

Lecture 5: Neural Operators 1, Background

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Some papers/books to look at

- Courant and Hilbert *Methods of mathematical physics Volumes 1,2*
- Stuart et. al. *Fourier Neural Operator for PDEs*
- Kovachi et. al. *Operator learning: algorithms and analysis*

Motivation: Solution Operators

Have studied using **PINNS** to solve PDE problems of the form

$$u_t = F(\mathbf{x}, u, \nabla u, \nabla^2 u) \quad \text{with BC,}$$

$$u(0, x) = u_0(x)$$

At time T we have the solution $u_T(x) \equiv u(x, T)$.

Solution $u(x, t)$ for all x and t is obtained by minimising a function directly associated with the PDE eg. residual.

Neural Operator methods take a different approach

- Consider u_T as a function F of u_0 . $u_T = F(u_0)$
- F is an operator mapping one infinite dimensional function space to another $F : A \rightarrow B$. eg. $A, B = H^1(\Omega)$
- Train a Neural Operator NN to approximate this operator note infinite dimensions
- Train it by generating a (large) set of solution pairs (u_0^i, u_T^i)

Can generate solution pairs using a (conventional) numerical method eg. Finite Element, Pseudo-Spectral, Symplectic.

eg. ERA5 data for 24 hour weather forecasts.

Example 1: A linear ODE system

Consider the linear ODE

$$\frac{d\mathbf{u}}{dt} = A \mathbf{u}, \quad \mathbf{u}(0) = \mathbf{u}_0, \quad \mathbf{u} \in R^n.$$

Solution

$$\mathbf{u}(T) = e^{A T} \mathbf{u}_0 \equiv B \mathbf{u}_0$$

$$B \equiv e^{AT} = I + AT + \frac{A^2 T^2}{2!} + \frac{A^3 T^3}{3!} + \dots$$

Properties of the solution operator

- Operator is linear
- Operator is continuous over any subset of R^n
- Can easily learn the matrix B from data pairs if we assume that the operator is linear in advance!
- If we learn B from a subset of the data pairs then we can extrapolate this to ALL data pairs
- This is NOT true if don't make the linearity assumption. Many NN methods will locally approximate the operator to be linear, but will not give this as a global approximation.

tanh and linear picture

Latent space description of the operator

Let A have eigenvectors ϕ_i so that

$$A \phi_i = \lambda_i \phi_i$$

Set $\mathbf{u} = \sum a_i(t) \phi_i$ then

$$\frac{d\mathbf{u}}{dt} = \sum \frac{da_i}{dt} \phi_i = \sum A u = \sum \lambda_i a_i \phi_i$$

so that

$$\frac{da_i}{dt} = \lambda_i a_i \implies a_i = a_i(0) e^{\lambda_i t}$$

Assume A is colorblue symmetric. Then can set

$$\phi_i^T \phi_j = \delta_{ij}$$

Hence

$$\mathbf{u}(T) = \sum \phi_i^T \mathbf{u}(0) e^{\lambda_i T} \phi_i.$$

Takes the form of

- **Encoder:** $\phi_i^T \mathbf{u}_0$.
- **Latent space evolution:** $e^{\lambda_i T}$
- **Decoder** Multiply by ϕ_i

We will mimic this structure in the design of Neural Operators eg.
Deep-O-Net

Example 2: Parabolic PDEs

Consider the **parabolic PDE** [picture]

$$u_t = u_{xx} + f(x), \quad x \in [0, 2\pi], \quad u(0, x) = u_0(x), \quad \textit{periodicBC}$$

We can express $u(x, t)$ in terms of **convolutional integral operators**:

$$u(x, t) = G * u_0 + H * f \equiv \int_0^{2\pi} G(x-y, t) u_0(y) dy + \int_0^{2\pi} H(x-y, t) f(y) dy$$

These operators act on the **infinite dimensional space** $L^2[0, 2\pi]$.

Can find $G(z, t)$ and $H(z, t)$ **explicitly** using a **Fourier series**.

This construction will motivate the construction, and use, of the FNO (Fourier Neural Operator) in the next Lecture

Fourier Series

As u and f are 2π periodic we can set:

$$u(x, t) = \sum_j c_j(t) e^{ijx}, \quad f(x) = \sum_j f_j e^{ijx},$$

Substituting into the PDE we have

$$\frac{du_j}{dt} = -j^2 u_j(0) + f_j,$$

with

Hence

$$c_j(T) = e^{-j^2 T} \left(c_j(0) - \frac{f_j}{j^2} \right) + \frac{f_j}{j^2}, \quad c_0(T) = c_0(0) + f_0 T$$

with

$$c_j(0) = \frac{1}{2\pi} \int_0^{2\pi} e^{-ijy} u_0(y) dy, \quad f_j = \frac{1}{2\pi} \int_0^{2\pi} e^{-ijy} f(y) dy.$$

Hence

$$u(x, T) = \int_0^{2\pi} \frac{1}{2\pi} \sum_j e^{ij(x-y)} e^{-j^2 T} u_0(y) dy \\ + \int_0^{2\pi} \frac{1}{2\pi} \sum_j e^{ij(x-y)} j^{-2} f(y) dy + \dots$$

So we can see that this has the correct integral form with

$$G(z, T) = \sum_j \frac{1}{2\pi} e^{-j^2 T} e^{ijz}, \quad H(z, t) = \sum_j \frac{1}{2\pi} j^{-2} e^{ijz} + \dots$$

Trivially $G(z, T)$ has Fourier Coefficients

$$G_j = \frac{1}{2\pi} e^{-j^2 T}.$$

Learning G and H

- Suppose for a fixed $f(x)$ we have lots of solution pairs $(u_0^k(x), u_T^k(x))$ ($k = 1..N$ random set)
- Use FFT to find the Fourier coefficients $u_0^k \rightarrow u_0^{k,j}, u_T^k \rightarrow u_T^{k,j}, f \rightarrow f_j$
- For each j find the FCs of G and H by solving the minimisation problem

$$(G_j, H_j) = \operatorname{argmin}_k \|G_j u_0^{k,j} + H_j f_j - u_T^{k,j}\|$$

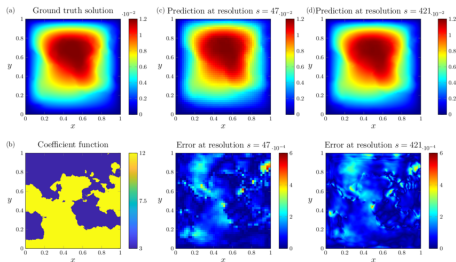
This motivates the construction of the **Fourier Neural Operator (FNO)** in the next lecture.

Example 3: Darcy Problem

The Darcy problem relates a permeability $a(x)$ to a velocity field $u(x)$

$$-\nabla \cdot (a(x) \nabla u) = f(x) \quad x \in \Omega, \quad u = 0 \quad x \in \partial\Omega.$$

This induces a (nonlinear) map $N : a \rightarrow u$, $N : L^2(\Omega) \rightarrow H_0^1(\Omega)$



We can approximate this map using the **Finite Element Method**

$$u(x) \approx U(x) = \sum U_i \phi_i(x).$$

$$-\nabla \cdot (a(x) \nabla u) = f \implies \int a(x) \nabla u(x) \cdot \nabla \phi_i(x) dx = \int f(x) \phi_i(x) dx \equiv f_i$$

Giving the **linear system**

$$\mathbf{AU} = \mathbf{f}, \quad \mathbf{U}_i = U_i, \quad \mathbf{f}_i = f_i, \quad A_{ij} = \int a(x) \nabla \phi_i \cdot \nabla \phi_j dx.$$

Hence we can approximate the nonlinear map via:

$$\mathbf{U} = \mathbf{A}^{-1} \mathbf{f}$$

And ...

We can **LEARN** this map by

- Doing lots of finite element calculations to find solution pairs $(a(x), u(x))$
- Learn the operator between these pairs (see next lecture).

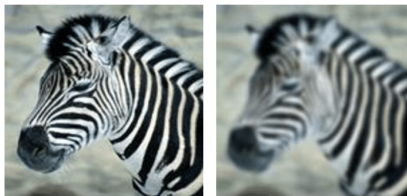
Pictures

In **image processing** a picture is often thought of as a high dimensional vector $\mathbf{z} \in R^n$.

Can also think of it as a **function** $f(x, y) : R^2 \rightarrow R$. Image processing is then an **operation** on an infinite dimensional **function space**.

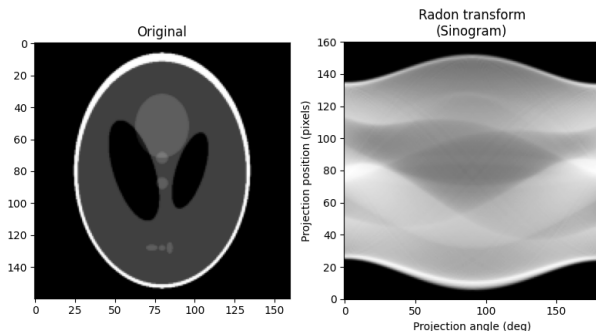
Example 1: Blurring

$$f \rightarrow G * f(x, y) = \int \int G(x - x', y - y') f(x', y') dx' dy'$$



Example 2: Radon Transform in Tomography

$$f(x, y) \rightarrow Rf(\theta, d) = \int f((z \sin(\theta) + d \cos(\theta)), (-z \cos(\theta) + d \sin(\theta))) dz$$



Methods such as FNO work as much as possible in the infinite-dimensional function space.

They Construct and train Neural Operators which are **approximations to the true operator (or its inverse)** which are **independent of the resolution of the underlying function/image**

Nonlinear problems and a warning

Consider now the nonlinear parabolic PDE

$$u_t = u_{xx} + f(x, u), \quad u(0) = u(1) \quad u(0, x) = u_0(x)$$

This does not always induce a continuous map from $u(0, x) \rightarrow u(1, x)$.

- If $f(x, u)$ is Globally Lipschitz in x and u then all is OK
- If not then we may have problems
- See Case Study One!

Example

Let

$$f(x, u) = u^2, \quad u_0(x) = \gamma > 0$$

Then

$$u(1, x) = \frac{\gamma}{1 - \gamma}.$$

Map is only continuous on the interval $\gamma \in [0, 1)$

If we train only on data with $\gamma < 1$ we will get a false result if we try to extend to $\gamma > 1$.

Case Study: Learning the Green's function of a linear elliptic operator

[Boullé + Townsend: <https://arxiv.org/pdf/2102.00491>]

If we have an elliptic PDE

$$-\Delta u = f(\mathbf{x}), \quad \mathbf{x} \in \Omega, \quad u = 0 \quad \mathbf{x} \in \partial\Omega$$

then there exists a Green's function $G(\mathbf{x}, \mathbf{y})$ so that

$$u(\mathbf{x}) = G * f \equiv \int_{\Omega} G(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y}.$$

$$G : C^{\alpha} \rightarrow C^{2,\alpha} \quad \text{Hölder Spaces}$$