# ECE 228 Spring 2025 Lecture 13: Neural Operators Part 1

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# Neural ODEs introduced us to this idea of learning continuous representations. How can we take this further?

Recall that Neural ODEs learn the flow field $f$ of a dynamical system

$$\frac{dz(t)}{dt} = f(z(t), t; \theta), \quad z(0) = \bar{z}_0 .$$

This is the first type of continuous learning representation we have discussed. However, there's more to be explored here. NeuralODEs require us to build a set of points $t \in [0, T]$ to learn the solution of which we use the final output time $T$.

> **Motivating question:** How can we design neural architectures that we can query at any time (or for PDEs, any space) location?

# First a little history: How do we simulate PDEs (See homework 3)

1. **Start with a PDE:**
$$\frac{\partial u}{\partial t} = \mathcal{F}(u, \nabla u, \nabla^2 u, \ldots)$$
This represents the evolution of a physical quantity $u$.

2. **Discretize Space and Time:** Replace continuous space/time with a grid:
$$x_0, x_1, \ldots, x_N \quad \text{and} \quad t_0, t_1, \ldots, t_M$$

3. **Approximate Derivatives:** Use finite differences, finite volumes, or finite elements to approximate spatial and temporal derivatives.

4. **Step Forward in Time:** Update the solution using a time-stepping method (e.g., Euler, Runge-Kutta).

5. **Repeat:** Continue iterating until the final time is reached.

# History: Key limitation of numerically simulating PDEs

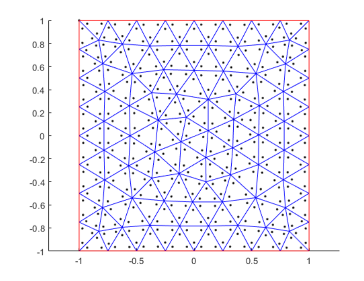



Figure: Example of a triangle mesh for a PDE.

- **Fixed Resolution:** Simulations are restricted to predefined spatial and temporal grid points. Fine grids increase accuracy but also computational cost and can lead to millions of simulation points

- **Poor Generalization:** Traditional solvers compute solutions only at grid points they're run on. New parameters require *re-running the simulation from scratch*.

# How do we *classically* solve PDEs?

Take the simplest PDE (1D transport):

$$
\begin{aligned}
\frac{\partial u(x,t)}{\partial t} &= \frac{\partial u(x,t)}{\partial x}\,, \quad x \in (0,1), t \in \mathbb{R}^+\,,\\
u(x,0) &= f(x)\,,\\
u(t,0) &= 0\,.
\end{aligned}
$$

This PDE just shifts the initial condition with space and time.

# Example of a transport PDE

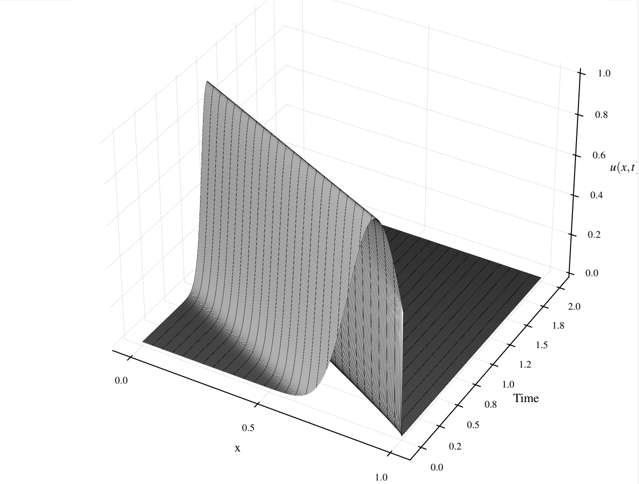



Figure: Transport PDE with Gaussian initial condition centered at $x = 0.9$.

# How do we *classically* solve PDEs?

Can apply Euler's method:

$$\frac{\partial u(x,t)}{\partial t} \approx \frac{u(x,t+\delta t) - u(x,t)}{\delta t} + \mathcal{O}(\delta t^2)\,,$$
$$\frac{\partial u(x,t)}{\partial x} \approx \frac{u(x+\delta x,t) - u(x,t)}{\delta x} + \mathcal{O}(\delta x^2)\,,$$

Combining yields the **finite difference** scheme

$$u(x,t+\delta t) = u(x,t) + \frac{\delta t}{\delta x}\left(u(x+\delta x,t) - u(x,t)\right)$$

where we impose the conditions

$$u(x,0) = f(x)\,,$$
$$u(t,0) = 0\,.$$

Then, to simulate until say $T = 5$, we just recursively run the above calculation until our desired timestep is reached.

# PDE solvers get very expensive very quickly

Unlike Euler's method for ODEs, PDE solvers become computationally costly extremely quickly.

- This is due to the fact we have both a spatial and temporal component, and thus we need to solve this PDE across both space and time.
- Furthermore, As with ODE's we require the step sizes $\delta x$ and $\delta t$ to be small. A reasonable choice is $\delta x = 0.01$ and $\delta t = 0.0005$ (for most numerical scheme $\delta t \ll \delta x$ as discussed in your homework).
- Then, to solve to $T = 5$, we require $(1/\delta x + 1) \times (5/\delta t + 1) = 1,010,101$ points of evaluation.

# Solving computationally becomes much worse as dimension scales

Consider the Navier Stokes PDE in 2D.

- For 1D, to solve to $T = 5$, we require $(1/\delta x + 1) \times (5/\delta t + 1) = 1,010,101$ points of evaluation.
- For 2D, to solve to $T = 5$, we require $(1/\delta y + 1) \times (1/\delta x + 1) \times (5/\delta t + 1) = 10,211,201$ points.
- For 3D, for $T = 5$, we rquire a billion points $(1,031,331,301)$ which is not possible on everyday machines.

Figure: Sierra supercomputer in Livermore California.

# How can we design a machine learning model that can learn PDE solutions and be queried at any grid location?

**Answer:** Design a machine learning model using *continuous representations*.

To do so, we need to introduce the mathematical notion of an **operator**. One reasonable viewpoint is too look at an operator as an abstraction of functions. That is, functions map vectors to vectors:

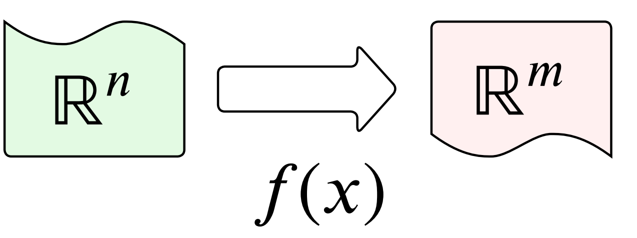



Figure: The function $f$ take an input vector $x \in \mathbb{R}^n$ and maps to an output vector in $\mathbb{R}^m$.

# What is an operator?

Now, imagine we considered a set of functions, for example all polynomials of degree 2 or all sin function of the form $f(x) = A\sin(Bx + C)$ where $A, B, C$ can very. Then, like a function that maps vectors to vectors, an operator maps *functions to functions:*

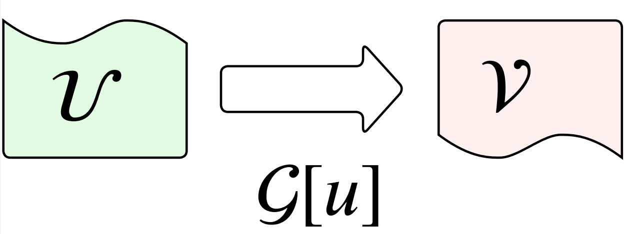
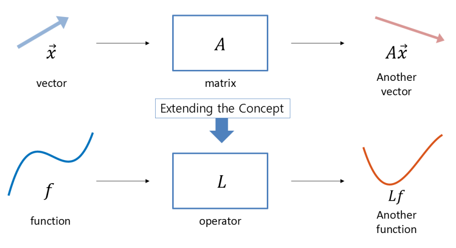



Figure: Let $\mathcal{U}$ be a set of functions and $\mathcal{V}$ be another set of functions. Then the operator $\mathcal{G}$ takes a function in $u \in \mathcal{U}$ and maps it to a function $v \in \mathcal{V}$.

# Examples of operators

You all (Y'all for the southerners) know many types of operators. Perhaps, the most famous are:

- The matrix multiplication $A$ is *linear* operator:




- The integral operator. Let $f \in \mathcal{F}$ and $g \in \mathcal{G}$, then the integral acts as

$$g = \int f(x)dx \,.$$

- Analogously the derivative of a function is an operator.
- Another operator is the shift operator. Given a parameter $c$, it acts as:

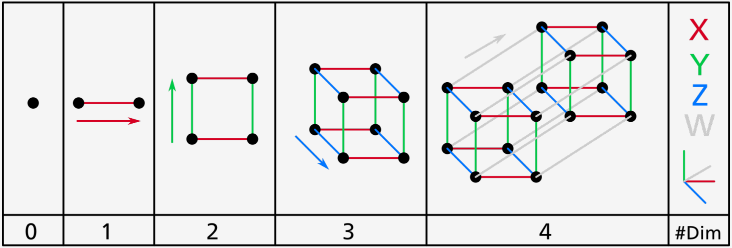
$$g(x) = \mathcal{G}[f](x) = f(x+c)$$

# An important property of vector spaces

In vector spaces, we had this important structure of dimension which essentially told us:

- We need exactly $d$ linearly independent vectors to create any vector in the space (recall this is a basis)

This essentially means that our vector field has $d$ degrees of information or one can think of this as $d$ values need to specify the object.



# Operators typically make function spaces, which in many cases have ???? dimension

Consider the set of all continuous functions $\mathcal{C}$.

> Using the fact that dimension says we need $d$ number of linearly independent objects to build any object in the space, what dimension do you think $\mathcal{C}$ is?

**Answer:** $\mathcal{C}$ is infinite dimensional! This will be an important property when we consider operator mappings, as we *cannot* write down an infinite dimensional object in the form of a finite number of basis vectors! This will become important in our neural network design.

# Approximation of operators

Neural networks approximate functions. Neural operators approximate operators.

What does it mean to approximate an operator?

Main questions:

- How do we input a function $f$ which is inherently continuous and (sometimes) a member of an infinite dimensional set into a computer?
- Say we can do this, what does it mean to get an output function from our neural network?
- Why would anyone want to do this?

Let's answer the third question before moving on. Do you see any advantages?

# Why do we care about approximating operators?

The solution to dynamical systems - both ODEs and PDEs is inherently an *operator*. For example consider ODEs

$$\frac{dz(t)}{dt} = f(z(t), t)\,, \quad z(0) = \bar{z}_0\,.$$

Then, one can write the solution as

$$z(t) = \int_0^t f(z(t), t)dt + \bar{z}_0\,.$$

The solution to an ODE is given by an **operator**!

Thus, imagine we want to learn $z(t)$ for any input $\bar{z}_0$. Then, if we can learn this implicit integral operator, we have a solution to the ODE for all times $t$ with all initial conditions $\bar{z}_0$ removing the expensive numerical schemes (Euler's, RK4, etc.)

# Perhaps you think ODEs are too simple

Consider the holy grail of PDE's: Navier-Stokes

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p + \mu\nabla^2\mathbf{u} + \mathbf{f}\,,$$

$$\nabla\cdot\mathbf{u} = 0\,,$$

where:

- $\mathbf{u}$ is the velocity field
- $p$ is the pressure field
- $\rho$ is the fluid density (constant for incompressible flow)
- $\mu$ is the dynamic viscosity
- $\mathbf{f}$ represents body forces (e.g., gravity)

First, if you can just prove that a solution exists congrats your a millionaire.[a]

[a] https://en.wikipedia.org/wiki/Millennium_Prize_Problems

# Operator formulation of Navier-Stokes

Given an initial velocity field at time 0, $\boldsymbol{u}(\boldsymbol{x}, 0) = \boldsymbol{g}(\boldsymbol{x})$, $\boldsymbol{x} \in \mathbb{R}^n$, then we can write the solution operator as

$$\boldsymbol{u}(\boldsymbol{x}, t) = \mathcal{G}[p, \rho, \mu, \boldsymbol{f}, \boldsymbol{g}](\boldsymbol{x}, t)$$

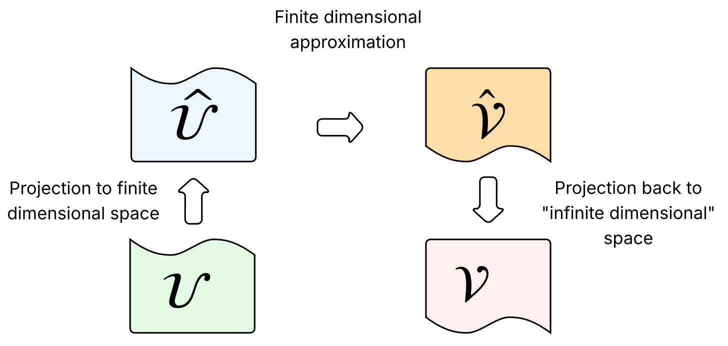
which takes an input of $\mathbb{R} \times \mathbb{R} \times \mathbb{R} \times C^0(\mathbb{R}^n \times \mathbb{R}^0; \mathbb{R}^n) \times C^0(\mathbb{R}^n; \mathbb{R}^n)$ to an output of some function $\boldsymbol{u}$ (of which we don't know if it's smooth. See Millennium problems).

- Notice, for PDEs, the operator learned is a mapping of function spaces.
- As with the ODE problem, if we can learn an approximation of this operator, then we obtain the Navier-Stokes equations at any desired $\boldsymbol{x}, t$. The grid independence or otherwise known as **discretization invariance** will enable us to perform calculations that are otherwise impossible with traditional solvers.

# So why learn an approximation of an operator

It gives us a framework to develop machine learning solutions to ODE and PDEs that can be queried at any desired $x, t$ location!

So what does this look like in practice? **Answer:** There are a variety of approaches, but they all follow the same structure.



# Let's walk through an example: Transport PDE and FNO

Consider the 1D transport PDE:

$$
\begin{aligned}
\frac{\partial u(x,t)}{\partial t} &= \frac{\partial u(x,t)}{\partial x}\,, \quad x \in (0,1], t \in \mathbb{R}^+\,, \\
u(x,0) &= f(x)\,, \\
u(t,0) &= 0\,.
\end{aligned}
$$

Given, $f(x)$, we want to know the solution of the PDE from time $T = 3$ to $T = 5$. That is, we want to learn the operator mapping

$$
f(x) \mapsto u(x,t)\,, \quad t \in [3,5], x \in [0,1]\,.
$$

Step 1: How do we encode $f(x)$ (project $f(x)$ to finite dimensional space)?

# Encoding: Simplest approach.

That is, consider points $x_1, x_2, ..., x_n \in [0, 1] = X$. One possible encoding of $f(x)$ is to evaluate the function at these points:

$$[f(x_1), f(x_2), ..., f(x_n)] \, .$$

More commonly, one extends this by a classical feedforward neural network with $[f(x_1), ...f(x_n)]$ as its input (sometimes, this projects to a *higher dimensional space* - you can think of the NN as performing interpolation between the $x_k$ points).

**Key:** This introduces error in our approximation as we can't pass the true functional form, but this is a representation which can be passed into a computer as a vector.

# How to do a finite dimensional approximation of an operator

Let a typical MLP for a neural network be given by

$$f(x) = \sigma(Wx + b)\,.$$

Then, a neural operator approximation is given by

$$\mathcal{L}(f)(x) := \sigma(Wf(x) + b + (\mathcal{K}_l f)(x))$$

where

$$(K_l f)(x) = \int_{y \in X} K_l(x, y) f(y) dy\,.$$

So what is new: Essentially, we added this non-local integral term which now depends on every point in the space and multiplies by the weight matrix $K_l$.

# Why this structure for the hidden layers?

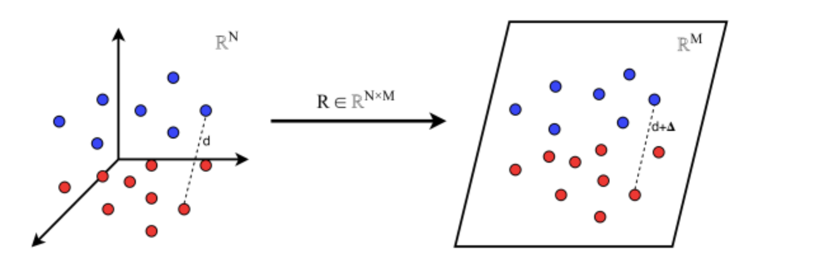
Two reasons:

- Theoretically, this structure has the nice *universal operator approximation* properties that we had for neural networks and functions
- In practice, it yields a very rich set of architectures based on the choice of $K_l$ which achieve state-of-the-art results.

> Can you think of any connection or differences to other architectures we have discussed (Transformers, ResNets, CNNs)?

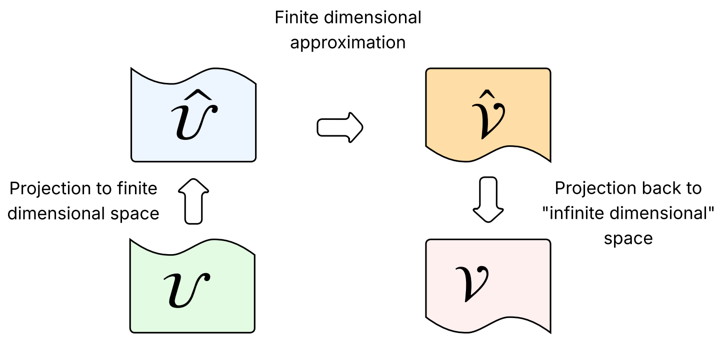
# Decoder structure

Take the output of the hidden layers and *project* back to the desired evaluation points.
How this projection is done can vary, and there are a variety of approaches (Example of one approach later today).



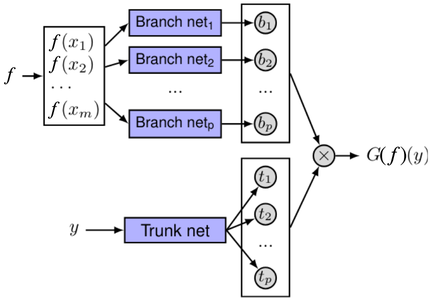
# Theory recap: Neural Operators

1. **Encoder:** Obtain some point-wise representation of our functional input.
2. **Hidden layers:** Perform *Non-local* finite dimensional approximation with our kernel matrix
3. **Decoder:** Project back to desired grid locations (architecture dependent)



# Architecture Example: Deep Operator Networks (DeepONet)

1. Encoder: Standard Point-wise function evaluations $[f(x_1), .., f(x_n)]$
2. Finite dimensional approximation: Let us consider $p$ different neural networks (MLP) that all take in $[f(x_1), ..., f(x_n)]$ as their input and output $\beta_1, ..., \beta_p$.
3. Decoder: To construct our target function $v$, we use a second NN that takes in the evaluation point $y$ which is where to evaluate the target function and perform a linear combination.



# Architecture Intuition: Deep Operator Networks (DeepONet)

**Main idea:** Use the finite dimensional approximation to learn a *basis* for the target function which can be queried at any point.
That is, from the functional inputs $f(x_1), ..., f(x_n)$, learn basis vectors $b_1, ...b_p$.
Then, to decode, pass in the target location $y$ and learn the coefficients $t_1, ..., t_p$ that act as the linear combination coefficients for $b_1, ..., b_p$ to obtain the result:

$$\mathcal{G}(f)(y) \approx \sum_{i=1}^{p} b_i([f(x_1), ..., f(x_n)] \times \tau_i(y)$$

- $b_i$ are given via neural networks (MLP, **Branch net**).
- $\tau_i$ are given via neural networks (MLP, **Trunk net**)

# Connection to the theoretical definition of Neural Operators

Think of the summation as the kernel component of the DeepONet:

$$\mathcal{G}(f)(y) \approx \sum_{i=1}^{p} b_i([f(x_1), ..., f(x_n)] \times \tau_i(y)$$

$$\mathcal{L}(f)(x) := \sigma(Wf(x) + b + (\mathcal{K}_l f)(x))$$

That is, treat $\sum_{i=1}^{p} b_i(f) \times \tau_i(y)$ as the kernel function and let $W, b = 0$ and simplify $\sigma =$ Identity. Then the DeepONet is a simplified form of the abstract Neural Operator definition. [1]

[1] See Section 3.6 of https://arxiv.org/pdf/2304.13221 for more detail.

# Key features of DeepONet

- Can query the NN at any desired location $y$ *without retraining* (Super-resolution). Branch and trunk NNs are independently computable.
- Easily extended where the two networks are of any form.
- Theoretical universal approximation guarantees.
- "Notion of interpretability" for the basis vectors.

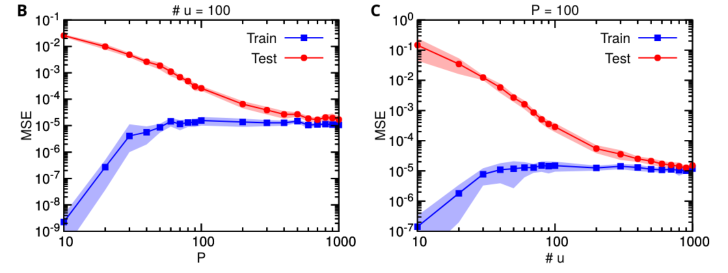



Figure: (Left) scaling with respect to number of evaluation points $x_1, ..., x_P$. (Right) Scaling with respect to number of training data. Both for a reaction diffusion PDE.

# Disadvantages of DeepONet

What can you think of?

- The linear combination structure is less expressive Do these types of dot products have issues in other architectures?
- Can struggle with generalization and be very sample inefficient due to its very generic architecture.
- Resolution mismatch - if your training data is given at uniform grid, will struggle to evaluate on non-uniform grids.

# Extensions of DeepONet

There have been a variety of extensions enhancing DeepONet.

- NOMAD - Generalizes the dot-product in DeepONet to be the input to a third NN (Paper link).
- Use DeepONet with pretrained encoder-decoder structure of functional evaluations for better encoding/decoding. (Paper link)
- Multiscale DeepONet that solves the non-uniform grid challenge (Paper link).
- Integration with RNNs for temporal dependence (Paper link)
- Uncertainty quantification ingrained DeepONets (Paper link)

# Next time...

- Introduce other types of neural operator architectures (Fourier Neural Operator)

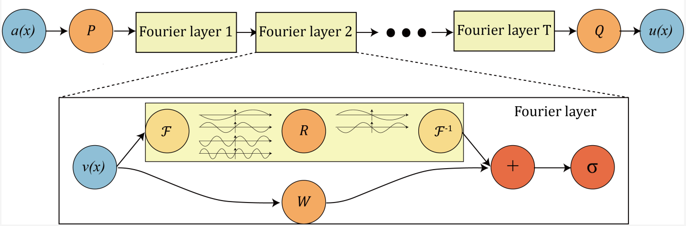



Figure: Fourier Neural Operator Architecture

- Discuss whether super-resolution really works?
- If time permits, a few examples of how these can be applied in climate modeling, robotics, and earthquakes (See your homework).