbb{R}^d) := \text{span}\{\prod_{j=1}^d x_j^{\nu_j} : \sum_{j=1}^d \nu_j \leq p\}$ the space of multivariate polynomials of degree at most p . As has been observed in [19], networks employing the ‘‘ReLU’’² activation

$$\rho_r(x) := \rho(x)^r = \max\{0, x\}^r$$

²Also referred to as ‘‘rectified power unit’’ (RePU).

for some fixed integer $r \geq 2$, can be used to express multivariate polynomials in $\mathbb{P}_p(\mathbb{R}^d)$ exactly. We use here a formulation of this result from [21]³, extended to vector-valued polynomials by parallelization:

Proposition 7.1 ([21, Proposition 2.14]) *Fix $d, k \in \mathbb{N}$, $r \in \mathbb{N}$, $r \geq 2$ and a polynomial degree $p \in \mathbb{N}$.*

Then there exists a constant $C > 0$ independent of d, k and p but depending on r such that for any multivariate polynomial $f \in [\mathbb{P}_p(\mathbb{R}^d)]^k$ there is a NN Φ_f , employing ReLU^r activation, such that $\mathbf{R}(\Phi_f)(x) = f(x)$, for all $x \in \mathbb{R}^d$ and such that $M(\Phi_f) \leq Ck(p+1)^d$ and $L(\Phi_f) \leq Cd \log_2(p)$.

Combining Proposition 7.1 with Proposition 2.8 and Lemma 2.9, by a similar argument as in Lemma 3.1 we obtain a generalization of this result to piecewise polynomial functions on regular, simplicial partitions for all interelement-conformities which arise from compatibility with the complex (1.1).

Proposition 7.2 (Emulation of piecewise higher order polynomial elements) *Let $r \in \mathbb{N}$, $r \geq 2$. For $d, s, k, p \in \mathbb{N}$ let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz polytope and \mathcal{T} be a regular, simplicial partition of Ω with $s = \#(\mathcal{T})$ elements, $\mathcal{T} = \{T_i\}_{i=1, \dots, s}$. Let $u : \Omega \rightarrow \mathbb{R}^k$ be a function which for all $i = 1, \dots, s$ satisfies that $u|_{T_i} \in [\mathbb{P}_p(\mathbb{R}^d)]^k$.*

Then there exists a NN Φ_u^{PwP} employing ReLU , ReLU^r and BiSU activations and satisfies $u(x) = \mathbf{R}(\Phi_u^{PwP})(x)$ for a.e. $x \in \Omega$. Moreover,

$$L(\Phi_u^{PwP}) \leq Cd \log_2(p), \quad M(\Phi_u^{PwP}) \leq Csk(p+1)^d.$$

Here the constant C is independent of d, s, k and p but depends on r .

Our results thus straightforwardly extend to piecewise polynomial spaces of arbitrarily high order, covering all De Rham compatible element families on simplicial partitions on polytopes as described in [17]. Importantly, as in the case of low-order finite elements, the network size only scales linearly in the number $s = \#(\mathcal{T})$ of simplices of the triangulation \mathcal{T} . Similarly, also the results of Section 6 extend to higher order polynomials.

Remark 7.3 *ReLU NNs are known to be efficient at approximating multivariate polynomials, see e.g. [22, 28]. Thus, also ReLU+BiSU (rather than ReLU+ReLU^r+BiSU) networks could be employed to extend our results to higher order polynomial spaces, however only in an approximate sense.*

7.2 Crouzeix-Raviart elements CR_0

While this work focused on conformal discretization of functions in the compatible spaces in (1.1), the result of Lemma 3.1 is more general and includes the non-conformal Crouzeix-Raviart elements (e.g. [16, Section 7.5]) of lowest order for $d \geq 2$. Due to the importance and widespread use of the Crouzeix-Raviart elements (e.g. [13, 8, 5] and the references there), we state a NN emulation result of these elements. The lowest order Crouzeix-Raviart FE space is defined as

$$\text{CR}_0(\mathcal{T}, \Omega) := \{v \in L^1(\Omega) : v|_T \in \mathbb{P}_1 \ \forall T \in \mathcal{T} \text{ and } \int_f [v]_f = 0 \ \forall f \in \mathcal{F}\}. \quad (7.1)$$

Analogously to the case of Raviart-Thomas FE, the space $\text{CR}_0(\mathcal{T}, \Omega)$ has one degree of freedom per face $f \in \mathcal{F}$: the corresponding shape functions are, for $f \subset \partial\Omega$, $\theta_f^{\text{CR}}(x) := d(\frac{1}{d} - (1 -$

³We apply this result here with the multiindex set $\Lambda := \{(\nu_1, \dots, \nu_d) \in \mathbb{N}_0^d : \sum_{j=1}^d \nu_j \leq p\}$, which has cardinality bounded by $(p+1)^d$.

$\frac{|f|(x-a)\cdot n_f}{d|T|})\mathbb{1}_T$, where $f \subset \bar{T}$, $T \in \mathcal{T}$ and a is the only vertex of T that does not belong to \bar{f} . For interior faces $f \subset \Omega$ we construct θ_f^{CR} by assembling local shape functions of the neighboring simplices T_1, T_2 with $\bar{f} = \bar{T}_1 \cap \bar{T}_2$,

$$\theta_f^{CR}(x) := \begin{cases} d(\frac{1}{d} - (1 - \frac{|f|(x-a_1)\cdot n_f}{d|T_1|})) & \text{if } x \in T_1, \\ d(\frac{1}{d} - (1 + \frac{|f|(x-a_2)\cdot n_f}{d|T_2|})) & \text{if } x \in T_2, \\ 0 & \text{if } x \notin \bar{T}_1 \cap \bar{T}_2, \end{cases} \quad (7.2)$$

where a_1, a_2 are the the only vertices of T_1, T_2 , respectively, not belonging to \bar{f} .

Proposition 7.4 *Given $f \in \mathcal{F}$, $f \subset \partial\Omega$, let $T \in \mathcal{T}$ be the simplex adjacent to f and $a := (\mathcal{V} \cap \bar{T}) \setminus \bar{f} \in \mathbb{R}^d$.*

Then there exist $A_{f,T} \in \mathbb{R}^{1 \times d}$, $b_{f,T} \in \mathbb{R}$ such that

$$\Phi_f^{CR} := \Phi_{1,\kappa}^\times \odot \text{P}(\Phi_{1,2}^{\text{Id}} \odot ((A_{f,T}, b_{f,T}, \text{Id}_{\mathbb{R}})), \Phi_T^{\mathbb{1}}) \quad (7.3)$$

satisfies $\theta_f^{CR}(x) = \text{R}(\Phi_f^{CR})(x)$ for a.e. $x \in \Omega$, for any

$$\kappa \geq d - 1. \quad (7.4)$$

Given $f \in \mathcal{F}$, $f \subset \Omega$, let T_1, T_2 be the simplices adjacent to f and let $a_i := (\mathcal{V} \cap \bar{T}_i) \setminus \bar{f} \in \mathbb{R}^d$, $i = 1, 2$. Then, there exist $A_{f,T_i} \in \mathbb{R}^{1 \times d}$, $b_{f,T_i} \in \mathbb{R}$, $i = 1, 2$ such that

$$\Phi_f^{CR} := \sum_{i=1,2} \Phi_{1,\kappa}^\times \odot \text{P}(\Phi_{1,2}^{\text{Id}} \odot ((A_{f,T_i}, b_{f,T_i}, \text{Id}_{\mathbb{R}})), \Phi_{T_i}^{\mathbb{1}}) \quad (7.5)$$

satisfies $\theta_f^{CR}(x) = \text{R}(\Phi_f^{CR})(x)$ for a.e. $x \in \Omega$, for any κ as in (7.4). In addition, there exists an absolute constant $C > 0$ such that for all $f \in \mathcal{F}$

$$L(\Phi_f^{CR}) = 5, \quad M(\Phi_f^{CR}) \leq Cd^2.$$

Proof. The values of A_{f,T_i}, b_{f,T_i} can be read from (7.2) and also $A_{f,T}, b_{f,T}$ can be read from the definition of θ_f^{CR} . Similar to Proposition 3.2, $\theta_f^{CR}(x) = \text{R}(\Phi_f^{CR})(x)$ for all $x \in \Omega \setminus \partial\mathcal{T}$, where $\partial\mathcal{T} := \bigcup_{T \in \mathcal{T}} \partial T$.

We conclude applying Lemma 3.1 with $k = 1$ and $m = d + 1$, and with $s = 1$ in (7.3) and $s = 2$ in (7.5). \square

The same idea carries over to higher order Crouzeix-Raviart elements and canonical hybrid elements [16, Section 7.6], along the lines of Section 7.1.

7.3 Conclusions

The present construction of deep NN emulations of De Rham compatible Finite Element spaces was given for the lowest order Finite Element families on regular, simplicial partitions \mathcal{T} of Ω . Generalizing recent work [18], we provided exact emulation of continuous piecewise linear functions (“Courant” Finite Elements) on arbitrary, regular simplicial partitions in any space dimension by ReLU networks. As shown, the network size in this construction merely scales linearly with the number of elements.

As is well known (e.g. [17] and the reference there) the presently emulated, lowest order element families are embedded in hierarchies of higher-order Finite Element families for arbitrary polynomial order. We argued that admitting higher order, so-called ReLU^r activations with $r \in \mathbb{N}$, $r \geq 2$ allows to exactly emulate the higher order element families from [17] along the lines of the present constructions.

Compatible constructions similar to the ones developed here are also possible on *affine partitions* \mathcal{T} (comprising elements that are affine images of reference elements) which contain other element shapes, in particular quadrilaterals ($d = 2$) and hexahedral elements ($d = 3$). We refer to [17, Sec. 4 and 6] for details on the shape functions.

The present results, in particular Proposition 6.1, can be the basis to extend the recently proposed frameworks of “PiNN” [24] and “DeepRitz” [14] for DNN discretization of PDEs to larger classes of PDEs, and to corresponding boundary integral formulations (see, e.g., [25] for such methods, and [4] for a realization of this approach for a model problem). While in this paper we mainly concentrated on the De Rham formalism, our ideas and proofs naturally extend also to compatible discretizations of more general structures, as occur in the so-called Finite Element Exterior Calculus (FEEC) (e.g. [2] and the references there). Development of details is beyond the scope of the present work.

Similarly, with Proposition 7.2 other nonconforming FEM such as Hybridized, High Order (“HHO”) FEM can be emulated with appropriate functionals which account for element interface unknowns and reduced interelement conformity, see, e.g. [9, Prop. 1.8].

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References

- [1] A. Alonso and A. Valli. An optimal domain decomposition preconditioner for low-frequency time-harmonic Maxwell equations. *Math. Comp.*, 68(226):607–631, 1999.
- [2] D. N. Arnold, R. S. Falk, and R. Winther. Differential complexes and stability of finite element methods. II. The elasticity complex. In *Compatible spatial discretizations*, volume 142 of *IMA Vol. Math. Appl.*, pages 47–67. Springer, New York, 2006.
- [3] R. Arora, A. Basu, P. Mianjy, and A. Mukherjee. Understanding deep neural networks with rectified linear units. In *International Conference on Learning Representations*, 2018. arXiv: 1611.01491.
- [4] R. Aylwin, F. Henriquez, and C. Schwab. ReLU neural network Galerkin BEM. Technical Report 2022-01, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2022.
- [5] A. K. Balci, C. Ortner, and J. Storn. Crouzeix-Raviart finite element method for non-autonomous variational problems with Lavrentiev gap, 2021. arXiv 2106.06837.
- [6] A. Buffa, J. Dölz, S. Kurz, S. Schöps, R. Vázquez, and F. Wolf. Multipatch approximation of the de Rham sequence and its traces in isogeometric analysis. *Numerische Mathematik*, 144(1):201–236, 2020.
- [7] A. Buffa, R. Hiptmair, T. von Petersdorff, and C. Schwab. Boundary element methods for Maxwell transmission problems in Lipschitz domains. *Numer. Math.*, 95(3):459–485, 2003.
- [8] A. Chambolle and T. Pock. Crouzeix-Raviart approximation of the total variation on simplicial meshes. *J. Math. Imaging Vision*, 62(6-7):872–899, 2020.
- [9] M. Cicuttin, A. Ern, and N. Pignet. *Hybrid High-Order Methods : A Primer with Applications to Solid Mechanics*. SpringerBriefs in Mathematics Ser. Springer International Publishing AG, Cham, 2021.
- [10] M. Costabel. A coercive bilinear form for Maxwell’s equations. *J. Math. Anal. Appl.*, 157(2):527–541, 1991.
- [11] M. Costabel and M. Dauge. Maxwell and Lamé eigenvalues on polyhedra. *Math. Methods Appl. Sci.*, 22(3):243–258, 1999.

- [12] M. Costabel, M. Dauge, and S. Nicaise. Singularities of Maxwell interface problems. *M2AN Math. Model. Numer. Anal.*, 33(3):627–649, 1999.
- [13] M. Crouzeix and R. S. Falk. Nonconforming finite elements for the Stokes problem. *Math. Comp.*, 52(186):437–456, 1989.
- [14] W. E and B. Yu. The deep Ritz method: a deep learning-based numerical algorithm for solving variational problems. *Commun. Math. Stat.*, 6(1):1–12, 2018.
- [15] A. Ern and J.-L. Guermond. Finite element quasi-interpolation and best approximation. *ESAIM Math. Model. Numer. Anal.*, 51(4):1367–1385, 2017.
- [16] A. Ern and J.-L. Guermond. *Finite elements I—Approximation and interpolation*, volume 72 of *Texts in Applied Mathematics*. Springer, Cham, [2021] ©2021.
- [17] F. Fuentes, B. Keith, L. Demkowicz, and S. Nagaraj. Orientation embedded high order shape functions for the exact sequence elements of all shapes. *Computers & Mathematics with Applications*, 70(4):353–458, 2015.
- [18] J. He, L. Li, J. Xu, and C. Zheng. ReLU deep neural networks and linear finite elements. *J. Comp. Math.*, 38, 2020.
- [19] B. Li, S. Tang, and H. Yu. Powernet: Efficient representations of polynomials and smooth functions by deep neural networks with rectified power units. *Journal of Mathematical Study*, 53(2):159–191, 2020.
- [20] H. N. Mhaskar and T. Poggio. Deep vs. shallow networks: an approximation theory perspective. *Anal. Appl. (Singap.)*, 14(6):829–848, 2016.
- [21] J. A. A. Opschoor, Christoph Schwab, and J. Zech. Exponential ReLU DNN expression of holomorphic maps in high dimension. *Constructive Approximation*, 2021.
- [22] J. A. A. Opschoor, P. C. Petersen, and C. Schwab. Deep ReLU networks and high-order finite element methods. *Analysis and Applications*, 18(05):715–770, 2020.
- [23] P. Petersen and F. Voigtlaender. Optimal approximation of piecewise smooth functions using deep ReLU neural networks. *Neural Netw.*, 108:296 – 330, 2018.
- [24] M. Raissi, P. Perdikaris, and G. E. Karniadakis. Physics-informed neural networks: a deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *J. Comput. Phys.*, 378:686–707, 2019.
- [25] S. A. Sauter and C. Schwab. *Boundary element methods*, volume 39 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, 2011. Translated and expanded from the 2004 German original.
- [26] C. Schwab and J. Zech. Deep learning in high dimension: Neural network expression rates for generalized polynomial chaos expansions in UQ. *Analysis and Applications, Singapore*, 17(1):19–55, 2019.
- [27] L. Yang, X. Meng, and G. E. Karniadakis. B-PINNs: Bayesian physics-informed neural networks for forward and inverse PDE problems with noisy data. *Journal of Computational Physics*, 425:109913, Jan 2021.
- [28] D. Yarotsky. Error bounds for approximations with deep ReLU networks. *Neural Netw.*, 94:103–114, 2017.
- [29] D. Yarotsky. Universal approximations of invariant maps by neural networks. *Constructive Approximation*, 2021.