Operator learning for multi-patch domains

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Definition of Neural Operator

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$$\mathcal{N}_\theta : \mathcal{A}(D, \mathbb{R}^{d_a}) \to \mathcal{U}(D, \mathbb{R}^{d_u}), \quad \text{with } D \subset \mathbb{R}^d, \quad \mathcal{N}_\theta := \mathcal{Q} \circ \mathcal{L}_L \circ \cdots \circ \mathcal{L}_1 \circ \mathcal{P}.$$

1. **Lifting:** linear and local operator

$$\mathcal{P} : \mathcal{A}(D, \mathbb{R}^{d_a}) \to \mathcal{U}(D, \mathbb{R}^{d_v}), \quad \mathcal{P}(a)(x) = W_{\mathcal{P}} \cdot a(x) + b_{\mathcal{P}}, \; W_{\mathcal{P}} \in \mathbb{R}^{d_v \times d_a}, b_{\mathcal{P}} \in \mathbb{R}^{d_v}$$

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2. **Integral operator:** for $t = 1, \dots, L$

$$\mathcal{L}_t : \mathcal{U}(D, \mathbb{R}^{d_v}) \to \mathcal{U}(D, \mathbb{R}^{d_v})$$

$$\mathcal{L}_t(v)(x) := \sigma\Big(W_t v(x) + b_t + (\mathcal{K}_t(a, \theta)v)(x)\Big)$$

   with $\mathcal{K}_t(a, \theta)$ linear and non-local operator.

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   with $\mathcal{K}_t(a, \theta)$ linear and non-local operator.
3. **Projection:** linear and local operator

   $$\mathcal{Q} : \mathcal{U}(D_L, \mathbb{R}^{d_v}) \to \mathcal{U}(D, \mathbb{R}^{d_u}), \quad \mathcal{Q}(v)(x) = W_{\mathcal{Q}} + b_{\mathcal{Q}} \cdot v(x), \; W_{\mathcal{Q}} \in \mathbb{R}^{d_{v_u} \times d_v}, \; b_{\mathcal{Q}} \in \mathbb{R}^{d_u}.$$

Definition of Fourier Neural Operator

For defining the Fourier Neural Operator (FNO) we make the following assumptions

$$(\mathcal{K}_t(\theta_t, a)v)(x) = (\mathcal{K}_t(\theta_t)v)(x) = \int_{\mathbb{T}^d} \kappa_{t,\theta_t}(x, y)v(y)\, dy = (\kappa_{t,\theta_t} * v)(x).$$

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Using the convolution theorem we have

$$(\kappa_{t,\theta_t} * v)(x) = \mathcal{F}^{-1}\left(\mathcal{F}(\kappa_{t,\theta_t})(k) \cdot \mathcal{F}(v)(k)\right)(x),$$

and parameterizing $\mathcal{F}(\kappa_{t,\theta_t})$ with the parameters $R_{\theta,t}(k) \in \mathbb{C}^{d_v \times d_v}$ $\forall k \in \mathbb{Z}^d$, we have

$$(\mathcal{K}_t(\theta_t)v)(x) = \mathcal{F}^{-1}\left(R_{\theta,t}(k) \cdot \mathcal{F}(v)(k)\right)(x)$$

Universal approximation for FNOs [1]

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Universal approximation theorem

Given $s, s' \geq 0$ and

$$\mathcal{G} : H^s(\mathbb{T}^d, \mathbb{R}^{d_a}) \to H^{s'}(\mathbb{T}^d, \mathbb{R}^{d_u})$$

continuous operator. Given $K \subset H^s(\mathbb{T}^d, \mathbb{R}^{d_a})$ a compact subset and $\sigma \in \mathbb{C}^\infty(\mathbb{R})$ non-linear and globally Lipschitz activation function. Then, for all $\varepsilon > 0$, exists a Fourier Neural Operator

$$\mathcal{N} : H^s(\mathbb{T}^d, \mathbb{R}^{d_a}) \to H^{s'}(\mathbb{T}^d, \mathbb{R}^{d_u})$$

such that:

$$\sup_{a \in K} \|\mathcal{G}(a) - \mathcal{N}(a)\|_{H^{s'}} \leq \varepsilon.$$

[1] N. Kovachki, S. Lanthaler, S. Mishra, "On universal approximation and error bounds for fourier neural operators"

Pseudo Spectral Fourier Neural Operator

Pseudo Spectral Fourier Neural Operator (ψ-FNO) is a map

$$\mathcal{N}^* : \mathcal{A}(\mathbb{T}^d, \mathbb{R}^{d_a}) \to \mathcal{U}(\mathbb{T}^d, \mathbb{R}^{d_u}), \qquad a \mapsto \mathcal{N}^*(a),$$

defined by

$$\mathcal{N}^*(a) = \mathcal{Q} \circ I_N \circ \mathcal{L}_L \circ I_N \circ \cdots \circ \mathcal{L}_1 \circ I_N \circ \mathcal{R}(a),$$

where I_N denotes the pseudo-spectral projection on the Fourier polynomials of degree N

$$I_N : C(\mathbb{T}^d) \to L^2_N(\mathbb{T}^d), \quad u \mapsto I_N u.$$

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$$I_N : C(\mathbb{T}^d) \to L^2_N(\mathbb{T}^d), \quad u \mapsto I_N u.$$

So a ψ-FNO can be identified with a finite-dimensional map

$$\widetilde{\mathcal{N}}^* : \mathbb{R}^{d_a \times \mathcal{I}_N} \to \mathbb{R}^{d_u \times \mathcal{I}_N}, \quad \widetilde{\mathcal{N}}^*(a)_j = \mathcal{N}^*(a)(x_j) \quad \forall j \in \mathcal{I}_N,$$

where the input $a = \{a_j\}_{j \in \mathcal{I}_N}$, $a_j = a(x_j)$ and $\mathcal{I}_N = \{1, \dots, 2N\}^d$.

Universal approximation for ψ-FNOs[2]

Universal approximation for ψ-FNOs

Given $s > d/2$, $s' \geq 0$ and

$$\mathcal{G} : H^s(\mathbb{T}^d, \mathbb{R}^{d_a}) \to H^{s'}(\mathbb{T}^d, \mathbb{R}^{d_u})$$

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$$\mathcal{N}^* : L^2_N(\mathbb{T}^d, \mathbb{R}^{d_a}) \to L^2_N(\mathbb{T}^d, \mathbb{R}^{d_u})$$

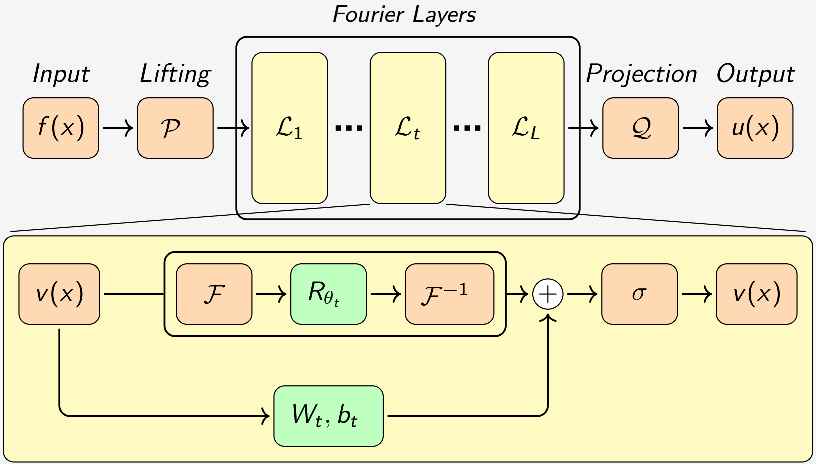
satisfy:

$$\sup_{a \in K} \|\mathcal{G}(a) - \mathcal{N}^*(a)\|_{H^{s'}} \leq \varepsilon.$$

[2] N. Kovachki, S. Lanthaler, S. Mishra, "On universal approximation and error bounds for fourier neural operators"

Representation of ψ-FNO

1 Fourier Neural Operator



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FNOs are limited to rectangular domains. To extend the operator to irregular domains, we can extend the domain to a larger rectangular domain and training the FNO to approximate the solution only on the original domain.

Periodic extension operator

Let $\Omega \subset \mathbb{R}^d$ be a bounded and Lipschitz domain. There exists a continuous. linear operator $\mathcal{E} : W^{m,p}(\Omega) \to W^{m,p}(B)$ for any $m \geq 0$ and $1 \leq p < \infty$, where B is an hyper-cube containing Ω, such that, for any $u \in W^{m,p}(\Omega)$:

- $\mathcal{E}(u)_{|\Omega} = u$,
- $\mathcal{E}(u)$ is periodic on B, including its derivatives.

Fourier continuation

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- $\mathcal{E}(u)$ is periodic on B, including its derivatives.

But this can be computationally expensive.

Chebyshev Neural Operator

Let $D \subset \mathbb{R}^d$ be a bounded domain. The Chebyshev Neural Operator (CNO) is a map

$$\mathcal{N}_\theta : \mathcal{A}(D, \mathbb{R}^{d_a}) \to \mathcal{U}(D, \mathbb{R}^{d_u}),$$

defined by

$$\mathcal{N}_\theta(a) = \mathcal{Q} \circ \mathcal{L}_L \circ \cdots \circ \mathcal{L}_1 \circ \mathcal{P}(a),$$

where is all defined as the FNO but in the integral operator we use the Chebyshev transform and anti-transform instead of the Fourier transform, i.e.

$$(\mathcal{K}_t(\theta_t)v)(x) = \mathcal{C}^{-1}\left(R_{\theta_t}(k) \cdot \mathcal{C}(v)(k)\right)(x), \quad R_{\theta_t}(k) \in \mathbb{R}^{d_v \times d_v} \ \forall k \in \mathbb{N}^d.$$

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At the discrete level, we can define the Pseudo Spectral Chebyshev Neural Operator (ψ-CNO) as before, with the difference that the grid $\mathcal{I}_N$ is defined on a Chebyshev grid and not on an uniform one.

Boundary adapted Chebyshev basis

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The one dimensional Chebyshev polynomials are defined on the interval $[-1, 1]$, as $T_n(\cos(\theta)) = \cos(n\theta)$, $n \in \mathbb{N}$ with the property that $T_n(1) = 1$ and $T_n(-1) = (-1)^n$.
We define the boundary adapted Chebyshev basis as $B_0(x) = \frac{1}{2}(-x+1)$, $B_1(x) = \frac{1}{2}(x+1)$ and for $n \geq 2$

$$B_n(x) = \begin{cases} T_n(x) - T_0(x) & n \text{ is even,} \\ T_n(x) - T_1(x) & n \text{ is odd.} \end{cases}$$

Boundary adapted Chebyshev basis

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For two dimensional Chebyshev polynomials we define $B_{n_1,n_2}(x,y) = B_{n_1}(x)B_{n_2}(y),\ 0 \leq n_1, n_2 \leq n.$ Considering the square domain $D = [-1,1]^2$ we notice that there is only a function not equal to zero in each vertex of the square and there are only n functions that are not zero on each edge, $B_{i,j}(x,y)$ $2 \leq i,j \leq n$ are zero on the boundary.

Multi-patch domains

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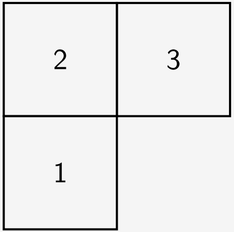
If we have the domain D divided in N patches D_k with $D = \bigcup_{k=1}^{N} D_k$ with $D_i \cap D_j = \emptyset$ or $D_i \cap D_j = \Gamma_{ij}$ for $i \neq j$.



We consider the L-domain

$$D = [-1,1]^2 \setminus ([0,1] \times [-1,0])$$

divided in $N = 3$ patches D_1, D_2, D_3. We define the boundary adapted Chebyshev basis on each patch D_k and denotes with $B^k_{i,j}$ with $k = 1,2,3$ and $0 \leq i,j \leq n$. To ensure the continuity on the interface $\Gamma_{1,2}$ and $\Gamma_{2,3}$ we have to impose that

$$b^0_{i,1} = b^1_{i,0}, \quad b^2_{0,i} = b^1_{1,i}, \quad \forall i = 1, \dots n$$

Multi-patch Neural Operator

The multi-patch neural operator is defined as the Chebyshev neural operator on each patch D_k and the continuity on the interface is imposed using the boundary adapted Chebyshev basis in the following way:

- compute the Chebyshev discrete transform of the function v on each patch D_k,
- moltiply with the parameters $R_{\theta,t}$,
- compute the boundary adapted Chebyshev coefficients on each patch,
- impose the continuity on the interface $\Gamma_{1,2}$ and $\Gamma_{2,3}$,
- go back to the Chebyshev coefficients on each patch,
- compute the Chebyshev inverse transform on each patch.

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For our numerical experiments we consider the Darcy problem:

$$\begin{cases} -\nabla(a \cdot \nabla u) = f, & \text{in } D \\ u = 0, & \text{on } \partial D \end{cases}$$

with the L-domain $D = [-1,1]^2 \setminus ((0,1) \times (-1,0))$, diffusion coefficient $a \in \mathcal{A} = L^\infty(D, \mathbb{R}^+)$, and $f \equiv 1$. With this settings exists a unique solution $u \in H_0^1(D, \mathbb{R})$ and so we can define the solution operator

$$\mathcal{G} : L^\infty(D, \mathbb{R}^+) \to H_0^1(D, \mathbb{R}), \qquad \mathcal{G} : a \mapsto u.$$

Dataset generation

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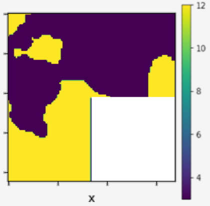
We have to generate the dataset $\left\{a^{(i)}, u^{(i)}\right\}_{i=1}^{N}$.

Dataset generation

3 Numerical experiments

We have to generate the dataset $\left\{a^{(i)}, u^{(i)}\right\}_{i=1}^{N}$.

For the input we use the push forward of a proper gaussian random fields $a^{(i)} \sim \mu = T_{\#}N(0, C)$ i.i.d. where $C = -(\Delta + 9I)^{-2}$ and $T : \mathbb{R} \to \mathbb{R}$ such that T gives 12 to the positive values and 3 to the negative ones.



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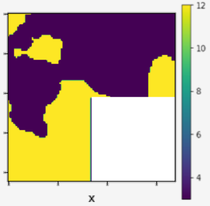

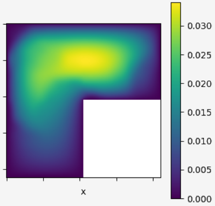

For the output we approximate the solution of the Darcy problem solution $u^{(i)} = \mathcal{G}(a^{(i)})$ using the isogeometric geoPDEs library.

Relative L^2 error

We define the relative L^2 error as

$$\left\|\frac{\mathcal{G}-\mathcal{N}_\theta^*}{\mathcal{G}}\right\|_{L^2_\mu(L^\infty,L^2)} = \mathbb{E}_{a\sim\mu}\frac{\|\mathcal{G}(a)-\mathcal{N}_\theta^*(a)\|^2_{L^2(D)}}{\|\mathcal{G}(a)\|^2_{L^2(D)}}$$

that can be approximated by

$$\left\|\frac{\mathcal{G}-\mathcal{N}_\theta^*}{\mathcal{G}}\right\|_{L^2_\mu(L^\infty,L^2)} \approx \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\sum_{k=1}^{M}\left|u^{(i)}(x_k)-\mathcal{N}_\theta^*\left(a^{(i)}\right)(x_k)\right|^2}{\sum_{k=1}^{M}\left|u^{(i)}(x_k)\right|^2}\right).$$

Where $\{x_k\}_{k=1}^M \subset D$ is the set of the discretization points. That is a uniform (or Chebyshev) grid of 42 points per direction in every square patches.

Fourier continuation numerical experiments

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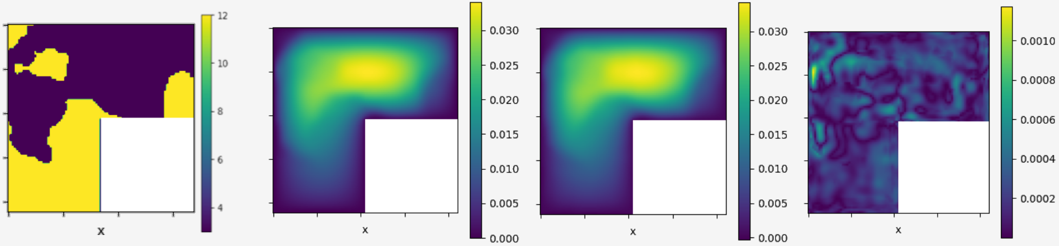
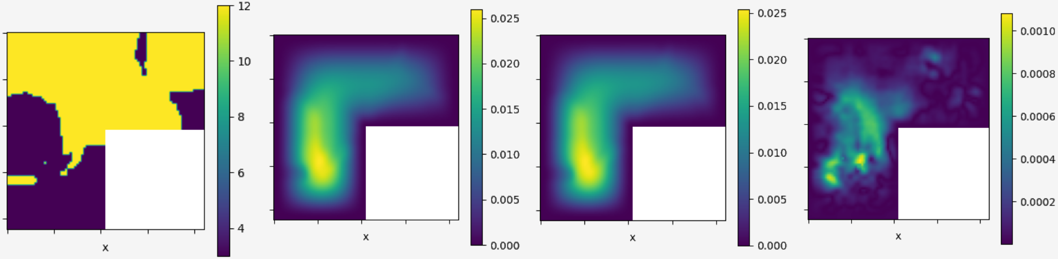


rel. train error L^2	rel. test error L^2	parameters	epochs
0.0282	0.0229	2 363 681	500

Multi-patch neural operator numerical experiments

3 Numerical experiments



rel. train error L^2	rel. test error L^2	parameters	epochs
0.0115	0.0212	2 372 233	500

Conclusions and future works

Achievements:

- We have constructed a multi-patch neural operator for the Darcy problem on the L-domain.
- The neural operator is easily parallelizable between the patches.

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Future works:

- Analyze if an universal approximation result can be obtained for the multi-patch neural operator.
- Use the multi-patch neural operator to approximate the solution of different PDEs.
- Extend the multi-patch neural operator to more complex geometries, with patches that are isomorphic to the square.

Operator learning for multi-patch domains

Thank you for your attention!

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Teorema

Given $s > d/2$, $\lambda \in (0,1)$ and we consider the solution operator for the Darcy problem

$$\mathcal{G} : \mathcal{A}_\lambda^s(\mathbb{T}^d) \to H^1(\mathbb{T}^d).$$

Given $\sigma \in C^3(\mathbb{R})$ non-polynomial, for any $N \in \mathbb{N}$ exists $C > 0$ and a ψ-FNO

$$\mathcal{N}^* : \mathcal{A}_\lambda^s(\mathbb{T}^d) \to H^1(\mathbb{T}^d)$$

such that

$$\sup_{a \in \mathcal{A}_\lambda^s} \|\mathcal{G}(a) - \mathcal{N}^*(a)\|_{H^1(\mathbb{T}^d)} \leq CN^{-k}$$

and $\mathrm{depth}(\mathcal{N}^*) \leq C \log(N)$, $\mathrm{lift}(\mathcal{N}^*) \leq C$, $\mathrm{size}(\mathcal{N}^*) \lesssim N^d \log(N)$.

Trasformata di Fourier

3 Numerical experiments

- Given $v \in L^2(\mathbb{T}^d)$, the Fourier transform is defined as

$$\begin{aligned} \mathcal{F} : L^2(\mathbb{T}^d, \mathbb{C}^n) &\to \ell^2(\mathbb{Z}^d, \mathbb{C}^n) \\ v &\mapsto \mathcal{F}(v) \end{aligned}$$

$$\mathcal{F}(v)(k) := \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} v(x) e^{-i\langle k, x\rangle} \, dx, \quad \forall k \in \mathbb{Z}^d.$$

- Given $\widehat{v} = \{\widehat{v}_k\}_{k \in \mathbb{Z}^d} \in \ell^2(\mathbb{Z}^d, \mathbb{C}^n)$, the anti-Fourier transform is defined as

$$\begin{aligned} \mathcal{F}^{-1} : \ell^2(\mathbb{Z}^d, \mathbb{C}^n) &\to L^2(D, \mathbb{C}^n) \\ \widehat{v} &\mapsto \mathcal{F}^{-1}(\widehat{v}) \end{aligned}$$

$$(\mathcal{F}^{-1}\widehat{v})(x) = \sum_{k \in \mathbb{Z}^d} \widehat{v}_k e^{i\langle k, x\rangle} \qquad \forall x \in D.$$

Discrete Fourier transform and anti-transform

We choose $N \in \mathbb{N}$ and fix an uniform grid $\{x_j\}_{j\in\mathcal{I}_N}$ with $x_j = (2\pi j)/(2N+1) \in \mathbb{T}^d$, $j \in \mathcal{I}_N = \{0,\dots,2N\}^d$, finally we define $\mathcal{K}_N := \{k \in \mathbb{Z}^d : |k|_\infty \leq N\}$. We define the discrete Fourier transform as

$$\mathcal{F}_N : \mathbb{R}^{\mathcal{I}_N} \to \mathbb{C}^{\mathcal{K}_N}$$

$$\mathcal{F}_N(v)(k) := \frac{1}{(2N+1)^d} \sum_{j\in\mathcal{I}_N} v(x_j) e^{-2\pi i\langle j,k\rangle/N}, \quad \forall k \in \mathcal{K}_N,$$

and we define the discrete version of the anti-Fourier transform as

$$\mathcal{F}_N^{-1} : \mathbb{C}^{\mathcal{K}_N} \to \mathbb{R}^{\mathcal{I}_N}$$

$$\mathcal{F}_N^{-1}(\widehat{v})(j) := \sum_{k\in\mathcal{K}_N} \widehat{v}_k e^{2\pi i\langle j,k\rangle/N}, \qquad \forall j \in \mathcal{J}_N.$$

Sketch of the proof of universal approximation theorem for FNOs

- The definition of the projection on the trigonometric polynomial is

$$P_N : L^2(\mathbb{T}^d) \to L^2_N(\mathbb{T}^d),$$

$$P_N\left(\sum_{k\in\mathbb{Z}^d} c_k e^{i\langle x,k\rangle}\right) = \sum_{|k|_\infty \le N} c_k e^{i\langle x,k\rangle}, \qquad \forall (c_k)_{k\in\mathbb{Z}^d} \in \ell^2(\mathbb{Z}^d).$$

- If the universal approximation theorem holds for $s' = 0$ then it holds for any value of $s' \ge 0$.
- We fix $s' = 0$

$$\mathcal{G}_N : H^s(\mathbb{T}^d, \mathbb{R}^{d_a}) \to L^2(\mathbb{T}^d, \mathbb{R}^{d_u}), \qquad \mathcal{G}_N(a) := P_N\mathcal{G}(P_N a),$$

holds that $\forall \varepsilon > 0$, $\exists N \in \mathbb{N}$ such that

$$\|\mathcal{G}(a) - \mathcal{G}_N(a)\|_{L^2} \le \varepsilon, \qquad \forall a \in K.$$

Sketch of the proof of universal approximation theorem for FNOs

Define the operator

$$\widehat{\mathcal{G}}_N : \mathbb{C}^{\mathcal{K}_N} \to \mathbb{C}^{\mathcal{K}_N}, \qquad \widehat{\mathcal{G}}_N(\widehat{a}_k) := \mathcal{F}_N(\mathcal{G}_N(Re(\mathcal{F}_N^{-1}(\widehat{a}_k)))),$$

holds the following identity

$$\mathcal{G}_N(a) = \mathcal{F}_N^{-1} \circ \widehat{\mathcal{G}}_N \circ \mathcal{F}_N(P_N a),$$

for any function $a \in L^2(\mathbb{T}^d, \mathbb{R}^{d_a})$. So we reconduce to demonstrate that FNO can approximate

$$\mathcal{F}_N^{-1}, \; \widehat{\mathcal{G}}_N, \; \mathcal{F}_N(P_N a).$$

Definition MLP

Let $d \in \mathbb{N}$ and $L \in \mathbb{N}$ with $L \geq 2$ and $\sigma : \mathbb{R} \to \mathbb{R}$ a non-linear activation function. Let $A_\ell \in \mathbb{R}^{n_\ell \times n_{\ell-1}}$, $b_\ell \in \mathbb{R}^\ell$ with $n_\ell \in \mathbb{N}$ for $\ell = 1, \ldots, L$ and $n_0 = d$. We call multilayer perceptron (MLP) the function defined as

$$\begin{cases} x_L = A_L x_{L-1} + b_L \\ x_\ell = \sigma\left(A_\ell x_{\ell-1} + b_\ell\right) \end{cases},$$

where x_0 is the input and x_L is the output of the function.

Universal approximation theorem for operator

Suppose that $\sigma \in TW$, X is a Banach space, $K_1 \subset X$, $K_2 \subset \mathbb{R}^d$ are two compact sets in X and $\mathbb{R}^d$ respectively, and V is a compact set in $C(K_1)$. Let G a nonlinear continuous operator which maps V into $C(K_2)$, then for any $\varepsilon > 0$, there are a positive integers n, p, m; real constants c_i^k, θ_i^k, ξ_{ij}^k, $\zeta^k \in \mathbb{R}$, points $w^k \in \mathbb{R}^d$ and $x_j \in K_1$, with $i = 1, \dots, n$, $j = 1, \dots, m$ and $k = 1, \dots, p$, such that

$$\left| G(u)(y) - \sum_{k=1}^{p} \sum_{i=1}^{n} c_i^k \sigma \left(\sum_{j=1}^{m} \xi_{ij}^k u(x_j) + \theta_i^k \right) \sigma(w^k \cdot y + \zeta^k) \right| < \varepsilon$$

holds for all $u \in V$ and $y \in K_2$.