Fourier Neural Operator

For Parametric Partial Differential Equations

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Organizational Details – Final Exam

Registration:

- Exam is available in **TUM Online**
- Registration deadline: **2 July 2025**

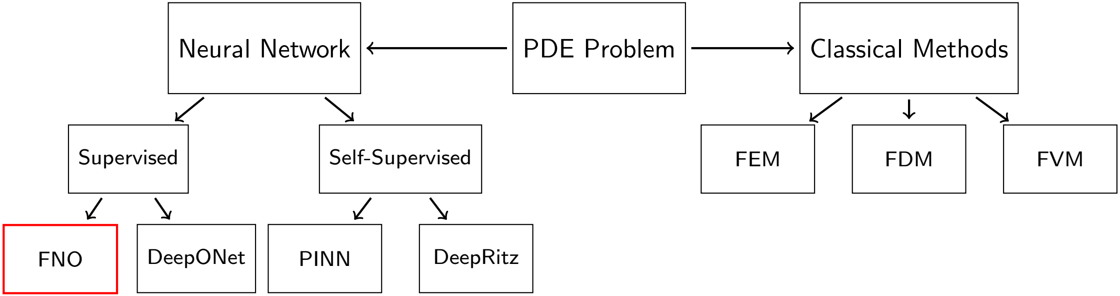
Exam Format:

- Exam task will be published on **2 July 2025** via **Moodle**
- You will:
  - Complete the assigned tasks
  - Submit a written report (template provided)
  - Submit your code (or link to code)
  - Give a short presentation (10–15 minutes, excl. Q&A)

Deadlines:

- Report & Code Submission: **23 July 2025**
- Presentation Day: **30 July 2025** (time slots will be assigned individually)

Overview



Neural Network
PDE Problem
Classical Methods
Supervised
Self-Supervised
FEM
FDM
FVM
FNO
DeepONet
PINN
DeepRitz

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Parametric PDE Problems

We consider a general **parametric PDE** in form:

$$F(x, y, u, u_x, u_y, u_{xx}, u_{yy}, \cdots, a) = 0, \quad (x, y) \in \Omega$$

Where:

- $u(x, y)$ is the **solution**
- $a(x, y)$ is a **parameter** (e.g., conductivity or source)
- Appropriate boundary conditions on $\partial\Omega$

Operator Learning Problem

Goal: Solve for $u(x, y; a)$ given any input parameter $a(x, y)$

This defines an **operator learning problem**:

$$\mathcal{G} : a(x, y) \in \mathcal{A} \longrightarrow u(x, y) \in \mathcal{U}$$

Where:

- $\mathcal{A}$: function space for inputs
- $\mathcal{U}$: function space for outputs
- $\mathcal{G}$: **solution operator** we want to approximate

From Vectors to Functions

Traditional neural networks work on **finite-dimensional vectors**:

$$\mathbf{v}_{l+1} = \sigma_l(W_l \mathbf{v}_l)$$

But in scientific computing, we often deal with **functions** rather than vectors.

Goal: Learn mappings between functions directly, without discretization.

This leads us to **neural operators** – networks that learn mappings of the form:

$$\mathcal{G} : v(x) \mapsto u(x)$$

Integral Operators (I)

Key idea: Process **function-to-function** mappings via integration.

An **integral operator** maps a function $v(y)$ to another function $u(x)$ by integrating over a kernel $k(x,y)$:

$$u(x) = \int_{\Omega} k(x,y)\, v(y)\, dy$$

Used extensively in:

- Inverse problems
- Gaussian processes
- PDE theory

Integral Operators (II): Visual Concept

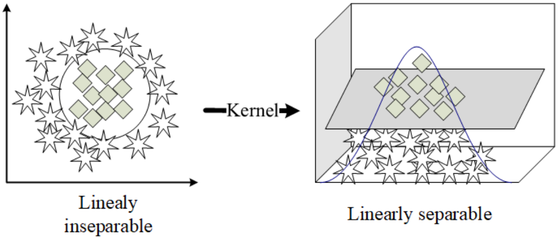


Figure: Illustration of a kernel-based operator acting on a function.

Kernel function: $k(x, y)$ describes how inputs y influence outputs at location x.

This is the foundation of **kernel-based neural operators**.

Kernel-Based Neural Operator

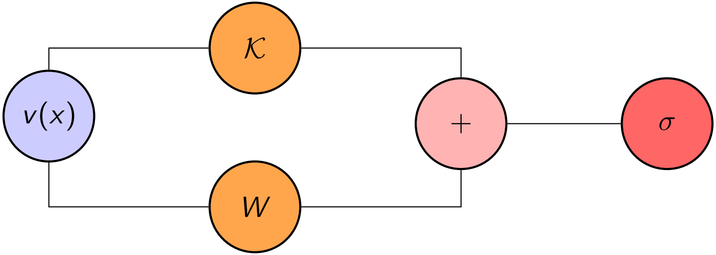
Extension to **function spaces** using **integral operators**:

$$v_{l+1}(x) = \sigma_l \left(\int_\Omega k_l(x, y) v_l(y)\, dy + W_l v_l(x) \right)$$

Where:

- $x, y \in \Omega$: spatial coordinates
- $k_l(x, y)$: learnable **kernel function**
- W_l: pointwise (local) linear transformation
- σ_l: nonlinear activation function

Kernel Operator: Computational Flow



Two pathways:

- **Non-local interaction** via kernel $\mathcal{K}(x, y)$
- **Local update** via W

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Motivation Behind FNO

Computer Vision: CNNs work well because images have **local patterns**

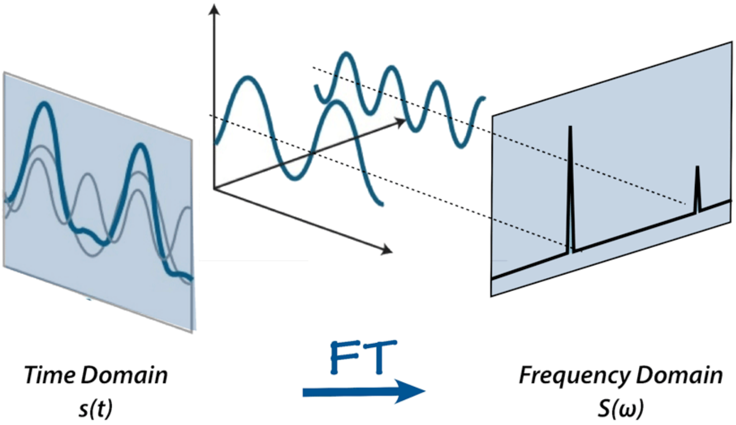
Parametric PDEs: Functions often exhibit **global correlations**

- Smooth variations across domain
- Long-range dependencies
- Local convolutions may be inefficient

FNO Solution:

- Replace local convolution with **global convolution**
- Use **Fourier transform** for efficiency
- Leverage compact representation in **frequency domain**

Fourier Transform Visualization



The Fourier Layer: Core Building Block

Why Fourier?

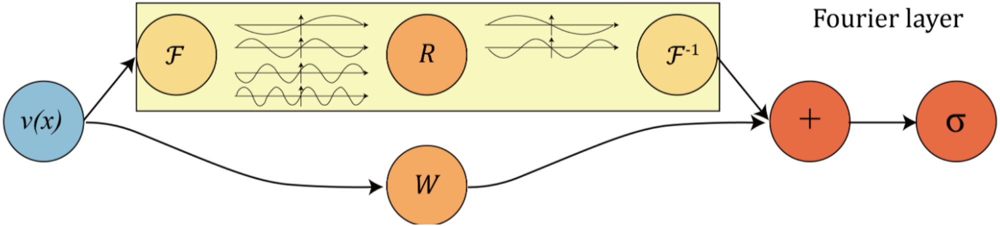
- **Speed**: $\mathcal{O}(n^2) \to$ quasilinear with FFT
- **Compactness**: PDE functions concentrated in low frequencies

Three-step process:

1. **Fourier Transform**: $v_l \to \mathcal{F}(v_l)$
2. **Linear Transformation**: Apply R to low-frequency modes
3. **Inverse Transform**: $\mathcal{F}^{-1} \to$ spatial domain

Fourier Layer Architecture

$$v_{l+1}(x) = \sigma\left(\mathcal{F}^{-1}\left(R \cdot \mathcal{F}(v_l)\right)(x) + W v_l(x)\right)$$



Key Design Choices

Remark A: Truncation

- **Discard high-frequency modes**
- Apply R only on lower modes
- Most useful information for PDEs in low frequencies

Remark B: Activation in Spatial Domain

- Activations applied **after** inverse Fourier transform
- Recovers **high-frequency details** omitted by truncation
- Captures **non-periodic boundary behaviors**

Complete FNO Architecture

Three main components:

1. **Input Layer**: **Lifting**

$$v_0 = P_\theta(a, x)$$

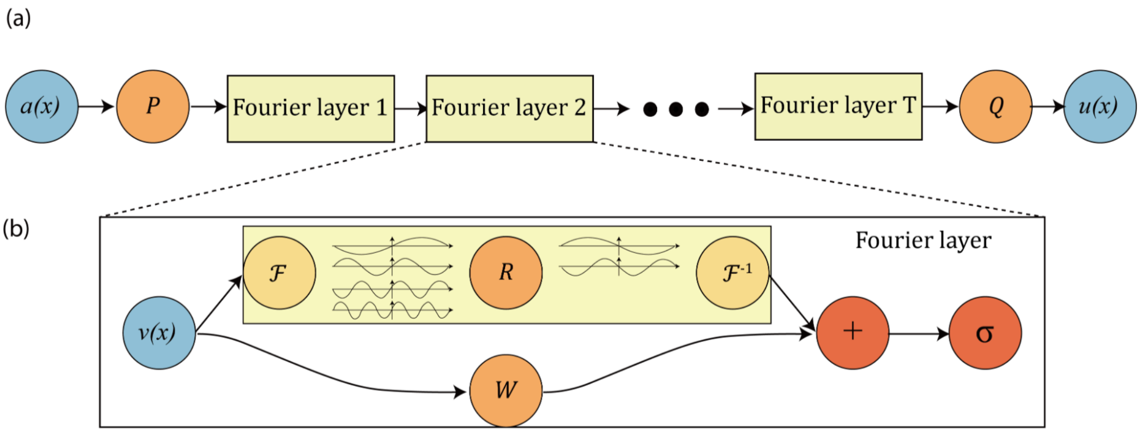
2. **Fourier Layers**: **Global Transformations**

$$v_{l+1} = \sigma\left(\mathcal{F}^{-1}(R \cdot \mathcal{F}(v_l)) + W v_l\right)$$

3. **Output Layer**: **Projection**

$$u = Q_\theta(v_L)$$

FNO Architecture



FNO Pipeline Summary

Input $a(x)$ $\rightarrow$ Lifting P_θ $\rightarrow$ Fourier Layers $\rightarrow$ Projection Q_θ $\rightarrow$ Solution $u(x)$

Key Innovation: Combines expressiveness of deep networks with efficiency of Fourier methods

Especially suitable for learning operators from parametric PDE problems

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Step 1: Prepare Training Data

FNO learns from **labeled training pairs** (a, u) on a **fixed regular mesh**:

- **Mesh**: $\Xi = \{\xi_1, \xi_2, \ldots, \xi_n\}$
- **Discretization**: $a(\Xi), u(\Xi)$
- **Dataset**: $\mathcal{D} = \{(a^{(i)}(\Xi), \Xi), u^{(i)}(\Xi)\}_{i=1}^{N_{\text{data}}}$

Note: FNO requires **uniform grid** for Fourier transforms

Data Generation:

- Inputs a sampled from function space $\mathcal{A}$
- Outputs u computed using accurate solvers (FEM/FDM)

Step 2: Build FNO Model

Forward pass through FNO model $\mathcal{G}_\theta$:

$$v_0 = P_\theta(a(\Xi), \Xi) \quad \text{(input lifting)} \tag{1}$$

$$v_{l+1} = \sigma\left(\mathcal{F}^{-1}(R \cdot \mathcal{F}(v_l)) + W v_l\right), \quad l = 0, \ldots, L-1 \tag{2}$$

$$u(\Xi) = Q_\theta(v_L) \quad \text{(projection to output)} \tag{3}$$

Parameters:

- P_θ, Q_θ: input/output networks
- R, W: learnable parameters in Fourier layers
- σ: activation function (e.g., ReLU)

Steps 3 & 4: Training Process

Loss Function (Mean Squared Error):

$$\theta^* = \arg\min_\theta L(\theta) = \frac{1}{N_{\text{data}}} \sum_{i=1}^{N_{\text{data}}} \left| \mathcal{G}_\theta(a^{(i)}(\Xi), \Xi) - u^{(i)}(\Xi) \right|^2$$

Optimization (SGD/Adam):

$$\theta_{t+1} = \theta_t - l_r \nabla_\theta L(\theta_t)$$

Where:

- l_r: learning rate
- t: training step

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Advantages of FNO

- **High accuracy and efficiency**
  - Typically outperforms DeepONet
  - Better prediction accuracy
  - Higher computational speed
- **Fast inference**
  - Rapid solving for any new input $a \in \mathcal{A}$
  - Suitable for real-time applications
  - Many-query scenarios
- **Global receptive field**
  - Captures long-range dependencies
  - Efficient frequency domain operations

Disadvantages of FNO

- **Data inefficiency**
    - Requires large number of labeled pairs (a, u)
    - Expensive numerical simulations
    - Costly experimental data collection
- **Limited generalization**
    - Struggles with out-of-distribution inputs
    - Performance degrades for unseen parameter ranges
- **Mesh dependence**
    - Requires regular grid for FFT
    - Less flexible for irregular domains
    - Complex geometries challenging
    - Reduced accuracy at non-mesh locations

Summary and Future Directions

FNO Summary:

- Powerful method for **parametric PDE operator learning**
- Combines deep learning with **Fourier efficiency**
- Excellent for **smooth, global** PDE solutions

Future Research Directions:

- Irregular domain handling
- Few-shot learning approaches
- Multi-scale and adaptive methods
- Integration with physics-informed constraints