Mapping properties of neural networks

Matti Lassas

in collaboration with Maarten de Hoop Ivan Dokmanic Takashi Furuya Konik Kothari Michael Puthawala





Outline:

- Neural networks and the manifold hypothesis
- Networks with injective layers
- Injective networks and approximation of manifolds
- Flow networks and approximation of probability distributions
- Applications in inverse problems
- Neural operators



Deep neural network with relu-functions

A deep neural network (DNN) is a function $f_{\theta} : \mathbb{R}^{d_0} \to \mathbb{R}^{d_{L+1}}$ defined by

$$\begin{array}{lll} y_0 &=& x, \\ y_{\ell+1} &=& \phi \left(W_{\theta}^{\ell} y_{\ell} + b_{\theta}^{\ell} \right), \quad \ell = 0, 1, \dots, L-1, \\ f_{\theta}(x) &=& W_{\theta}^{L} y_L + b_{\theta}^{L}. \end{array}$$



We denote the set of such functions f_{θ} by $\mathcal{NN}(d_0, d_{L+1})$. Above,

•
$$\ell = 0, 1, 2, \dots, L$$
: the layer index.

•
$$y_\ell \in \mathbb{R}^{d_\ell}$$
: the state at layer ℓ .

• Weight matrixes $W^\ell_ heta \in \mathbb{R}^{d_{\ell+1} imes d_\ell}$ and bias vectors $b^\ell_ heta \in \mathbb{R}^{d_{\ell+1}}$

• ϕ is the activation function, the Rectified Linear Unit (relu)

$$\phi: \mathbb{R}^d \to \mathbb{R}^d, \quad \phi(x_1, \dots, x_d) = (\max(0, x_1), \dots, \max(0, x_d))$$

Basic mapping properties of neural networks

We consider the following topics

• Examples of injective neural networks $f_{\theta} : \mathbb{R}^n \to \mathbb{R}^m$ that are one-to-one, that is,

$$f_{ heta}(z_1) = f_{ heta}(z_2) \implies z_1 = z_2$$

Let K ⊂ ℝⁿ be a compact set and f_θ : ℝⁿ → ℝ^m be injective (and continuous). Then,

$$f_{ heta}: K o f_{ heta}(K)$$

is a homeomorphism, and hence, K and $f_{\theta}(K)$ have the same topology.



Manifold hypothesis and a generative model

Let $M \subset \mathbb{R}^m$ be a *d*-dimensional surface (that is, a manifold) and $\mu_0 = \mu_{data}$ be a probability distribution supported on M. Let us assume that the topology of M is known and let $K \subset \mathbb{R}^n$ be a 'model space' that has the same topology as M. Let $Z \sim \text{Unif}(K)$ be a random variable. Here, $d \leq n < m$. Our aims are to

- Find a neural network $f_{\theta} : \mathbb{R}^n \to \mathbb{R}^m$ such that $f_{\theta} : \mathbb{R}^n \to \mathbb{R}^m$ is one-to-one and $f_{\theta}(K) = M$ (or $f_{\theta}(K) \approx M$).
- **2** Find $f_{\theta} : \mathbb{R}^n \to \mathbb{R}^m$ such that $f_{\theta}(Z)$ has the distribution μ_0 .



Figures: Goldt et al Phys. Rev. X 2020 and Bukhari et al Sci. Rep. 2022.

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Injective of layer of a relu-neural network

Consider function $N: \mathbb{R}^n \to \mathbb{R}^m$ defined by

$$N(x) = \phi (Wx + b)$$

where

• $W \in \mathbb{R}^{m \times n}$ is a weight matrix and $b \in \mathbb{R}^n$ is a bias vector,

• ϕ is the Rectified Linear Unit (relu)

$$\phi: \mathbb{R}^m \to \mathbb{R}^m,$$

$$\phi(x_1, \ldots, x_m) = (\max(0, x_1), \ldots, \max(0, x_m)) = \max(x, 0).$$

Examples of injective layers

• The map
$$N : \mathbb{R}^n \to \mathbb{R}^{2n}$$
,

$$N(x) = \begin{bmatrix} \phi(x) \\ \phi(-x) \end{bmatrix} = \begin{bmatrix} \max(x,0) \\ \max(-x,0) \end{bmatrix}$$

is injective.

② Let
$$W \in \mathbb{R}^{2n imes n}$$
 be

$$W = \begin{bmatrix} B \\ -B \end{bmatrix}$$

where $B \in \mathbb{R}^{n \times n}$ is an invertible matrix. Then

$$N: \mathbb{R}^n \to \mathbb{R}^{2n}$$
$$N(x) = \phi(Wx)$$

is injective.

Conditions for injectivity

Theorem (Conditions for injectivity of relu(Wx))

Let $W \in \mathbb{R}^{m \times n}$ be a matrix with row vectors $\mathcal{W} = \{w_j\}_{j=1}^m$, and relu $(y) = \max(y, 0)$. The function relu $(W(\cdot)) \colon \mathbb{R}^n \to \mathbb{R}^m$ is injective if and only if

$$span\{w \in \mathcal{W}: w \cdot x \ge 0\} = \mathbb{R}^n$$
 for all $x \in \mathbb{R}^n$.

If W is injective, then $m \ge 2n$.

Theorem (Conditions for injectivity of relu(Wx + b))

Let $W \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$ and $\mathcal{W} = \{w_j\}_{j=1}^m$ be the row vectors of W. The function relu $(W(\cdot) + b)$: $\mathbb{R}^n \to \mathbb{R}^m$ is injective if and only if $\{w_j \in \mathcal{W} : b_j \ge 0, w_j \cdot x \ge 0\}$ spans \mathbb{R}^n for every $x \in \mathbb{R}^n$.

Reference: [Puthawala-Kothari-L.-Dokmanic-de Hoop JMLR 2022]

(1)

$$W = \begin{bmatrix} \cos(\pi/8) & \sin(\pi/8) \\ \cos(5\pi/8) & \sin(5\pi/8) \\ \cos(-5\pi/8) & \sin(-5\pi/8) \\ \cos(-\pi/8) & \sin(-\pi/8) \end{bmatrix}$$



$$W = \begin{bmatrix} \cos(\pi/8) & \sin(\pi/8) \\ \cos(5\pi/8) & \sin(5\pi/8) \\ \cos(-5\pi/8) & \sin(-5\pi/8) \\ \cos(-\pi/8) & \sin(-\pi/8) \end{bmatrix}$$



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$$f_{ heta}(K) = M, \quad K \subset \mathbb{R}^2, \ M \subset \mathbb{R}^m$$



A	A	A	P	2	8	7	V	V	4	4	1	A	L	Þ	Þ	V
A	A	A	A	2	7	7	V	A	4	4	1	4	L	Þ	Þ	V
A	A	A	P	P	7	7	V	P	4	4	1	4	A	Þ	V	V
A	A	A	P	P	2	7	P	Y	4	4	*	4	L	Þ	V	V
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Universal Approximation by Injective Neural Networks

By using injective neural networks we are able to approximate any continuous function that maps a low dimensional space into a higher one.

Theorem (Puthawala-Kothari-L.-Dokmanic-de Hoop JMLR 2022)

Let $f : \mathbb{R}^n \to \mathbb{R}^m$ be a continuous function, where $m \ge 2n + 1$, and $L \ge 2$. Then for any $\varepsilon > 0$ and compact subset $K \subset \mathbb{R}^n$ there exists a relu-neural network $N_{\theta} \in \mathcal{NN}(n, m)$ of depth L such that $N_{\theta} : \mathbb{R}^n \to \mathbb{R}^m$ is injective (that is, a one-to-one function) and

 $|f(x) - N_{\theta}(x)| < \varepsilon$, for all $x \in K$.

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$$|f(x) - N_{\theta}(x)| < \varepsilon$$
, for all $x \in K$.

Combining our results with [Yarotsky, Neural Networks 2017], see also [Guhring-Raslan, Neural Networks 2022], we can estimate the depth, the width, and the inverse Lipschitz constant of N_{θ} in terms of ε , K and the C^1 -norm of f.

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$$f_{\theta}(K) = M, \quad f_{\theta}(Z) \sim \mu_0$$



A	A	A	P	2	7	7	V	V	4	4	1	A	L	Þ	V	V
A	A	A	A	P	7	7	V	A	4	4	4	4	L	Þ	V	V
A	A	A	P	P	7	7	V	P	4	4	1	4	A	Þ	V	V
A	A	A	A	2	7	7	A	Y	4	4	4	4	L	Þ	V	V
A	A	A			7	7	A	Y	4	4	A	4	4	Þ	V	V
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A	A	A			7	7	4	¥	*	4	A	L	4	Þ	Þ	V
A	A	A	>		7	7	4	A	*	*	4	4	4	Þ	Þ	V
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A	A	N	۲	7	7	7	4	¥	*	4	*	Ā.	4	Þ	Þ	v
A	٨	N	N	4	7	Ŧ	4	4	<	4.	A	L	4	Þ	Þ	v
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Diffeomorphic neural networks

The affine coupling flows are the maps $g : \mathbb{R}^n \to \mathbb{R}^n$,

$$g(x_1,...,x_{n-1},x_n) = \left(x_1,...,x_{n-1},e^{a_{\theta}(x_1,...,x_{n-1})}\cdot x_n + b_{\theta}(x_1,...,x_{n-1})\right)$$

where a_{θ} and b_{θ} are neural networks, e.g., relu-neural networks. It is easy to compute the inverse function of g,

$$g^{-1}(x_1,\ldots,x_n) = \left(x_1,\ldots,x_{n-1},e^{-a_{\theta}(x_1,\ldots,x_{n-1})}\cdot(x_n-b_{\theta}(x_1,\ldots,x_{n-1}))\right)$$

Functions $g : \mathbb{R}^n \to \mathbb{R}^n$ and $g^{-1} : \mathbb{R}^n \to \mathbb{R}^n$ are continuous bijective maps.

References: Dinh et al ICLR 2015, Teshima et al NeurIPS 2020.

Universal approximation of diffeomorphisms

The diffeo-networks are finite compositions of linear invertible maps $L_i : \mathbb{R}^n \to \mathbb{R}^n$ and affine coupling flows $g_i : \mathbb{R}^n \to \mathbb{R}^n$, that is,

$$T_{\theta} = L_k \circ g_k \circ \cdots \circ L_1 \circ g_1 : \mathbb{R}^n \to \mathbb{R}^n.$$

We denote the set of diffeo-networks by \mathcal{T}_n . Observe that

$$T_{\theta}^{-1} = g_1^{-1} \circ L_1^{-1} \circ \cdots \circ g_k^{-1} \circ L_k^{-1}.$$

Teshima et al, NeurIPS 2020 (c.f. Bogachev 2007), proved the following:

Theorem

Let $f : \mathbb{R}^n \to \mathbb{R}^n$ be a C^k -smooth diffeomorphism, $k \ge 2$, and $1 \le p < \infty$. Then for any $\varepsilon > 0$ and compact subset $K \subset \mathbb{R}^n$ there exists a neural network $T_{\theta} \in \mathcal{T}_n$

$$\|f-T_{\theta}\|_{L^p(K)}<\varepsilon.$$

Similar result holds for deep sigmoidal flows with $p = \infty$.

Definition of injective flow networks

Let $n, m \in \mathbb{N}$. An injective flow network is function

$$f = T_2 \circ R \circ T_1 : \mathbb{R}^n \to \mathbb{R}^m$$
, where

- $T_1: \mathbb{R}^n \to \mathbb{R}^n$ is a diffeo-network,
- 2 $R: \mathbb{R}^n \to \mathbb{R}^m$ be an injective linear map, e.g., R(x) = (x, 0),
- **③** $T_2 : \mathbb{R}^m \to \mathbb{R}^m$ is a diffeo-network.

We denote the set of injective flow networks by $\mathcal{IN} = \mathcal{IN}_{n,m}$

When are these networks universal approximators for all embeddings?

When $K \subset \mathbb{R}^n$ is compact, we say that a function $f : K \to \mathbb{R}^m$ is an embedding if $f : K \to \mathbb{R}^m$ is continuous and injective. We denote embeddings by

$$\mathrm{emb}^k(K,\mathbb{R}^m)=\mathrm{emb}(K,\mathbb{R}^m)\cap C^k(K,\mathbb{R}^m).$$



All embeddings are not given by flow networks

Let $K = S^1 \subset \mathbb{R}^2$ be a circle, and $f : K \to \mathbb{R}^3$ be an embedding of K to a trefoil knot to \mathbb{R}^3 . There are no map $E = T_2 \circ R \circ T_1$, where $T_1 : \mathbb{R}^2 \to \mathbb{R}^2$ is a diffeomorphism, $R : \mathbb{R}^2 \to \mathbb{R}^3$ is an injective linear map and $T_2 : \mathbb{R}^3 \to \mathbb{R}^3$ is a diffeomorphism, so that E(K) = f(K).



Example: the manifold of 3×3 patches of pixels of natural images can be well modelled by a Klein bottle [Carlsson et al 2008].

Practical implication: It is difficult to learn a prior distribution that is supported on a general submanifold. Next we show that this difficulty can be avoided by choosing a finer discretization in the inverse problem.

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All embeddings are extendable when $m \ge 3n + 1$

Definition (Extendable Embedding)

Let $K \subset \mathbb{R}^n$ be compact set. The set of extendable embeddings is

$$\mathcal{I}^{k}(K, \mathbb{R}^{m}) \coloneqq \{ \Phi \circ R \in C(K, \mathbb{R}^{m}) \colon \Phi \in \mathsf{Diff}^{k}(\mathbb{R}^{m} \to \mathbb{R}^{m}), \\ R : \mathbb{R}^{n} \to \mathbb{R}^{m} \text{ is injective and linear} \}$$

Theorem (Puthawala-L.-Dokmanic-de Hoop ICML 2022)

When $m \ge 3n + 1$, $k \ge 1$, and $K \subset \mathbb{R}^n$ is compact, it holds that

 $\mathcal{I}^k(K,\mathbb{R}^m) = emb^k(K,\mathbb{R}^m).$

When $p < \infty$, for any C^k -embedding $f \in emb^k(\mathbb{R}^n, \mathbb{R}^m)$ there is a map E in the L^p -closure of the injective flow neural networks \mathcal{IN} such that $E(\mathcal{K}) = f(\mathcal{K})$.

The proof is based on the "clean trick" in algebraic topology, see e.g. Madsen-Tornehave 1997

Matti Lassas (University of Helsinki)

Approximation of probability measures

Theorem (Puthawala-L.-Dokmanic-de Hoop ICML 2022)

Suppose $m \ge 3n + 1$. Let ν be a probability measure on a compact set $K \subset \mathbb{R}^n$ that is absolutely continuous w.r.t. Lebesgue measure, $f : K \to \mathbb{R}^m$ a C^1 -embedding, and

- **1** $R: \mathbb{R}^n \to \mathbb{R}^m$ is an injective linear map
- **2** \mathcal{T}_m is universal approximator of diffeomorphisms in L^{∞} ,
- **③** \mathcal{T}'_n is universal approximator of diffeomorphisms in L^p , $p \ge 1$.

Then, there are $E_i = T_i \circ R \circ T'_i$, $T_i \in \mathcal{T}_m$, $T'_i \in \mathcal{T}'_n$, i = 1, 2, ... such that

$$\lim_{i\to\infty}\mathsf{W}_2\left(f_{\#}\nu,(E_i)_{\#}\nu\right)=0,$$

where W_2 is the Wasserstein distance and $F_{\#}\nu(A) = \nu(F^{-1}(A))$.

This means the following: if $Z \sim \nu$ and $X = f(Z) \sim \mu_0$ then the distribution of $X_i = E_i(Z)$ is close to μ_0 .

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Credit on figure: Kothari-Khorashadizadeh-de Hoop-Dokmanic UAI 2021.

Solving an inverse problem with a learned prior

Let μ_0 be a distribution supported on manifold $M \subset \mathbb{R}^m$. Let x_j , j = 1, 2, ..., N be independent samples from the distribution μ_0 and $Z \sim N(0, I)$ in \mathbb{R}^n .

We aim to find a neural network $f_{\theta} : \mathbb{R}^n \to \mathbb{R}^m$ such that $f_{\theta}(Z) \sim \mu_0$.

Then, we will consider the following inverse problem: Let $A: \mathbb{R}^m \to \mathbb{R}^k$ and

$$\begin{split} Y &= AX + \varepsilon, \\ X &= f_{\theta}(Z) \in \mathbb{R}^{m}, \quad \text{where } Z \sim N(0, I) \text{ in } \mathbb{R}^{n}, \\ \varepsilon &\sim N(0, I). \end{split}$$

Let y be a sample of the random variable Y. The Maximum A Posteriori estimate for X is

$$x_{MAP} = \operatorname{argmax}_{x} \pi_{X|Y}(x|y)$$

We seek a solution of the form $x = f_{\theta}(z)$.

Numerical results

Figure below shows numerical the results with iFlow and iFlow-L in [Kothari-Khorashadizadeh-de Hoop-Dokmanic UAI 2021] when $Y = AX + \varepsilon$ and A is a down-sampling operator or a random mask.



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Definition (Neural operators, by Kovachki-Lanthaler-Mishra 2021) Let $D \subset \mathbb{R}^d$ is bounded open set. A neural operator is a function $F: L^2(D)^{n_0} \to L^2(D)^{n_k}, \quad F = \mathcal{L}_{k-1} \circ \mathcal{L}_k \circ \cdots \circ \mathcal{L}_0$ where layers $\mathcal{L}_\ell: L^2(D)^{n_\ell} \to L^2(D)^{n_{\ell+1}}$ are

$$\mathcal{L}_{\ell}(u)(x) = \sigma(W_{\ell}u(x) + K_{\ell}(u)(x)),$$

and $W_\ell \in C(\overline{D}, \mathbb{R}^{n_{\ell+1} imes n_\ell})$ and K_ℓ are non-linear integral operators

$$\mathcal{K}_{\ell}(u)(x) = \int_{D} k_{\ell}(x, y, u(x), u(y))u(y)dy,$$

where k_{ℓ} are bounded and C^3 -smooth (or a generalized function), and $\sigma : \mathbb{R}^n \to \mathbb{R}^n$ is pointwise activation function (e.g. a leaky relu).

A leaky relu is
$$\sigma_a(x) = \operatorname{relu}_a(x) = \begin{cases} x, x > 0, \\ ax, x \le 0, \end{cases}$$
 for $x \in \mathbb{R}, a \ge 0$.

Analogous continuous generative networks based on wavelets by Alberti, Santacesaria, and Sciutto 2022.

A non-linear operator $G: L^2(D)^n \to L^2(D)^n$ is coercive if $\lim_{\|u\|_{L^2(D)^n} \to \infty} \langle G(u), \frac{u}{\|u\|_{L^2(D)^n}} \rangle_{L^2(D)^n} = \infty.$

Theorem (de Hoop-Furuya-L.-Puthawala, NeurIPS 2023)

Let $\sigma : \mathbb{R} \to \mathbb{R}$ be surjective (e.g., a leaky relu), values of $W \in C^1(\overline{D}; \mathbb{R}^{n \times n})$ be invertible matrixes, and $K : L^2(D)^n \to L^2(D)^n$ be a non-linear integral operator with a C^3 -smooth kernel. Moreover, assume that the map $u \mapsto \alpha u + W^{-1}K(u)$ is coercive with some $0 < \alpha < 1$. Then, the operator

$$F: L^{2}(D)^{n} \to L^{2}(D)^{n},$$

$$F(u) = \sigma(Wu + K(u))$$

is surjective.

The proof is based on Leray-Schauder degree theory. If K is a non-linear Volterra operator, then $u \rightarrow Wu + K(u)$ is injective. Next we consider the case n = 1 and the non-linear integral operator

$$K(u)(x) := \int_D k(x, y, u(x))u(y)dy, \ x \in D.$$

Assume that

$$k(x,y,t) = \sum_{j=1}^{J} c_j(x,y)\phi(a_j(x,y)t + b_j(x,y)),$$

where ϕ is a wavelet activation function $\phi_{wire} : \mathbb{R} \to \mathbb{R}$, see Saragadam et al. 2023,

$$\phi_{wire}(t) = \operatorname{Im}\left(e^{i\omega t}e^{-t^2}\right),$$

and $a, b, c \in C(\overline{D} \times \overline{D})$, $a_j(x, y) \neq 0$. For $\alpha > 0$, the operators $u \mapsto \alpha u + W^{-1}K(u)$ are coersive and the operator

$$F: L^{2}(D) \to L^{2}(D),$$

$$F(u) = \sigma(Wu + K(u))$$

is surjective.

Let n=1 and $D\subset \mathbb{R}$ be a bounded interval. Let

$$F(u) = \sigma_a \circ G(u), \quad G(u)(x) = W(x)u(x) + \int_D k(x, y, u(y))u(y)dy,$$

where a > 0. Assume that $W \in C^1(\overline{D})$ satisfies $0 < c_1 \le W(x) \le c_2$ and

$$\|k\|_{C^{3}(\overline{D}\times\overline{D}\times\mathbb{R})} \leq c_{0}, \quad \|W\|_{C^{1}(\overline{D})} \leq c_{0}$$
(2)

and for all $u_0 \in H^1(D)$, the Frechet derivatives satisfy

$$DG|_{u_0}: H^1(D) o H^1(D)$$
 is an injective operator. (3)

Theorem (de Hoop-Furuya-L.-Puthawala, NeurIPS 2023)

Assume that F satisfies the above assumptions (2) and (3) and that $F : H^1(D) \to H^1(D)$ is a bijection. Let $\mathcal{Y} \subset \sigma_a(\overline{B}_{C^{1,\alpha}(\overline{D})}(0,R))$ where $\alpha > 0$. Then the inverse of $F : H^1(D) \to H^1(D)$ in \mathcal{Y} can written as a limit as a limit of integral neural operators having distributional kernels.

Idea of the proof

The inverse of $F = \sigma_a \circ G$ is $F^{-1} = G^{-1} \circ \sigma_{1/a}$. When w is sufficiently near to $w_j = G(u_j)$ in $H^1(D)$, the Banach fixed point theorem implies that

$$\begin{pmatrix} G^{-1}(w) \\ w \end{pmatrix} = \lim_{m \to \infty} \mathcal{H}_j^{\circ m} \begin{pmatrix} u_j \\ w \end{pmatrix},$$
$$\mathcal{H}_j \begin{pmatrix} u \\ w \end{pmatrix} = \begin{pmatrix} u - A_{u_j}^{-1}(G(u) - w) \\ w \end{pmatrix}, \quad A_{u_j} = DG|_{u_j}.$$

When we cover $\sigma_{1/a}(\mathcal{Y})$ with small neighborhoods of w_j in $H^1(D)$, and define a partition of unity Φ_j for these neighborhoods.

The operators $\Phi_j = \psi_{j,k} \circ \cdots \circ \psi_{j,1}$ are products operators of the form

$$\psi_{j,k} \begin{pmatrix} u \\ w \end{pmatrix} (x) = \begin{pmatrix} \int_D m_{j,k}(x, y, v(x), w(y)) dy \\ w(x) \end{pmatrix}$$

where $m_{j,k}(x, y, v(x), w(y)) = v(x) \mathbf{1}_{[s_{j,k}, s_{j,k}+h)}(w(y)) \delta(y - z_{j,k}).$

Idea of the proof

Combining the above operators, we have for $w \in \sigma_{1/a}(\mathcal{Y})$

$$\begin{pmatrix} G^{-1}(w) \\ w \end{pmatrix} = \lim_{m \to \infty} \sum_{j \in \mathcal{I}} \Phi_j \mathcal{H}_j^{\circ m} \begin{pmatrix} u_j \\ w \end{pmatrix}$$

Thus, $G^{-1}|_{\sigma_{1/a}(\mathcal{Y})}$ can be written as a limit of neural operators which kernels are generalized functions.

Summary

- Neural operators are generalization of neural networks where matrix multiplication is replaced by integral operators.
- Compactness of integral operators make it possible to analyze mapping properties of neural operators.
- Neural operators are non-linear operators which share some properties of pseudodifferential operators:
 - Neural operators and pseudodifferential operators are algebras
 - If pseudodifferential operator is invertible (more precisely, elliptic) then the inverse operator is a pseudodifferential operator.
 Similarly, if a neural operator is invertible then the inverse operator is a neural operator.

Thank you for your attention

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