Neural and operator network approximations for elliptic PDEs

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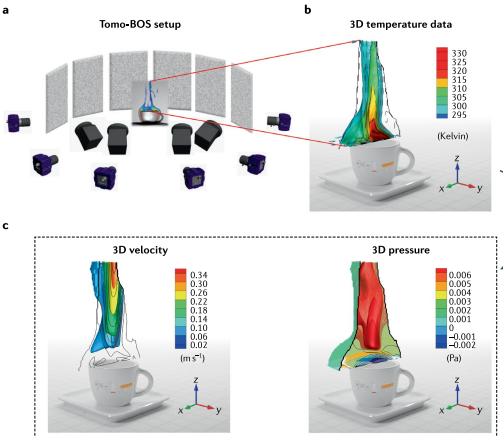
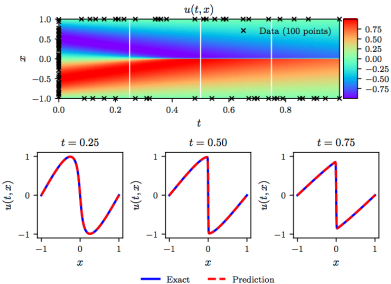
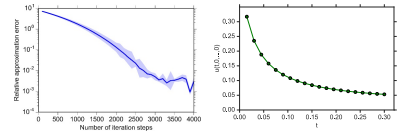
Neural Networks and PDEs



Flow reconstruction [Karniadakis et al., Nature (2021)]



Burgers [Raissi et al., JCP (2019)]



100-dim. Allen-Cahn [Han et al., PNAS (2018)]

Neural networks

Fully connected NN with $L \in \mathbb{N}$ layers and input dim. d

Sequence of matrix-vector couples

$$\Phi = ((A_1, b_1), \dots, (A_L, b_L))$$

with weights $A_\ell \in \mathbb{R}^{n_{\ell-1} \times n_\ell}$ and biases $b_\ell \in \mathbb{R}^{n_\ell}$, for $\ell = 1, \dots, L$ ($n_0 = d$).

Degrees of freedom:

$$\mathrm{depth}(\Phi) := L \qquad \mathrm{size}(\Phi) := \sum_{\ell=1}^{L} (\|A_\ell\|_0 + \|b_\ell\|_0)$$

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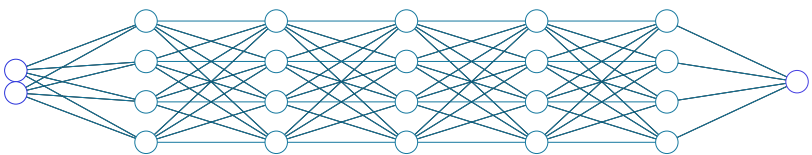

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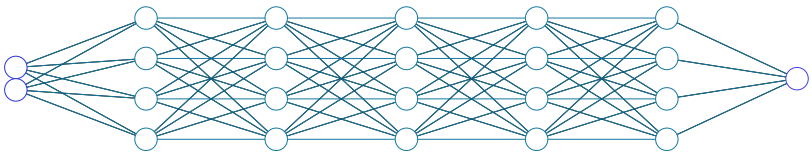

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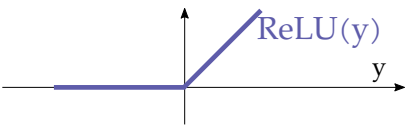
Neural networks

Realization with ReLU activation

$$\mathbb{R}^d \ni x \mapsto \mathrm{R}(\Phi)(x) = (A_L \cdot + b_L) \circ \rho \circ (A_{L-1} \cdot + b_{L-1}) \circ \cdots \circ \rho \circ (A_1 x + b)$$

with $\rho(y) = \mathrm{ReLU}(y) = \max(y, 0)$ (componentwise)



Some observations

- A ReLU NN is a piecewise linear function
- Every piecewise linear function can be represented as a ReLU NN [Arora et al., ICLR (2018)]
- Automatic differentiation: cheap to compute (exact) derivatives

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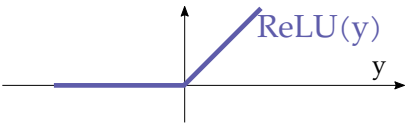

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Operator networks

- Mapping between infinite dimensional spaces $\mathcal{X}$ and $\mathcal{Y}$

$$\mathcal{X} \xrightarrow{\text{Encoding}} \mathbb{R}^n \xrightarrow{\text{Approximation}} \mathbb{R}^m \xrightarrow{\text{Reconstruction}} \mathcal{Y}$$

- Approximation and reconstruction involve NNs

Outline

Theoretical analysis of NNs and ONs for PDEs:

Approximation rates | Convergence of training algorithms

Approximation rates for

1. NN emulation of functions with isolated singularities
2. ON solution of smooth elliptic problems

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NN approximation rates

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Goal: Quantitative approximation rates

Given a class of functions $\mathcal{A}$ and a norm $\|\cdot\|_X$, for any $\varepsilon \in (0,1)$, find $L(\varepsilon), M(\varepsilon)$ such that

$$\sup_{u\in\mathcal{A}} \inf_{\Phi\in\mathcal{B}_{L(\varepsilon),M(\varepsilon)}} \|u - \mathrm{R}(\Phi)\|_X \leq \varepsilon$$

where

$$\mathcal{B}_{L,M} = \{\Phi \in NN : \mathbf{depth}(\Phi) \leq L,\ \mathbf{size}(\Phi) \leq M\}$$

- We look for uniform rates over $\mathcal{A}$
- Results for PDEs: we want the energy norm $\|\cdot\|_X$

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Some results in NN approximation theory

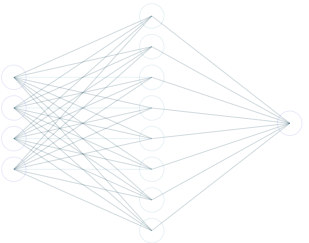
Universal approximation theorem
[Cybenko, Math. Control Signals Systems (1989), Hornik et al., Neural Netw. (1989)]

Let σ be any continuous sigmoidal function. Then, finite sums of the form

$$G(x) = \sum_{j=1}^{N} \alpha_j \sigma(y_j \cdot x + \theta_j), \qquad y_j, \theta_j \in \mathbb{R}^d,\ \alpha_j \in \mathbb{R}$$

are dense in $C((0,1)^d)$.

- Shallow network: $L = 2$
- $\mathcal{A} \subset C((0,1)^d)$
- $X = L^\infty((0,1)^d)$
- $M(\varepsilon) = ?$



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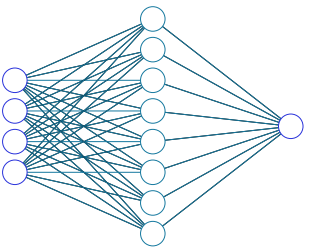

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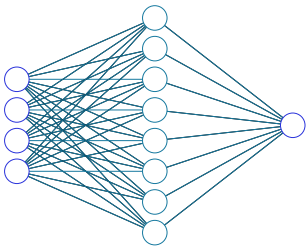

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Shallow networks

"Universal approximation bounds" [Barron, IEEE Trans. Inf. Theory (1993)]

Sigmoidal σ, $\mathcal{A}$ set of functions with finite integrals of Fourier transforms, any choice of measure $\|\cdot\|_X$ in bounded sets in $\mathbb{R}^d$. Then, $L = 2$ and

$$M(\varepsilon) = \mathcal{O}(\varepsilon^{-2}).$$

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- Dimension independent (except the hidden constant)
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Deep ReLU networks

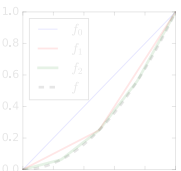
ReLU network approximation in Sobolev spaces [Yarotsky, Neural Netw. (2017)]

ReLU activation, $X = L^\infty((0,1)^d)$, $\mathcal{A} \subset W^{n,\infty}((0,1)^d)$. Then,

$$L(\varepsilon) = \mathcal{O}(|\log(\varepsilon)|), \qquad M(\varepsilon) = \mathcal{O}(\varepsilon^{-d/n}\,|\log(\varepsilon)|).$$

A crucial step:

The function $f(x) = x^2$ on the segment $[0,1]$ can be approximated with any error $\varepsilon > 0$ by a ReLU network having the depth and the number of weights and computation units $\mathcal{O}(|\log \varepsilon|)$.



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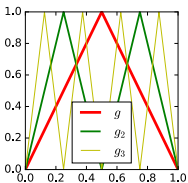

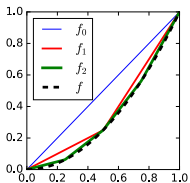

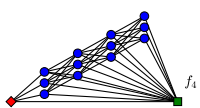

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- Going beyond $-d/n$ requires discontinuous weight assignment,
- Rates higher than $-d/2n$ are not achievable with ReLU networks,
- But for smaller $\mathcal{A}$:

Exponential convergence for analytic functions [E & Wang, Science China Math. (2018)]

ReLU activation, $X = L^\infty((0,1)^d)$, $\mathcal{A}$ subset of analytic functions in $[0,1]^d$. Then,

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Almost everything so far in L^∞ norm, but:

Approximation in Sobolev norms [Gühring et al., Anal. Appl. (2020)]

ReLU activation, $X = W^{s,p}((0,1)^d)$, $\mathcal{A} \subset W^{m,p}((0,1)^d)$. Then,

$$L(\varepsilon) = \mathcal{O}(\varepsilon^{-n/(n-s)}), \qquad M(\varepsilon) = \mathcal{O}(\varepsilon^{-d/(n-s)} \log(\varepsilon^{-n/(n-s)}))$$

When elliptic PDEs have smooth coefficients (or potentials)

- their solutions can have isolated singularities due to the domain
- low regularity in Sobolev spaces, but analytic outside the singular set

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NN approximation of functions with isolated singularities

Exponential convergence of NN approximation for some elliptic PDEs
[M & Opschoor & Petersen & Schwab, Found. Comp. Math (2022)]

ReLU activation, $X = H^1(\Omega)$ in polygonal or polyhedral Ω, $\mathcal{A}$ solutions to elliptic equation with smooth coefficients. Then,

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$\mathcal{A}$ contains weighted analytic functions with point and edge singularities, such as

- Solutions of elliptic PDEs with analytic coefficients and analytic rhs in
  - polygons
  - axiparallel polyhedra
- Eigenfunctions of elliptic eigenvalue problems with singular potentials
  - Linear & nonlinear Schrödinger
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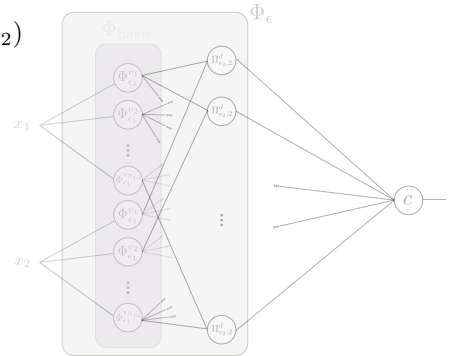
- NN concatenation: $\mathbf{R}(\Phi_1 \odot \Phi_2) = \mathbf{R}(\Phi_1) \circ \mathbf{R}(\Phi_2)$
- NNs can approximate
  - multiplication
  - one dim. piecewise polynomials
- Construct a tensor product *hp* approximation
- Approximate one dim. polynomials with NNs
- Multiply with NNs to construct a basis
- Multiply by *hp* coefficients
- Error and size bounds from the components



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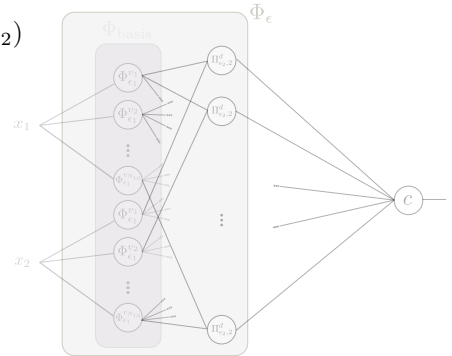

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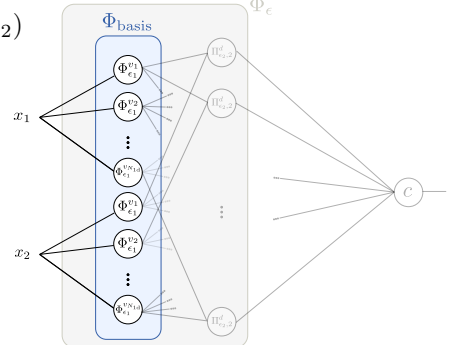

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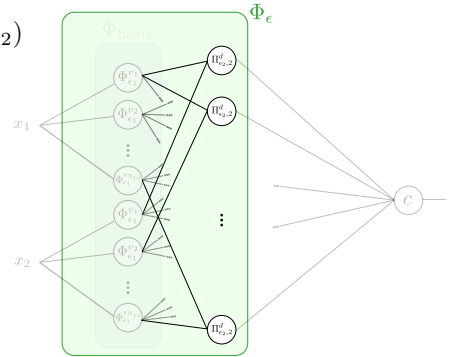

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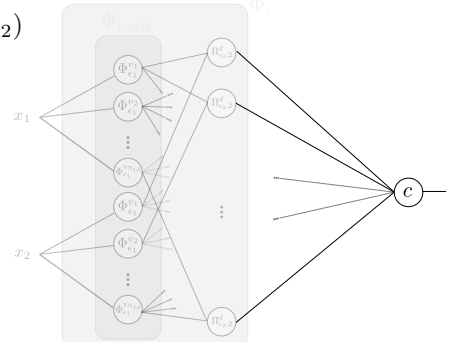

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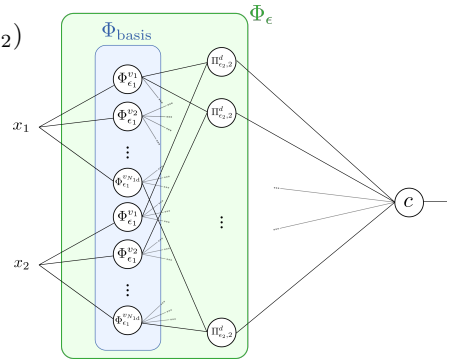

Operator Networks

Operator Networks

Universal approximation theorem for operators [Chen & Chen, IEEE Trans. Neural Netw. (1995)]

σ continuous non-polynomial function, X Banach space, $K_1 \Subset X$, $K_2 \Subset \mathbb{R}^d$, $V \subseteq C(K_1)$, $G : V \to C(K_2)$ nonlinear continuous operator. Then for any $\varepsilon > 0$,

$$\left| G(a)(y) - \sum_{k=1}^{m} \sum_{i=1}^{p} c_i^k \sigma \left(\sum_{j=1}^{n} \xi_{ij}^k a(x_j) + \theta_i^k \right) \sigma(w_k \cdot y + \zeta_k) \right| < \varepsilon \qquad \text{for all } a \in V,\ y \in K_2.$$

Operator Networks

Universal approximation theorem for operators [Chen & Chen, IEEE Trans. Neural Netw. (1995)]

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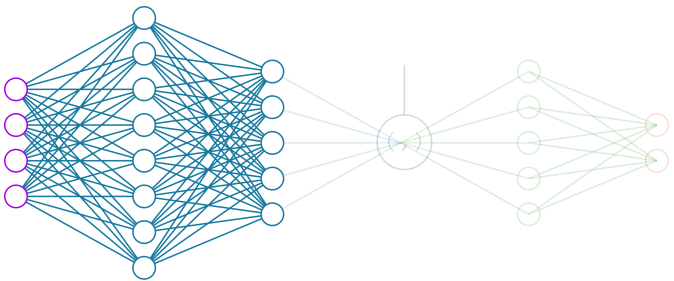

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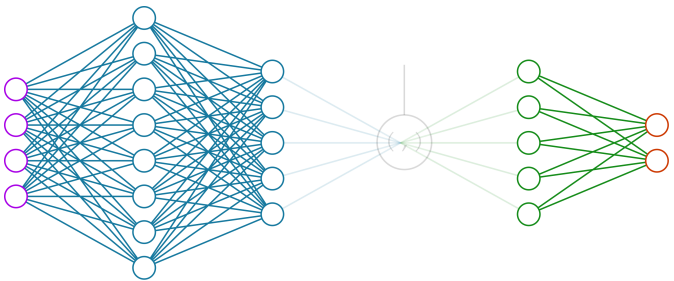

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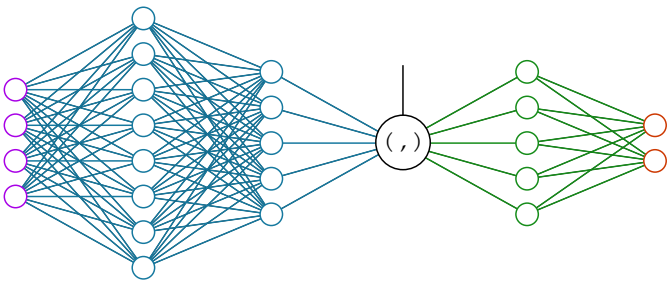

Deep Operator Networks

- More general structure [Lanthaler et al., Trans. Math. Appl. (2022)]:

$$\mathcal{X} \xrightarrow{\mathcal{E}} \mathbb{R}^n \xrightarrow{\mathcal{A}} \mathbb{R}^m \xrightarrow{\mathcal{R}} \mathcal{Y}$$

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A model elliptic PDE

$$-\nabla \cdot (a \nabla u^a) = f \quad \text{in } (\mathbb{R}/\mathbb{Z})^d$$

- Set of coefficients

$$\mathcal{D} = \left\{ \text{periodic } v : v(x) \geq a_{\min} > 0 \text{ and } \|v\|_{W^{k,\infty}(\Omega)} \leq A_{\mathcal{D}}^{k+1} k! \right\}$$

- Space of solutions ($Q = (0,1)^d$)

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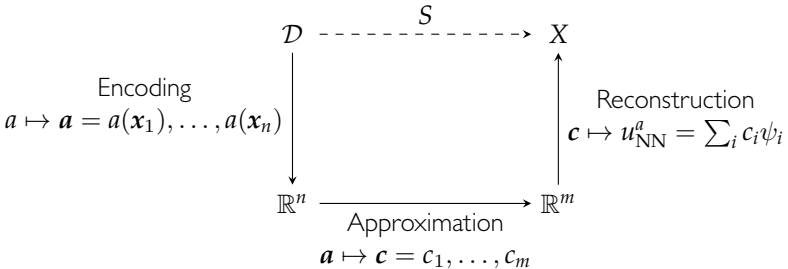

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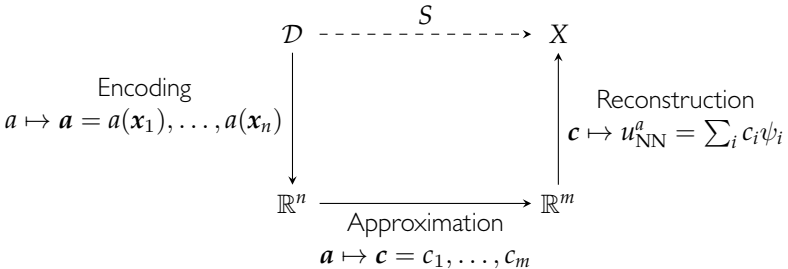

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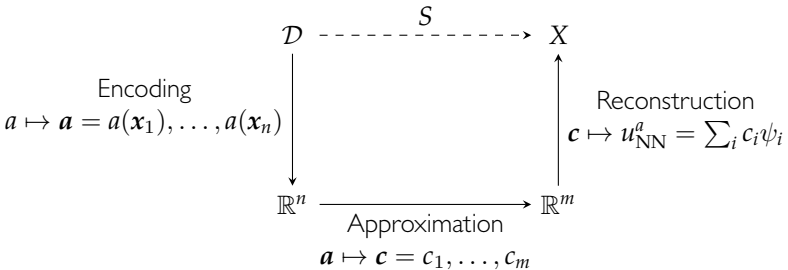

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Operator network approximation

Approximation rates [M & Schwab, Submitted (2021)]

There exists $C > 0$ such that, for all $\varepsilon \in (0, 1)$, there exist

- $n_{\mathrm{b}}, n_{\mathrm{q}} \in \mathbb{N}$ and points $\boldsymbol{x}_{\mathrm{enc}} := \{\boldsymbol{x}_1, \dots \boldsymbol{x}_{n_{\mathrm{q}}}\} \subset \overline{Q}$,
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Sketch of the proof

Idea: Approximate the fully discrete spectral-Galerkin solution

$$u^a_{n_\mathrm{b},n_\mathrm{q}}: \quad \sum_{k=1}^{n_\mathrm{q}} w_k a(x_k)(\nabla u^a_{n_\mathrm{b},n_\mathrm{q}})(x_k)(\nabla\varphi_i)(x_k) = \int_Q f\varphi_i, \qquad \forall i = 1,\dots,n_\mathrm{b},$$

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- φ_i Legendre polynomials.

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Approximation network

- $a(x_1), \dots a(x_{n_q})$
- $\mathrm{R}(\Phi^{A}_{n_b,n_q}) : a(x_1), \dots, a(x_{n_q}) \mapsto \sum_{k=1}^{n_q} w_k a(x_k)(\nabla\varphi_j)(x_k)(\nabla\varphi_i)(x_k) =: \left[A^a_{n_b,n_q}\right]_{ij}$
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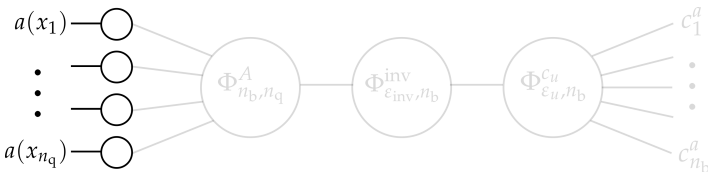

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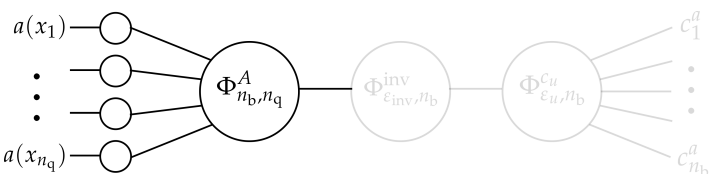

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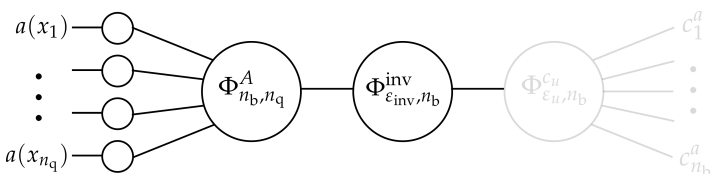
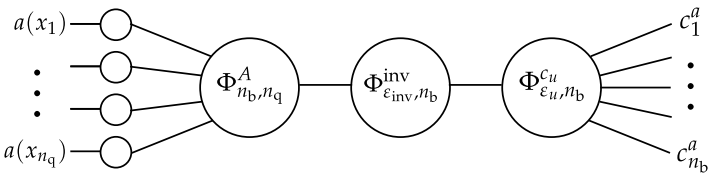
- $\mathrm{R}(\Phi^{\mathrm{inv}}_{\varepsilon_{\mathrm{inv}}}) : A^a_{n_\mathrm{b},n_\mathrm{q}} \mapsto A^a_{\mathrm{inv};\varepsilon_{\mathrm{inv}},n_\mathrm{b}} \simeq \left(A^a_{n_\mathrm{b},n_\mathrm{q}}\right)^{-1}$ [Kutyniok et al., Constr. Approx. (2021)]
- $\mathrm{R}(\Phi^{c_u}_{\varepsilon_u,n_\mathrm{b}}) : A^a_{\mathrm{inv};\varepsilon_{\mathrm{inv}},n_\mathrm{b}} \mapsto A^a_{\mathrm{inv};\varepsilon_{\mathrm{inv}},n_\mathrm{b}} \left[\int_Q f\varphi_i\right]_i \simeq c^a$



Approximation network

- $a(x_1), \dots a(x_{n_q})$
- $\mathrm{R}(\Phi^{A}_{n_b,n_q}) : a(x_1), \dots, a(x_{n_q}) \mapsto \sum_{k=1}^{n_q} w_k a(x_k)(\nabla\varphi_j)(x_k)(\nabla\varphi_i)(x_k) =: \left[A^{a}_{n_b,n_q}\right]_{ij}$
- $\mathrm{R}(\Phi^{\mathrm{inv}}_{\varepsilon_{\mathrm{inv}}}) : A^{a}_{n_b,n_q} \mapsto A^{a}_{\mathrm{inv};\varepsilon_{\mathrm{inv}},n_b} \simeq \left(A^{a}_{n_b,n_q}\right)^{-1}$ [Kutyniok et al., Constr. Approx. (2021)]
- $\mathrm{R}(\Phi^{c_u}_{\varepsilon_u,n_b}) : A^{a}_{\mathrm{inv};\varepsilon_{\mathrm{inv}},n_b} \mapsto A^{a}_{\mathrm{inv};\varepsilon_{\mathrm{inv}},n_b} \left[\int_Q f\varphi_i\right]_i \simeq c^a$



Extensions

- Parametric PDEs

$$-\nabla \cdot (a(\boldsymbol{y})\nabla u) = f \qquad \boldsymbol{y} \in \mathbb{R}^{n_{\mathrm{P}}} \text{ parameter}$$

- Anistropic diffusion-reaction

$$-\nabla \cdot (\mathbf{A}\nabla u) + cu = f$$

- Linear elasticity

$$-\nabla \cdot (\boldsymbol{\sigma}[\boldsymbol{u}]) = \boldsymbol{f}$$

Some open questions & perspectives

- Operator networks for problems with boundary
- High-dimensional problems
- General activation functions
- Training (and computations)

Thank you for your attention