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AI for Partial Differential Equations (PDEs) and Neural Operators

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My Work: AI for Science (AI4Sci)

AI4Sci refers to the use of recent advances in artificial intelligence and deep learning to solve problems in natural sciences: computational chemistry, PDEs, material science, drug design, etc..

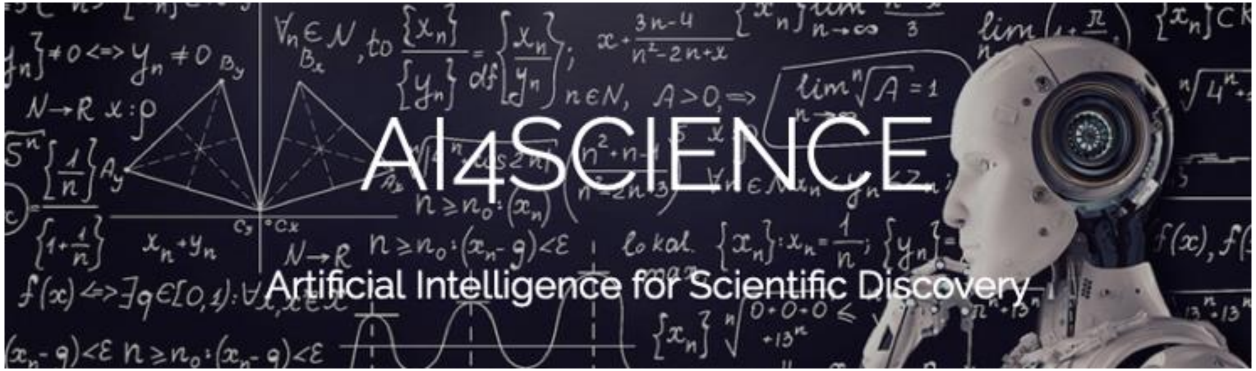

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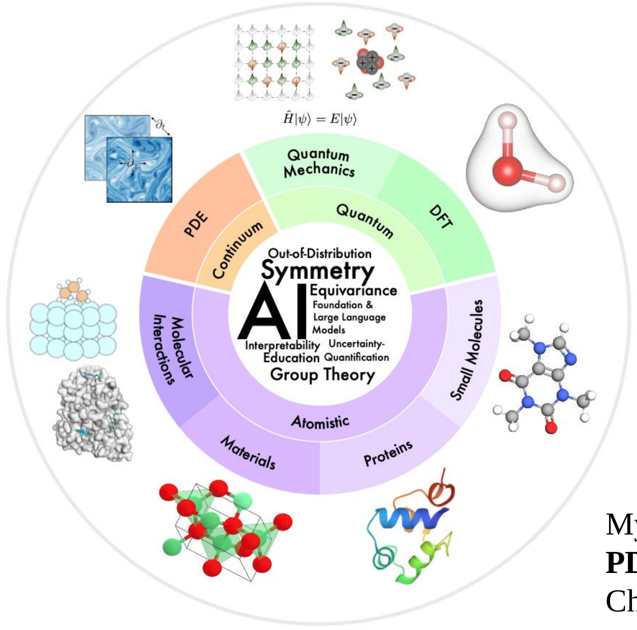
Image Source: My advisor, Dr. Yi Liu.

My Work: AI for Science (AI4Sci)



Key mission:

- How to properly (and efficiently) integrate domain knowledge in science (such as symmetry) into AI models.
- Developing new AI models that involve innovations in both AI and science.

Other perspectives:

- Explainability
- Out-of-distribution generalization
- Large language models
- Uncertainty estimation

My research in general focuses on AI for Science, particularly **AI for solving PDEs**, **symmetries in AI models**, and **applications** in Computational Physics, Chemistry, and Biology (e.g., **molecular property prediction, drug design, molecular dynamics**).

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Image Source: My advisor, Dr. Yi Liu.

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My Work: AI for Science

My recent work in AI for Science focuses on three main topics:

- ❑ AI for PDEs: Efficiently solving partial differential equations accelerates simulations in physics and engineering applications.
- ❑ Equivariant Neural Networks: The nature is full of symmetries. Preserving symmetries in models improves generalization and reduces data requirements for scientific problems.
- ❑ Generative Models: Many scientific tasks require generation such as generating new proteins.

I’m also broadly interested and have done works in:

- ❑ Explainability in AI Models: Understanding model decisions ensures trust and interpretability in critical scientific domains.
- ❑ Large Language Models: LLMs aid in scientific discovery to serve as a bridge between domain experts and AI scientists.

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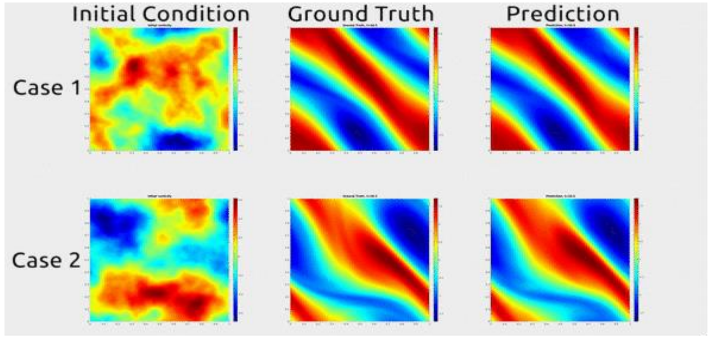
Today’s Talk: PDEs and Neural PDE Solvers

A PDE mathematically describes the behavior of a system by prescribing constraints relating partial derivatives.

Example: The Wave Equation $\frac{\partial^2 u}{\partial t^2} = D\nabla^2 u,$ where D is the diffusion coefficient. We can visualize, by solving the PDE, a disturbance in the medium which will then propagate in all directions.

Or the famous Navier-Stokes Equation.



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Traditional PDE solvers

- Solve one instance
- Require the explicit form
- Speed-accuracy trade-off on resolution
- Slow on fine grids; fast on coarse grids
- Suffers from the Curse of Dimensionality (CoD)

PINN

- Solve one instance
- Incorporate known physics
- Can train without data
- Mesh-free
- Can be slow to train
- Lessen the CoD issue

Neural Operator PDE solver

- Learn a family of PDEs
- Compatible with physics-informed ideas
- Black-box, data-driven
- Can be resolution-invariant
- Slow to train; fast to evaluate (can be several orders of magnitudes faster)
- Many neural operators suffer from CoD

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PINNs (Solving One Instance)

Consider the following general form of a PDE for $u(\boldsymbol{x})$:

$$\begin{cases} \mathcal{D}u(\boldsymbol{x}) = f(\boldsymbol{x}), & \text{in } \Omega, \\ \mathcal{B}u(\boldsymbol{x}) = g(\boldsymbol{x}), & \text{on } \partial\Omega, \end{cases}$$

we wish to approximate $u(\boldsymbol{x})$ with a neural network, denoted by $\phi(\boldsymbol{x};\boldsymbol{\theta})$. We can train the neural network with physics-informed loss. That is, we aim to solve the following optimization problem:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) : = \arg\min_{\boldsymbol{\theta}} \underbrace{\|\mathcal{D}\phi(\boldsymbol{x};\boldsymbol{\theta}) - f(\boldsymbol{x})\|_2^2}_{\text{Difference between the L.H.S. and R.H.S. of the differential equation.}} + \lambda\|\mathcal{B}\phi(\boldsymbol{x};\boldsymbol{\theta}) - g(\boldsymbol{x})\|_2^2$$

Intuition: We penalize the neural network by the extend to which it violates the PDE/boundary/initial conditions.

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Neural Operators (Solving a Family of PDEs)

- In numerous fields, we seek to **study the behavior of physical systems under various parameters**, such as different initial conditions, boundary values, and forcing functions.
- Neural operators approximate the mapping from parameter function space to solution function space.
- Once trained, obtaining a solution can be several orders of magnitude faster than numerical methods.

Function: A function is a mapping between **finite-dimensional** vector spaces.

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu k}{\sigma}\right)^2}, x \in \mathbf{R}.$$

Operator: An operator is a mapping between in**finite-dimensional** function spaces.

$$G(f(x)) = u(x).$$

Examples: Derivative Operator, Nabla Operator, Differential Operator, Integral Operator, etc..

A neural operator refers to the use of neural networks to approximate or learn an operator in infinite-dimensional function spaces.

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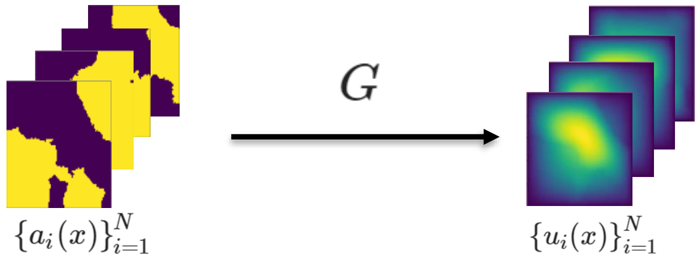
Parametric PDEs and the Learning Task

Consider a parametric PDE of the form:

$$\begin{aligned} \mathcal{N}(a,u)(x) &= f(x), \qquad && x \in \Omega \\ u(x) &= 0, && x \in \partial\Omega \end{aligned}$$

where $\Omega \subset \mathbb{R}^d$ is a bounded open set, $\mathcal{N}$ is a, possibly non-linear, differential operator, a is the parametric input function, f is a given fixed function in an appropriate function space determined by the structure of $\mathcal{N}$, and u is the PDE solution. A concrete example of $\mathcal{N}(a,u)(x) = f(x)$ can be $u(x)u_x(x) - a(x)u_{xx}(x) = f(x)$.

The PDE solution operator is defined as $G(a) = u$. We are interested in learning the operator $G(\cdot)$ through a given finite collection of observations of input-output pairs $\{a_j, u_j\}_{j=1}^N$, where each a_j and u_j are functions, in practice, that come with a discretization.



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Summary of Operator Learning Task

- Domain
  - $\Omega \subset \mathbb{R}^d$ be a bounded open set of spatial coordinates
- Input and output function spaces on Ω (e.g., Banach spaces, Hilbert spaces)
  - $\mathcal{A}$ and $\mathcal{U}$
- Ground truth solution operator
  - $G : \mathcal{A} \to \mathcal{U}$ with $G(a) = u$
- Training data
  - Observed (possibly noisy) function pairs $(a_i, u_i) \in \mathcal{A} \times \mathcal{U}, u_i = G(a_i)$ with measures $a_i \sim \nu_a, u_i \sim \nu_u$, where ν_u is the pushforward measure of ν_a by G
- Task: Learn operators from data
  - $G_\theta(a) \approx u$

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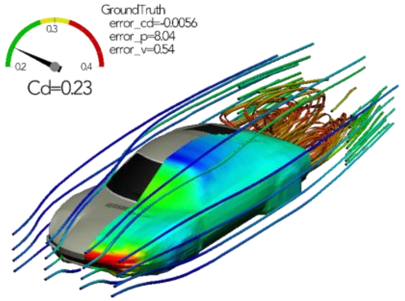
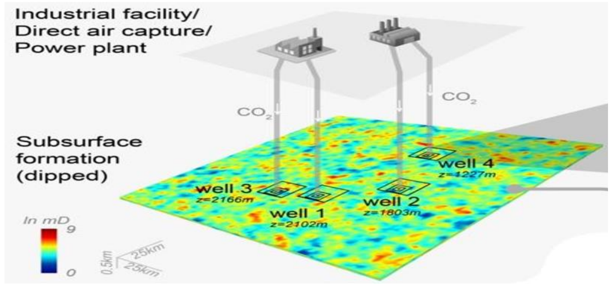
Applications of Operator Learning





Computational Fluid Dynamics [a]

Carbon Storage Modeling [b]

Weather Modeling [c]

[a] Geometry-informed neural operator for large-scale 3D PDEs. arXiv, 2023. Zongyi Li, et al..
[b] Fourier-MIONet: Fourier-enhanced multiple-input neural operators for multiphase modeling of geological carbon sequestration. arXiv, 2023. Zhongyi Jiang, et al..
[c] DeepPhysiNet: Bridging deep learning and atmospheric physics for accurate and continuous weather modeling. arXiv, 2024. Wenyuan Li, et al..

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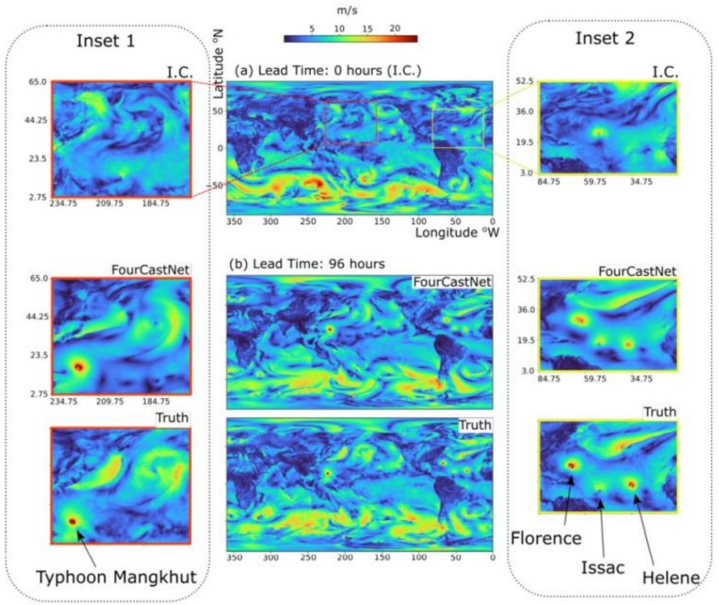
Weather Forecasting: FourCastNet



Pathak et al. (2022), FourCastNet: A Global Data-driven High-resolution Weather Model using Adaptive Fourier Neural Operators, arXiv: https://arxiv.org/abs/2202.11214

- Motivation: **Climate change** is making storms both stronger and less predictable, leading to more frequent natural disasters.
- Task: **Emulate the dynamics of global whether patterns** and predict extreme whether events like atmospheric rivers.
- Training Data: 10TB of earth system data from the past.
- Input: The current state of atmospheric fields.
- Result: **Predict the precise path of catastrophic atmospheric rivers a full week in advance**, with only a fraction of a second on powerful GPUs.

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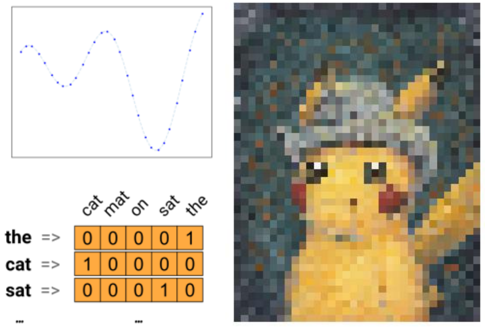
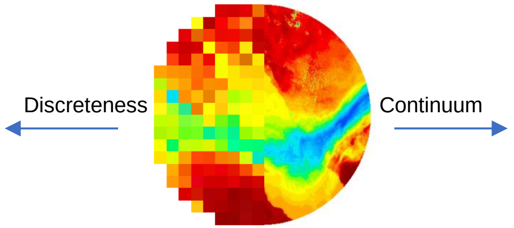
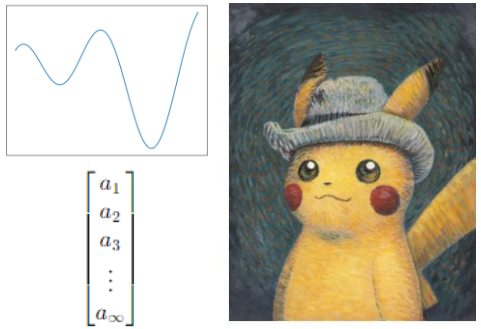
A Challenge in Operator Learning

Deep neural networks can only take finite-dimensional inputs and produce finite-dimensional outputs: $\phi_{\text{network}} : \mathbb{R}^{d_{in}<\infty} \mapsto \mathbb{R}^{d_{out}<\infty}$



		cat	mat	on	sat	the
the	=>	0	0	0	0	1
cat	=>	1	0	0	0	0
sat	=>	0	0	0	1	0
...		...				





Finite-dimensional Features

Infinite-dimensional Features

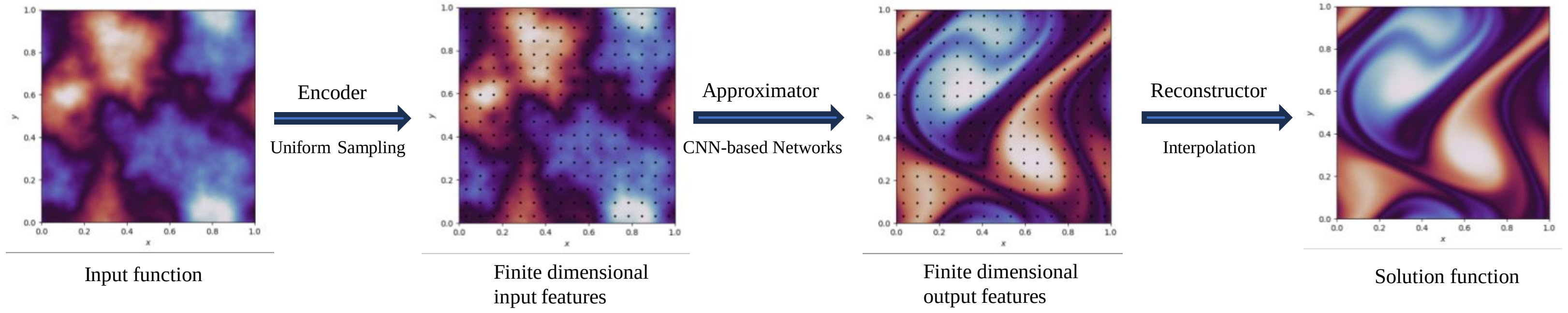
There are different ways of thinking about this challenge and approaching the design of neural operators:

- ❑ Finite-dimensional Learning: Following the same workflow as numerical schemes, functions are encoded into finite-dimensional features.

- ❑ Infinite-dimensional Learning: Extending the concept of linear layers in deep neural networks to infinite-dimensions.

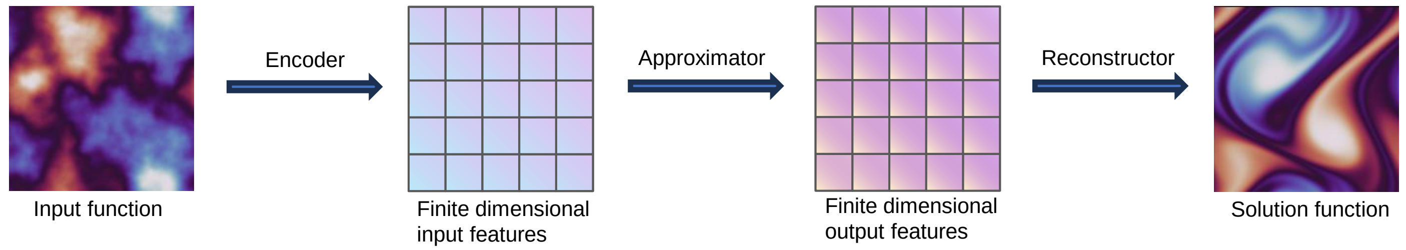
Finite-Dimensional Features and Learning

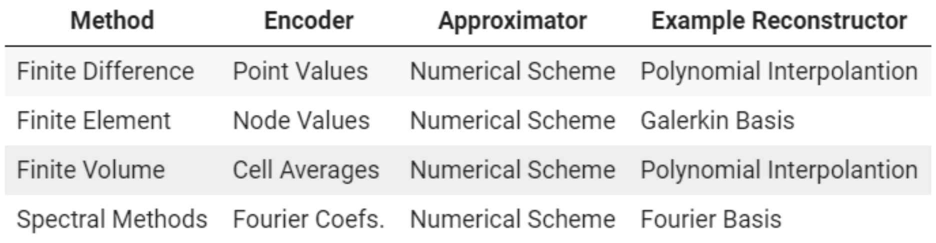
To adapt neural networks to learn operators, a workaround is to use **a simplified setting in which functions are characterized by finite-dimensional features.**



Finite-Dimensional Features and Learning

Many numerical schemes can be represented by this diagram as well:


Input function
Encoder
Finite dimensional input features
Approximator
Finite dimensional output features
Reconstructor
Solution function



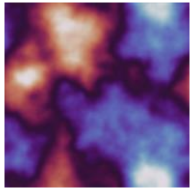
Method	Encoder	Approximator	Example Reconstructor
Finite Difference	Point Values	Numerical Scheme	Polynomial Interpolantion
Finite Element	Node Values	Numerical Scheme	Galerkin Basis
Finite Volume	Cell Averages	Numerical Scheme	Polynomial Interpolantion
Spectral Methods	Fourier Coefs.	Numerical Scheme	Fourier Basis

How we make choices of encoders, decoders, and approximators gives rise to different neural operators. Moreover, different choices may lead to different properties or various pros and cons for a particular neural operator.

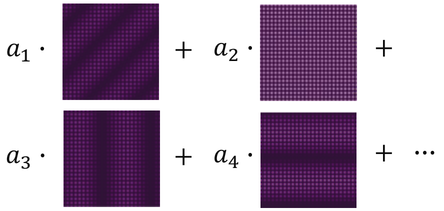
Neural Operator Instantiation: Spectral Neural Operator

(Generalized) Spectral neural operators [1] encodes a function as function coefficients with respect to a predefined function basis such as Fourier, Chebyshev, etc..
Given appropriate bases, under fairly general assumptions, function can be written in function series forms: $f = \sum_{i=0}^{\infty} c_i f_i$

Encoder:

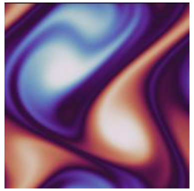

Input function

=

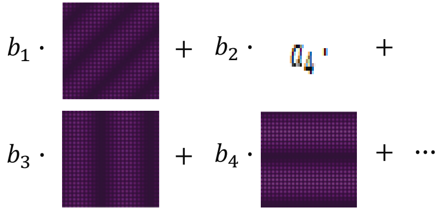


Coefs. with respect to a given basis

Reconstructor:


Solution function

=

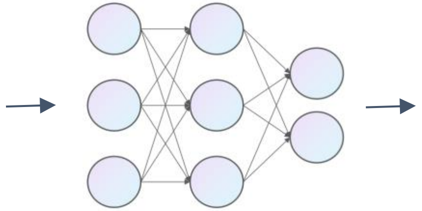


Coefs. with respect to a given basis

Approximator:

a_1
a_2
a_3
a_4
…
a_m

Input Coefs.



b_1
b_2
b_3
b_4
…
b_n

Output Coefs.

[1] Spectral neural operators. arXiv, 2022. V. Fanasko and I. Oseledets.

Neural Operator Instantiation: DeepOnet

Spectral Neural Operators specifies the function bases. However, this requirement can pose limitations from a data-driven standpoint. DeepOnet [2] is an architecture, based the universal approximation theorem for operators [3], that can overcome this limitation by **learning some function basis**.

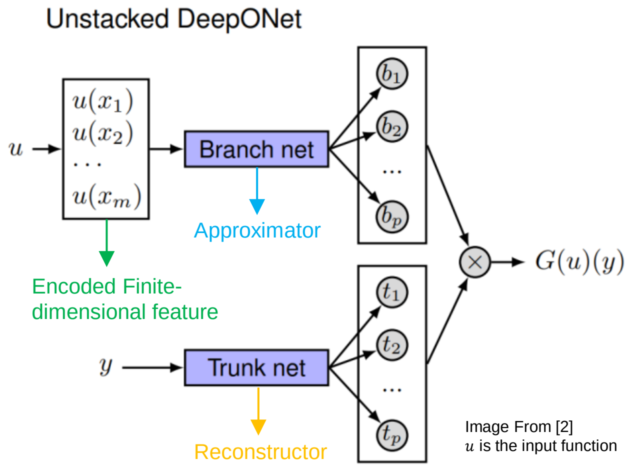


Image From [2]
u is the input function

Encoder	Point Values
Approximator	Neural networks that map fixed sensor point values to coefficients
Decoder	Neural networks that map an inference coordinate point to basis function values at these points

The learned solution function is given by:

$$f(y) \approx G(u)(y) = \sum_{i=0}^{p} b_i \tau_i(y) = \sum_{i=0}^{p} b_i t_i$$

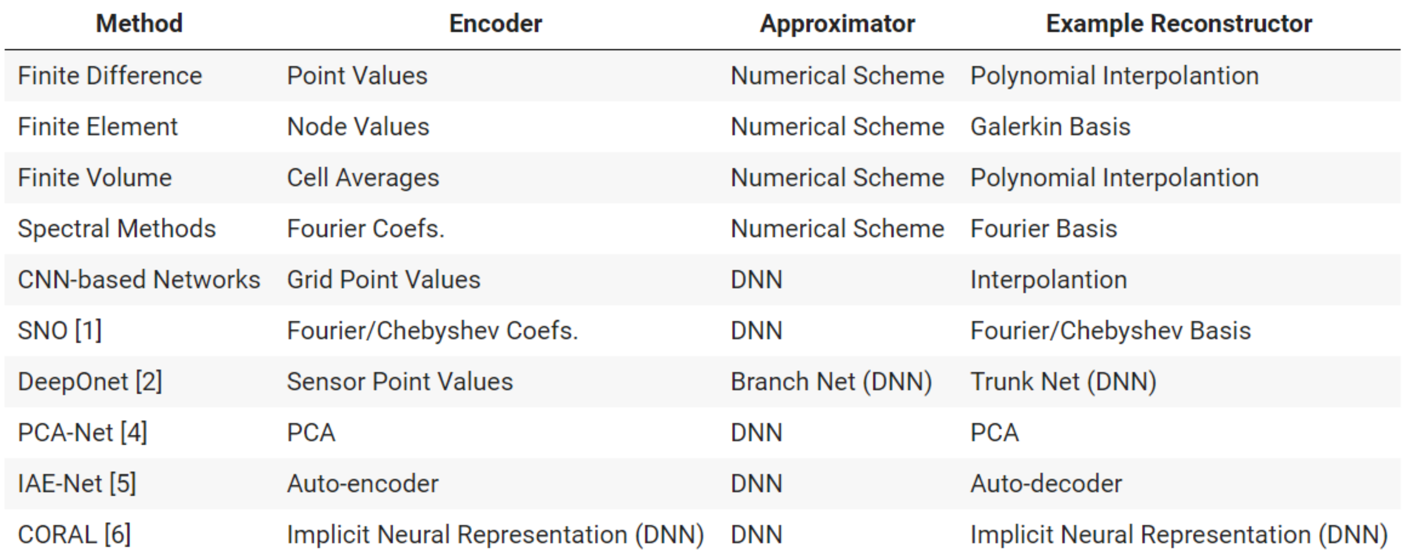
where $\{\tau_i\}_{i=1}^{p}$ are p basis function learned by the trunk network.

Thus, DeepOnet takes in function values at fixed locations, but we can infer the learned solution function at any point in the domain.

[2] Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators. NMI, 2021. Lu Lu, Pengzhan Jin, Guofei Pang, Zhongqiang Zhang, and George Em Karniadakis.
[3] Universal approximation to nonlinear operators by neural networks with arbitrary activation functions and its application to dynamical systems. Chen T, Chen H.

Finite-Dimensional Learning: Summary

There have been a lot of work done in this direction, and to name a few: PCA-Net [4], IAE-Net [5], and CORAL [6].



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Finite Volume	Cell Averages	Numerical Scheme	Polynomial Interpolantion
Spectral Methods	Fourier Coefs.	Numerical Scheme	Fourier Basis
CNN-based Networks	Grid Point Values	DNN	Interpolantion
SNO [1]	Fourier/Chebyshev Coefs.	DNN	Fourier/Chebyshev Basis
DeepOnet [2]	Sensor Point Values	Branch Net (DNN)	Trunk Net (DNN)
PCA-Net [4]	PCA	DNN	PCA
IAE-Net [5]	Auto-encoder	DNN	Auto-decoder
CORAL [6]	Implicit Neural Representation (DNN)	DNN	Implicit Neural Representation (DNN)

[4] Model Reduction And Neural Networks For Parametric PDEs. The SMAI Journal of computational mathematics, Volume 7 (2021), pp. 121-157. Kaushik Bhattachary et al..
[5] Integral autoencoder network for discretization-invariant learning. JMLR, 2022. Yong Zheng Ong, Zuowei Shen, and Haizhao Yang
[6] Operator learning with neural fields: Tackling PDEs on general geometries. arXiv, 2023. Louis Serrano, et al..

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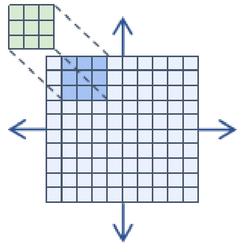
Infinite-Dimensional Learning: Introduction

For some of the methods we previously discussed, such as DeepOnet and CNN-based models, the network is **highly dependent on the resolution of the data and/or sensor locations**.



In CNN-based methods, fixed size kernels converge to a point-wise operator as the resolution increases.

Another perspective on operator learning is to think in terms of the continuum. Since we are learning an operator, the network should be independent of the discretization of the input and output functions, and the learned parameters should be transferable between discretizations.

In this perspective, we parameterize the model in infinite-dimensional spaces, so it learns continuous functions instead of discretized vectors.

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Motivation: Green's Function Method

Under fairly general conditions on $\mathcal{L}_a$, a linear differential operator, we may define the Green's function $G : \Omega \times \Omega \to \mathbb{R}$, where Ω is the domain of the PDE, as the unique solution to the problem

$$\mathcal{L}_a G(x, \cdot) = \delta_x$$

where δ_x is the delta measure on $\mathbb{R}^d$ centered at x. Note that G will depend on the coefficient a thus we will henceforth denote it as G_a.

Then operator $\mathcal{F}_{\text{true}}$ can be written as an integral operator of green function:

$$u(x) = \int_\Omega G_a(x, y) f(y) dy.$$

Here, the green function is called the kernel of the integral operator. We can verify that the integral operator of green function gives the solution.

$$\begin{aligned}(\mathcal{L}_a u)(x) &= \int_\Omega (\mathcal{L}_a G(x, \cdot))(y) f(y) dy \\ &= \int_\Omega \delta_x(y) f(y) dy \\ &= f(x)\end{aligned}$$

Generally the Green's function is continuous at points $x \neq y$, for example, when $\mathcal{L}_a$ is uniformly elliptic. Hence it is natural to model the kernel via a neural network κ. Just as the Green function, the kernel network κ takes input (x, y). Since the kernel depends on a, we let κ also take input $(a(x), a(y))$.

$$u(x) = \int_D \kappa(x, y, a(x), a(y)) f(y) dy.$$

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Kernel Integral Operators

In a standard deep neural network, a layer can be written as:

$$\text{Input: } v_t \longrightarrow \text{Linear Transformation: } W^T v_t + b \longrightarrow \text{ Non-linearity } \longrightarrow \text{ Output: } v_{t+1}$$

Here the input, v_t, and the output, v_{t+1}, are both vectors.

However, we wish to learn continuous functions instead of discretized vectors. We need to adjust the formulation of our linear layers as it must be able to **take functions as input**:

$$v_t(x) \longrightarrow \text{Integral Linear Operator: } \int \kappa(x,y) v_t(y) dy + b(x) \longrightarrow \text{ Non-linearity } \longrightarrow v_{t+1}(x)$$

Integral operators take functions as inputs and produce functions as outputs. Integral operators are discretization-invariant as numerical integration which will converge, under fairly general conditions, to the true integral.

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Kernel Integral Operators: GNO

Assuming a uniform distribution of y, the integral can be approximated by a discrete sum

$$v(x) = \int \kappa(x,y)v(y)dy \approx \frac{1}{|N(x)|}\sum_{y_i \in N(x)} k\left(x, y_i\right) v\left(y_i\right).$$

$N(x)$ denotes the neighbors of x. If we construct a graph based on the physical domain using these sensor points, this integration **can be viewed as message passing** on the graph. Graph Neural Operator [7] has been developed with this perspective in mind.

For the full integration, the graph is a n^2 fully connected graph, we may redefine the connectivity to make it more efficient:

$$\frac{1}{|B(x,r)|}\sum_{y_i \in B(x,r)} k\left(x, y_i\right) v\left(y_i\right)$$

Here $B(x,r)$ defines the neighbors of x to be within a certain radius r for connectivity.

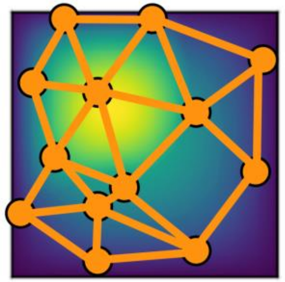
Image Source: https://zongyi-li.github.io/blog/2020/graph-pde/

[7] Neural operator: Graph kernel network for partial Differential equations. arXiv, 2020. Zongyi Li, et al..

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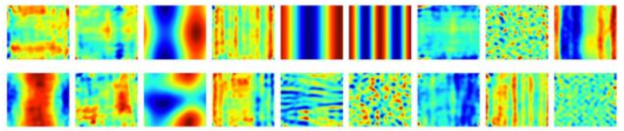
Kernel Integral Operators: FNO

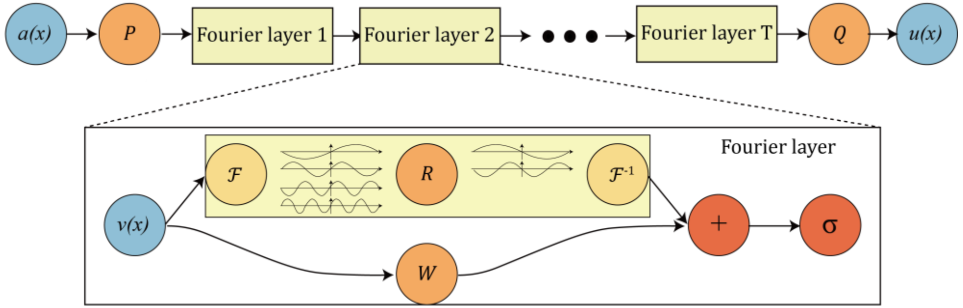
While GNO may encounter challenges related to computational complexity and accuracy, FNO, another widely recognized kernel integral operator [8], stands out for its **efficiency and precision**.

Integral Linear Operator	$\int \kappa(x, y) v(y) dy$
Convolution Operator	$\int \kappa(x - y) v(y) dy$
Solving Convolution in Fourier domain	$\mathcal{F}^{-1}(\mathcal{F}(\kappa) \cdot \mathcal{F}(v))$

"Filters in convolution neural networks are usually local. They are good to capture local patterns such as edges and shapes. Fourier filters are global sinusoidal functions. They are better for representing continuous functions."

Filters in CNN


Fourier Filters



[8] Fourier neural operator for parametric partial differential equations. ICLR, 2021. Zongyi Li, et al..
Image Source: Stanford CS159: Representation Learning for Science

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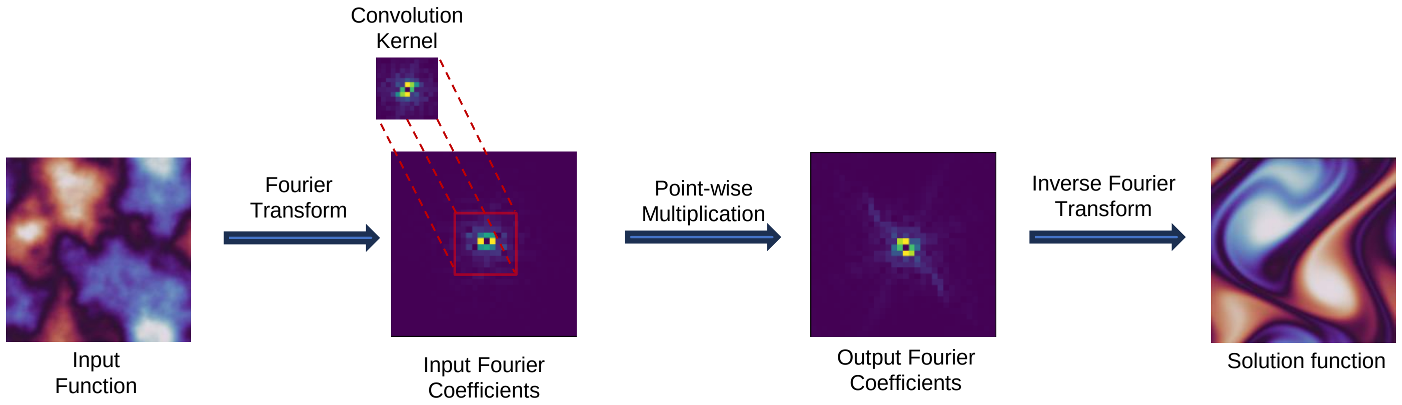
Kernel Integral Operators: FNO

Why Fourier:

1. Whereas approximating the full integral incurs a complexity of $O(n^2)$, the Fast Fourier Transform (FFT) operates with a complexity of $O(n \cdot \log n)$.
2. We can learn the kernel in the Fourier domain directly (convolution is point-wise multiplication in frequency domain).
3. Fourier transform is discretization invariant.
4. By using an orthogonal basis (Fourier) to represent the data, we can facilitate information compression, thereby further enhancing efficiency.


Convolution Kernel
Fourier Transform
Point-wise Multiplication
Inverse Fourier Transform
Input Function
Input Fourier Coefficients
Output Fourier Coefficients
Solution function

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