Fourier Neural Operator for Parametric Partial Differential Equations

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PDEs TODAY

Challenges in Science and Engineering

Solving complicated partial differential equations (PDE) systems is extremely important

Examples

Solving PDEs

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Molecular dynamics, micro-mechanics, turbulent flows, etc.

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Examples

Solving PDEs

Conventional solvers vs data-driven methods

Conventional solvers VS Data-Driven methods

Conventional solvers

VS

Data-Driven methods

Conventional solvers

Examples:

Finite Element Methods (FEM)

Finite Difference Methods (FDM)

Trade-off:

Coarse Grids: Faster but less accurate

Fine Grids: Accurate but slow

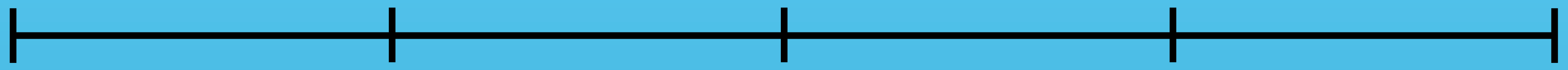
Challenge:

Complicated PDEs require fine discretization to capture the phenomenon

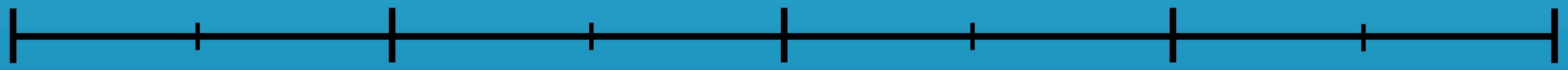
VS

Data-Driven methods

Coarse grid



Fine grid



Conventional solvers

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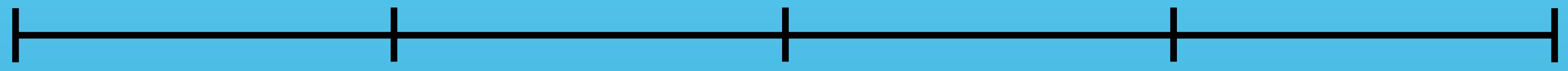

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- Finite Difference Methods (FDM)

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Data-Driven methods

Direct Learning:

- Learn trajectories directly from data
- Better runtime

Challenge:

- Classical Neural Networks (NNs) still limited by discretization

Solution:

- Develop discretization-invariant Neural Operators (NOs)

PAPER’S WORK

- New neural operator
- Parametrize the integral kernel in the Fourier space

Experiments on Burgers’ equation, Darcy flow, and Navier-Stokes equation

- Three orders of magnitude faster
- Superior accuracy

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New neural operator

NEURAL OPERATORS

Key features

- Infinite-Dimensional Operator
- Unified Parameters
  → Discretization-Invariance
    → Solution Transfer
- Data-Driven

New neural operator

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Fourier space

FOURIER SPACE

Differentiation → Multiplication

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Differentiation → Multiplication

Potentially a lot faster!

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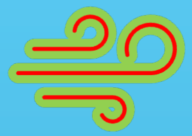
Navier-Stokes equation

NAVIER-STOKES EQUATION

- Models fluid dynamics



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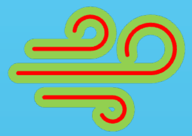

- Extremely useful
  - Airflow? → Planes, weather, etc.
  - Blood flow? → Medical diagnostics tools
  - Etc.

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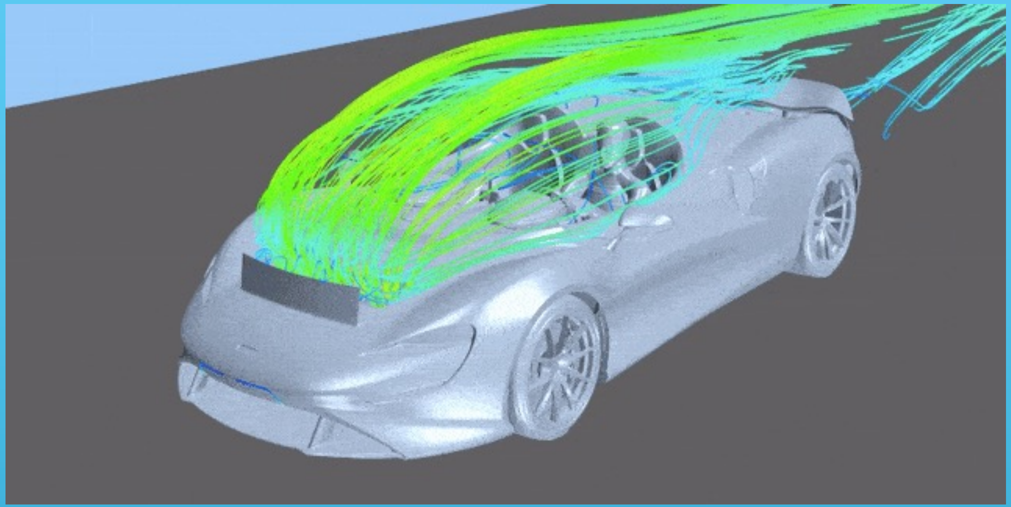

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NAVIER-STOKES EQUATION

$$\begin{cases} \partial_t w(x,t) + u(x,t) \cdot \nabla w(x,t) = \nu \Delta w(x,t) + f(x) \\ \nabla \cdot u(x,t) = 0 \\ w(x,0) = w_0(x) \end{cases}$$

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$\boldsymbol{u}$: velocity field

$\boldsymbol{w}$: vorticity

∇: gradient

Δ: Laplacian

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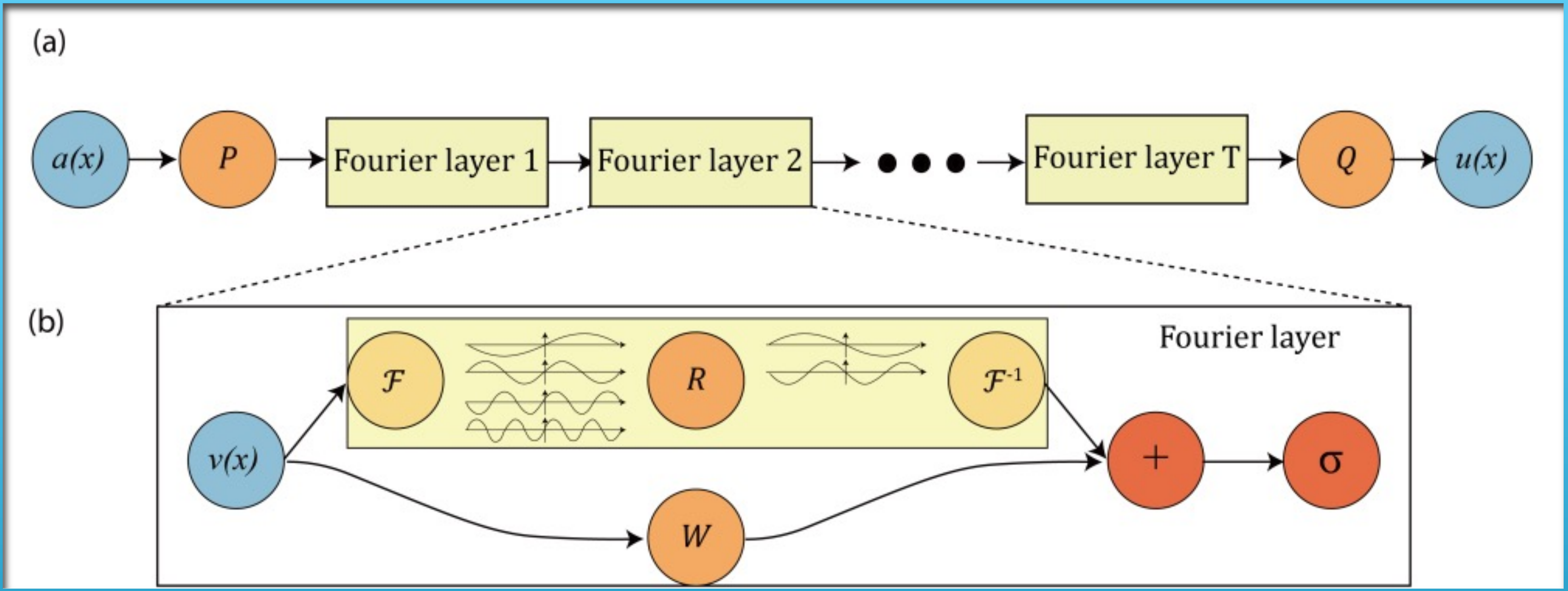
OPERATOR LEARNING



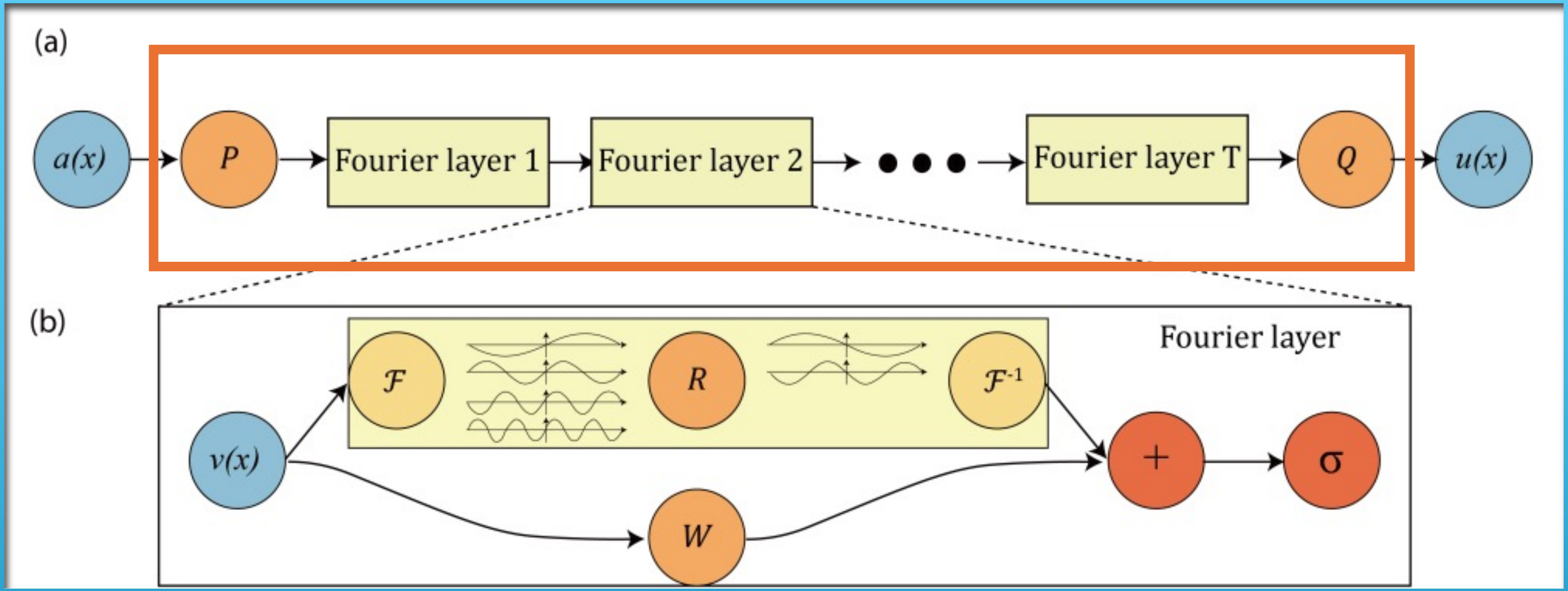
GOAL

Learn a mapping $\boldsymbol{G}^{\dagger}$

Inputs $\mathbf{a}(\mathbf{x}) \in \mathcal{A} = \mathcal{A}(D; \mathbb{R}^{d_a})$

Outputs $\mathbf{u}(x) \in \mathcal{U} = \mathcal{U}(D; \mathbb{R}^{d_u})$

OPERATOR LEARNING



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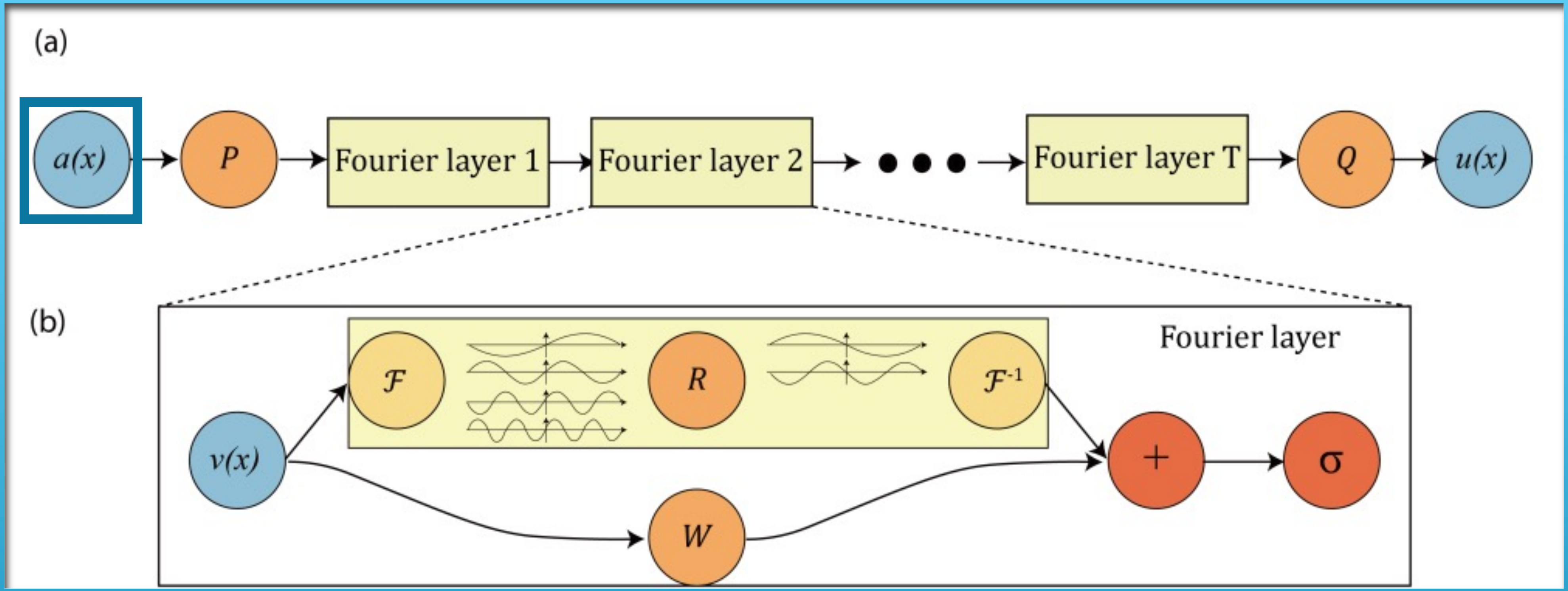

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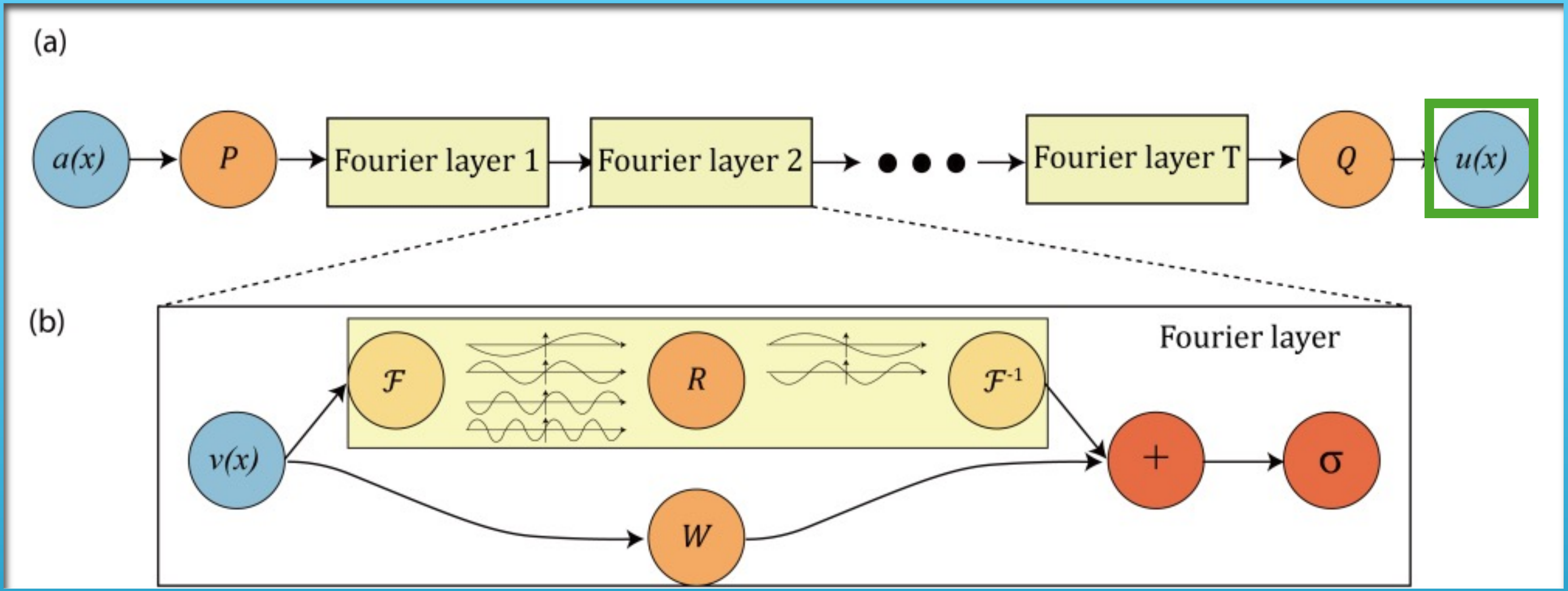

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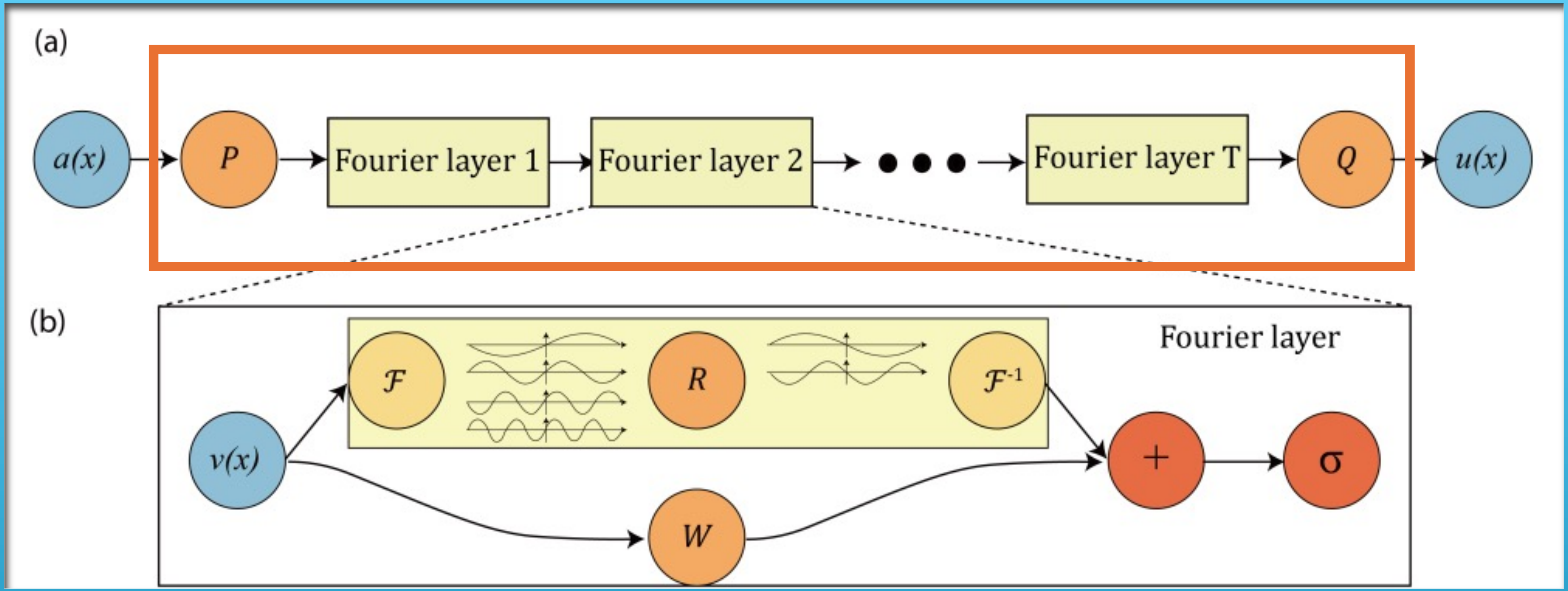
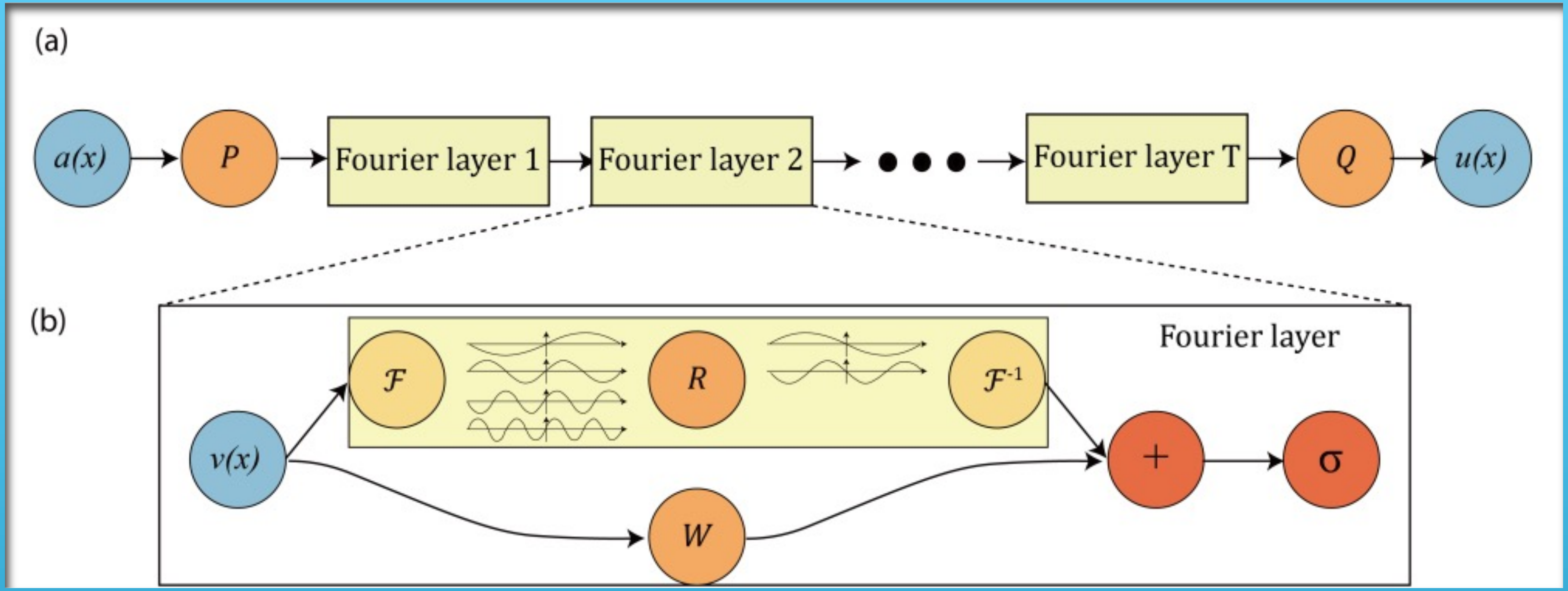


HOW Construct parametric map such that $G_{\theta^\dagger}$ is as close as possible to $G^\dagger$.

THE NEURAL OPERATOR



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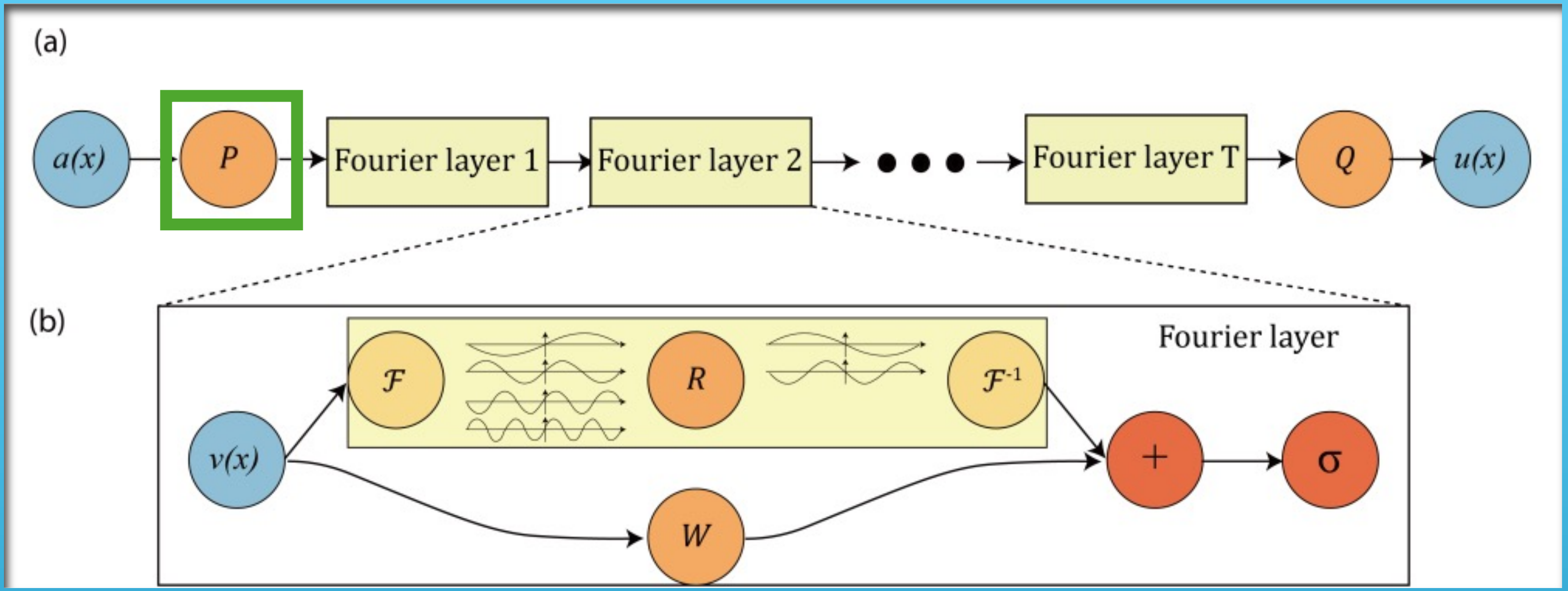
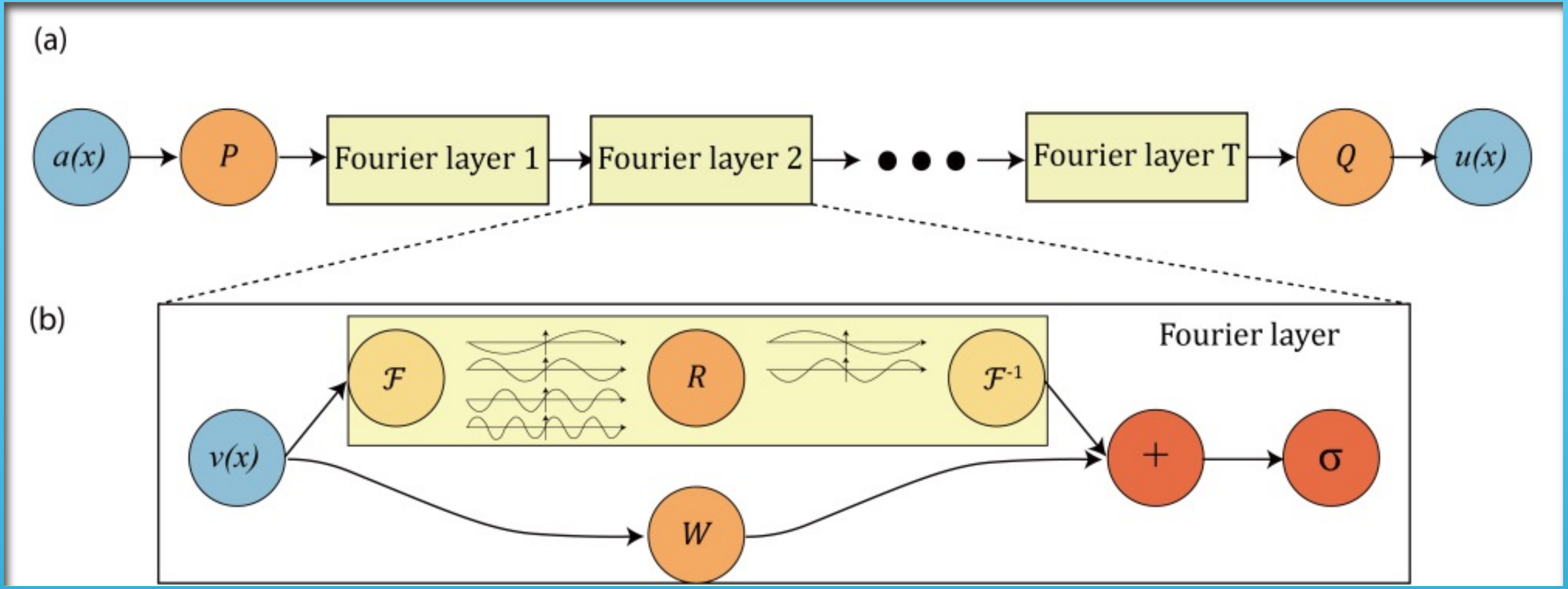
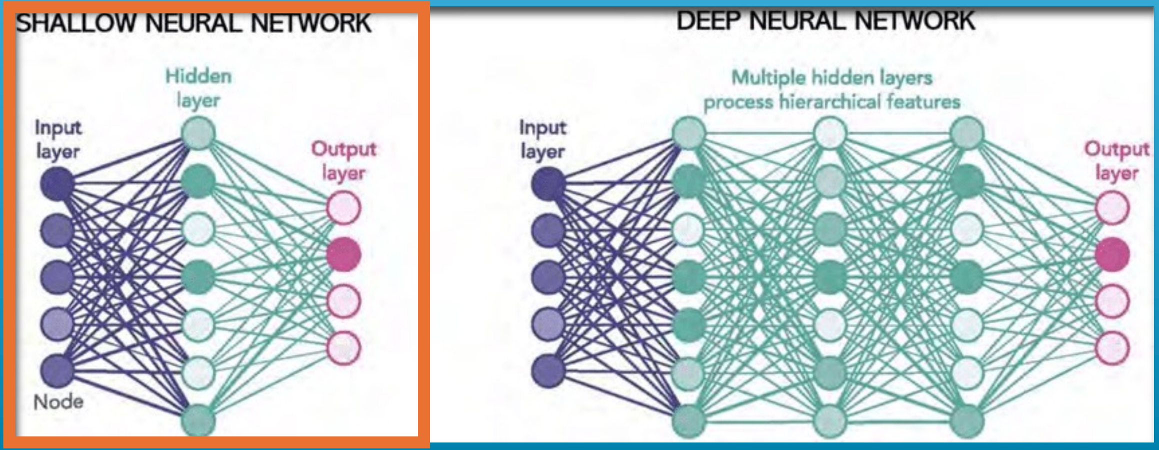


Lift input to higher dimension:
$v_0(x) = P(a(x))$

THE NEURAL OPERATOR



$P: \mathbb{R}^{d_u} \mapsto \mathbb{R}^{d_v}$, parametrized by a **shallow fully-connected NN**



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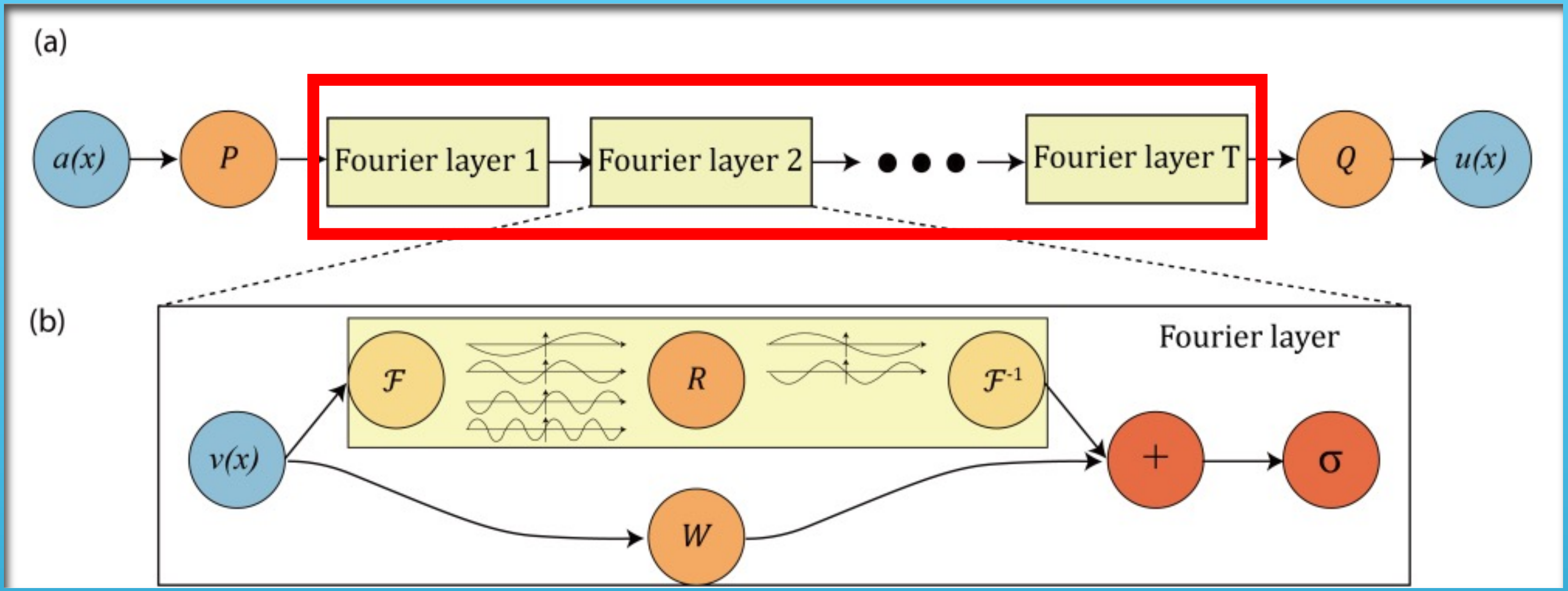
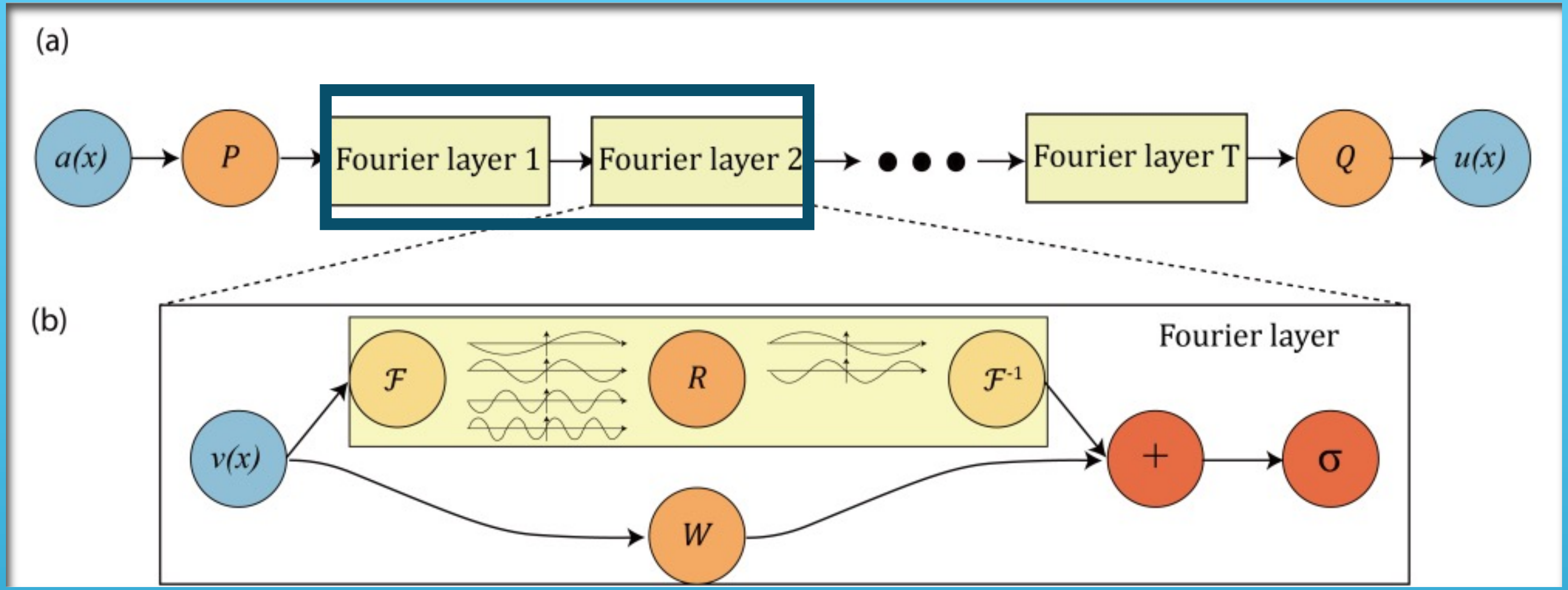


Iterative architecture:

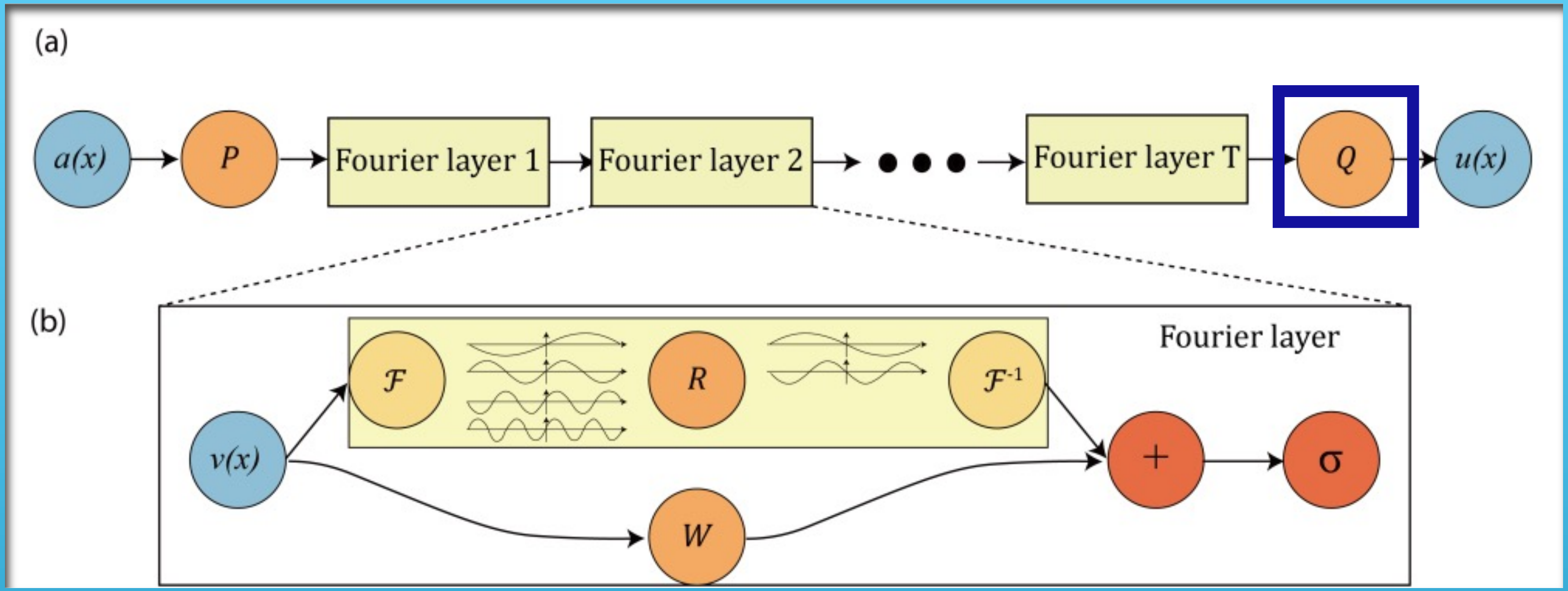
$v_0(x) \longmapsto \ \dots \ \mapsto \ v_T(x), x \in \ \mathbb{R}^{d_v}$

THE NEURAL OPERATOR



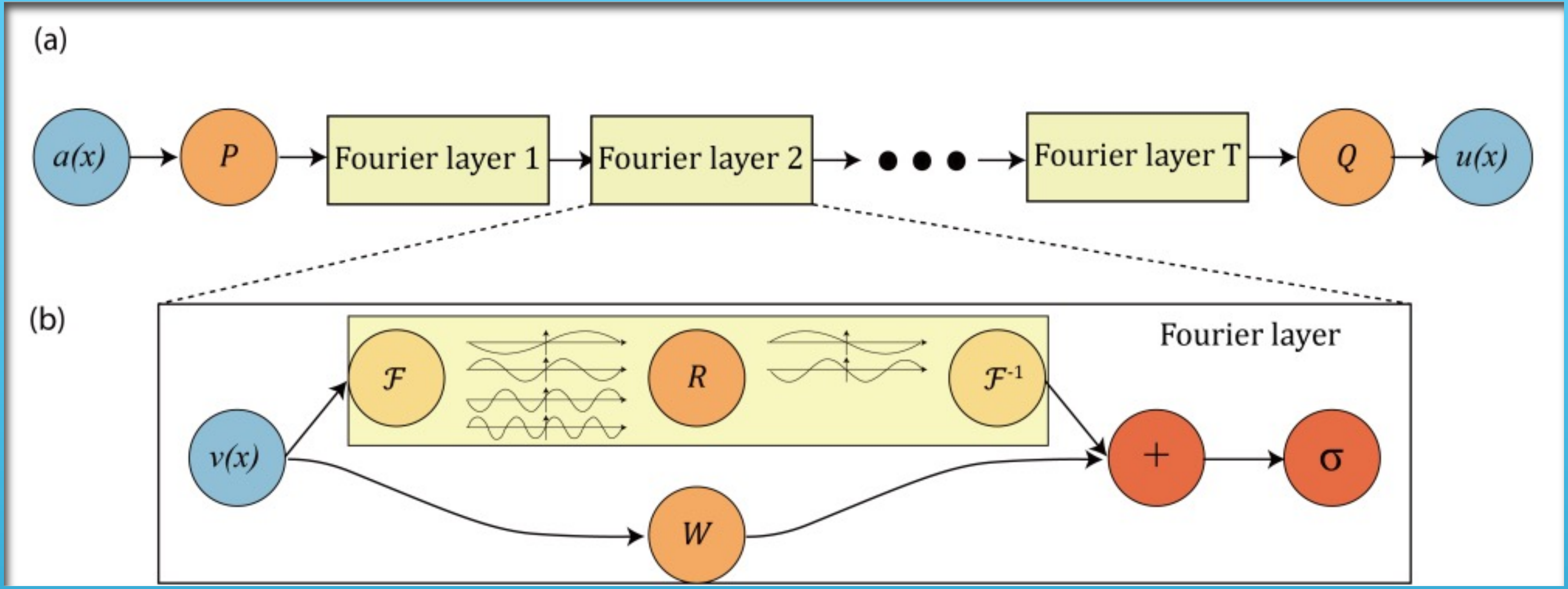
Iteration: $v_t \longmapsto v_{t+1}$

THE NEURAL OPERATOR



The $\boxed{\textbf{output } \boldsymbol{u(x) = Q(v_T(x))}}$,
$Q: \mathbb{R}^{d_v} \mapsto \mathbb{R}^{d_u}$

THE NEURAL OPERATOR



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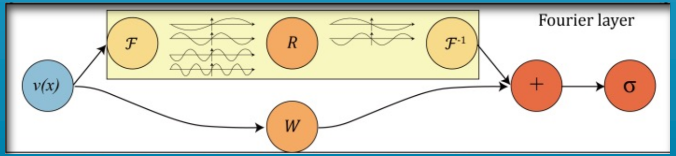
Iteration: $v_t \longmapsto v_{t+1}$

The **output** $u(x) = Q(v_T(x))$,
$Q: \mathbb{R}^{d_v} \mapsto \mathbb{R}^{d_u}$

$$v_{t+1}(x) \coloneqq \sigma\Big(Wv_t(x) + \big(\mathcal{K}(a;\, \phi)v_t\big)(x)\Big), \qquad \forall x \in D$$



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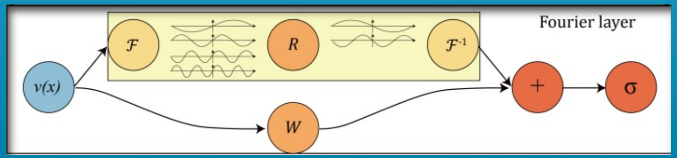
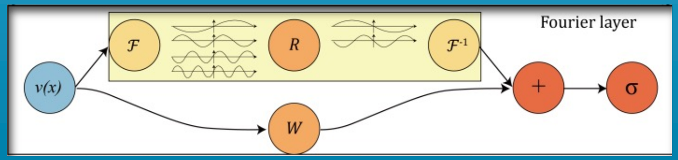


$$v_{t+1}(x) := \boldsymbol{\sigma}\Big(W v_t(x) + \big(\mathcal{K}(a;\ \phi)v_t\big)(x)\Big), \qquad \forall x \in D$$

$\sigma : \mathbb{R} \to \mathbb{R}$

Non-linear activation function

Component-wise operations



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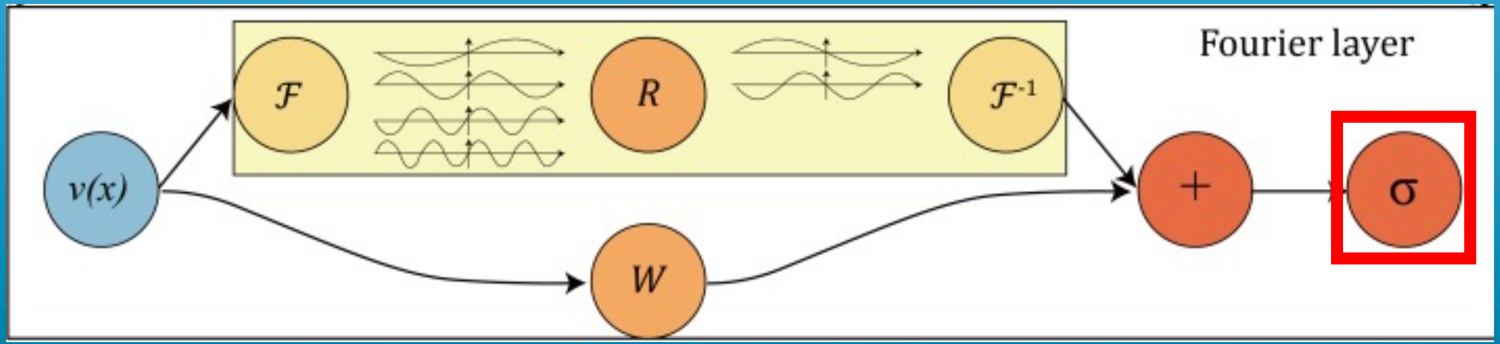

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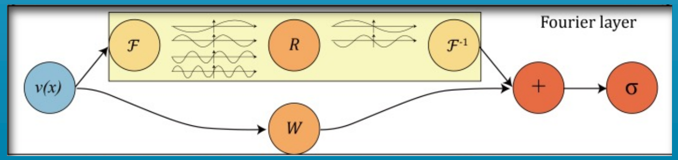
$W: \mathbb{R}^{d_v} \to \mathbb{R}^{d_v}$

Linear transformation

Spatial domain



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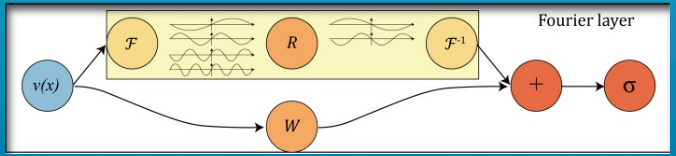

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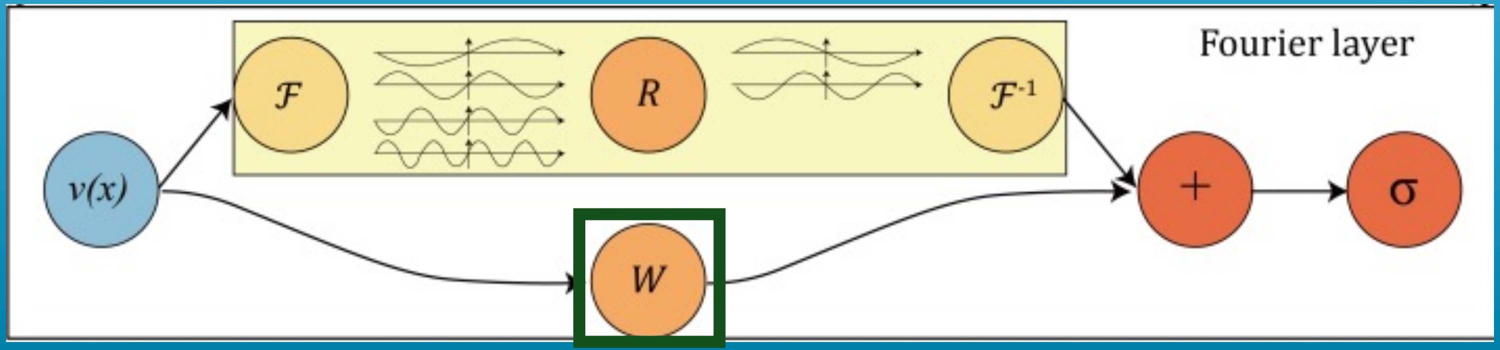

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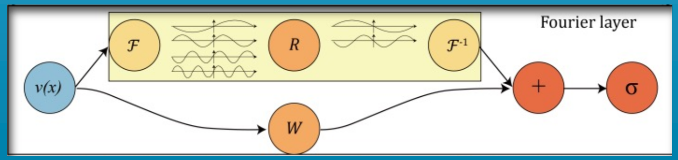
Linear transformation

Spatial domain

$$\mathcal{K}: \mathcal{A} \times \Theta_{\mathcal{K}} \to \mathcal{L}\big(\mathcal{U}(D;\ \mathbb{R}^{d_v}), \mathcal{U}(D;\ \mathbb{R}^{d_v})\big)$$

Maps to operators on $\mathcal{U}(D;\ \mathbb{R}^{d_v})$

parameterized by $\phi \in \Theta_{\mathcal{K}}$



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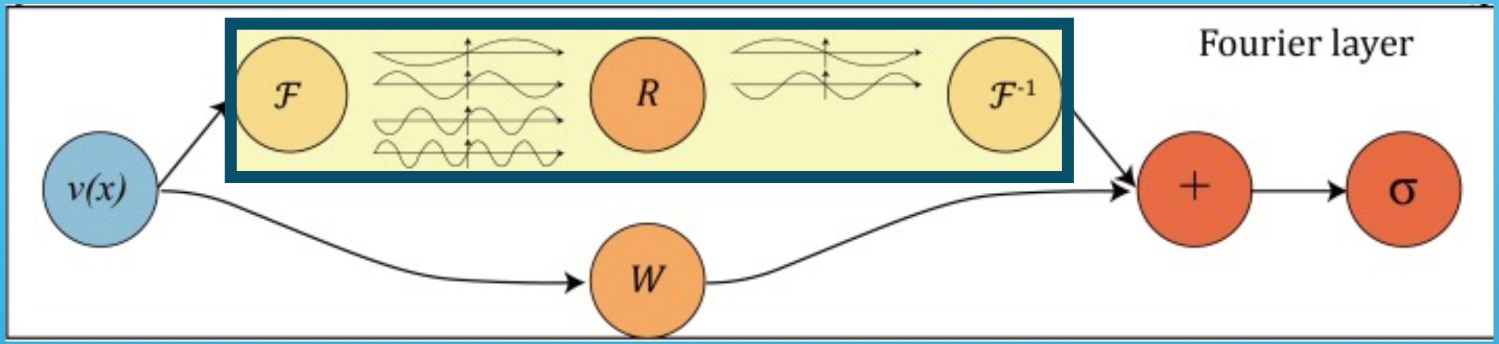

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$\sigma\colon\ \mathbb{R} \ \to\ \mathbb{R}$

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Component-wise operations

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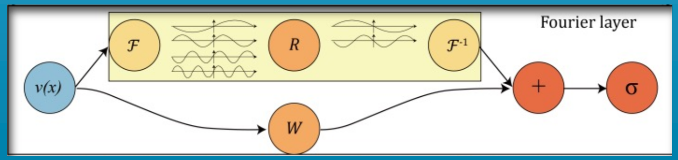

KERNEL INTEGRAL OPERATOR

$$(\mathcal{K}(a;\ \phi)v_t)(x) \ \coloneqq \int_D \kappa(x, y, a(x), a(y);\ \phi)v_t(y)\, dy, \qquad \forall x \ \in D$$

where $\kappa_\phi : \mathbb{R}^{2(d+d_a)} \to \mathbb{R}^{d_v \times d_v}$ is a NN parameterized by $\phi \in \Theta_{\mathcal{K}}$ ➔ kernel function

$$v_{t+1}(x) \coloneqq \sigma(Wv_t(x) + (\mathcal{K}(a;\ \phi)v_t)(x)), \qquad \forall x \in D$$

NEURAL OPERATOR

$$\boxed{v_{t+1}(x) \;:=\; \sigma\Big(W v_t(x) + \big(\mathcal{K}(a;\,\phi) v_t\big)(x)\Big)}$$

$$\boxed{\big(\mathcal{K}(a;\,\phi) v_t\big)(x) \;:=\; \int_D \kappa\big(x, y, a(x), a(y);\,\phi\big) v_t(y)\, dy}$$

NEURAL OPERATOR

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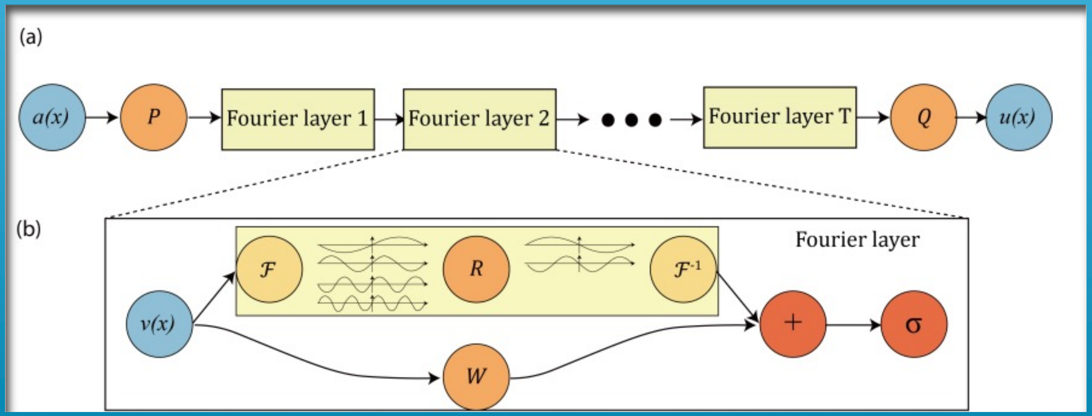

Linear integral operator

Neural Operator learns non-linear operators:

- Linear integral operators

+

- Non-linear activation functions

NEURAL OPERATOR

$$\boxed{\boldsymbol{v_{t+1}(x) := \sigma\big(W v_t(x) + (\mathcal{K}(a;\ \phi) v_t)(x)\big)}}$$

$$\boxed{\boldsymbol{(\mathcal{K}(a;\ \phi)v_t)(x) := \int_D \kappa(x, y, a(x), a(y);\ \phi) v_t(y)\, dy}}$$

Removing dependence of a

+

$$\kappa_\phi\big(x, y, a(x), a(y)\big) = \kappa_\phi\big(\mathrm{x} - \mathrm{y}, a(x), a(y)\big)$$

➔ Convolution operator

Removing dependence of a

+

$$\mathscr{k}_\phi\big(x, y, a(x), a(y)\big) = \mathscr{k}_\phi\big(\mathrm{x} - \mathrm{y}, a(x), a(y)\big)$$

CONVOLUTION THEOREM

Removing dependence of a

$+$

$$\mathscr{k}_\phi(x,y) = \mathscr{k}_\phi(\mathrm{x}-\mathrm{y})$$

Theorem

Fourier transform convolution ➔ pointwise product Fourier transforms

CONVOLUTION THEOREM

Removing dependence of a

$+$

$k_{\phi}(x, y) = k_{\phi}(\mathrm{x} - \mathrm{y})$

Theorem

$$r(x) = \{u * v\}(x) = \int u(x - \tau) v(\tau)\, d\tau$$

CONVOLUTION THEOREM

Removing dependence of a

$+$

$$k_\phi(x, y) = k_\phi(\mathrm{x} - \mathrm{y})$$

Theorem

$$r(x) = \{u * v\}(x) = \int u(x - \tau)v(\tau)\, d\tau$$

Theorem

$$r(x) = \{u * v\}(x) = \mathcal{F}^{-1}\{U \cdot V\}$$

$$Where\, U(f) \triangleq \mathcal{F}\{u\}(f);\ V(f) \triangleq \mathcal{F}\{v\}(f)$$

CONVOLUTION THEOREM

Removing dependence of a

$$+$$

$$k_{\phi}(x, y) = k_{\phi}(\mathrm{x} - \mathrm{y})$$

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Removing dependence of a

$+$

$k_\phi(x, y) = k_\phi(\mathrm{x} - \mathrm{y})$

Theorem

$$r(x) = \{u * v\}(x) = \mathcal{F}^{-1}\{U \cdot V\}$$

$$Where\, U(f) \triangleq \mathcal{F}\{u\}(f);\ V(f) \triangleq \mathcal{F}\{v\}(f)$$

$$(\mathcal{F}f)_j(k) = \int_D f_j(x) e^{-2i\pi\langle x,k\rangle}\, dx$$

$$(\mathcal{F}^{-1}f)_j(x) = \int_D f_j(k) e^{2i\pi\langle x,k\rangle}\, dk$$

APPLICATION

Removing dependence of a

$+$

$\mathscr{k}_{\phi}(x, y) = \mathscr{k}_{\phi}(x - y)$

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$r(x) = \{u * v\}(x) = \mathcal{F}^{-1}\{U \cdot V\}$

Where $U(f) \triangleq \mathcal{F}\{u\}(f);\ V(f) \triangleq \mathcal{F}\{v\}(f)$

$$(\mathcal{K}(a;\ \phi)v_t)(x) = \int_D \mathscr{k}(x - y;\ \phi)v_t(y)\,dy \quad , \quad \forall x \in D$$

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$$(\mathcal{K}(a;\, \phi)v_t)(x) = \int_D \Bbbk(x - y;\, \phi)v_t(y)\, dy = \int u(x - \tau)v(\tau)\, d\tau\,,$$

$$\forall x \in D$$

APPLICATION

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$$\forall x \in D$$

FOURIER INTEGRAL OPERATOR

$$(\mathcal{K}(a;\phi)v_t)(x) = \mathcal{F}^{-1}(\mathcal{F}(k_\phi)\cdot\mathcal{F}(v_t))(x)$$

$\rightarrow$ *directly parameterize* k_ϕ *in Fourier space*

FOURIER INTEGRAL OPERATOR

$$(\mathcal{K}(a;\phi)v_t)(x) = \mathcal{F}^{-1}\left(\boldsymbol{R}_\phi \cdot \mathcal{F}(v_t)\right)(x)$$

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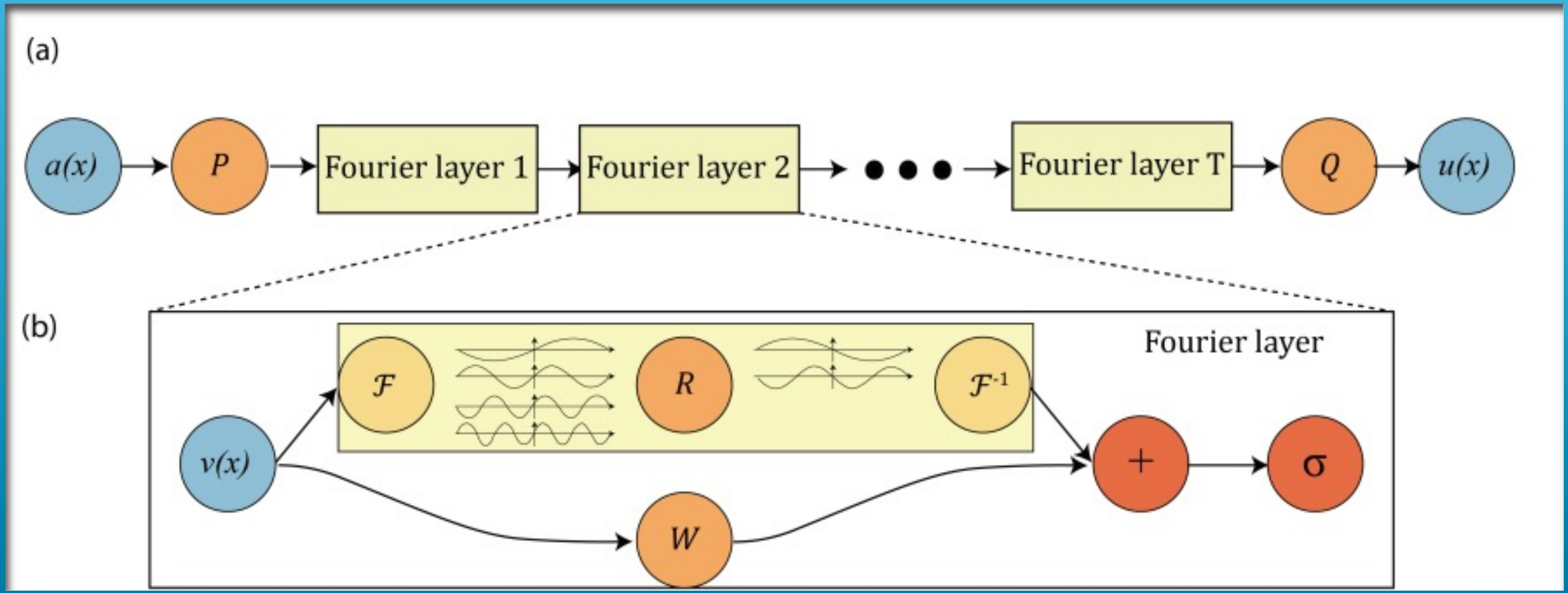
$$(\mathcal{K}(a;\phi)v_t)(x) = \mathcal{F}^{-1}\left(\boldsymbol{R_\phi} \cdot \mathcal{F}(v_t)\right)(x)$$

R_ϕ Fourier transform of periodic function κ



FOURIER INTEGRAL OPERATOR

$$\boxed{(\mathcal{K}(a;\phi)v_t)(x)} = \mathcal{F}^{-1}\left(R_\phi \cdot \mathcal{F}(v_t)\right)(x)$$

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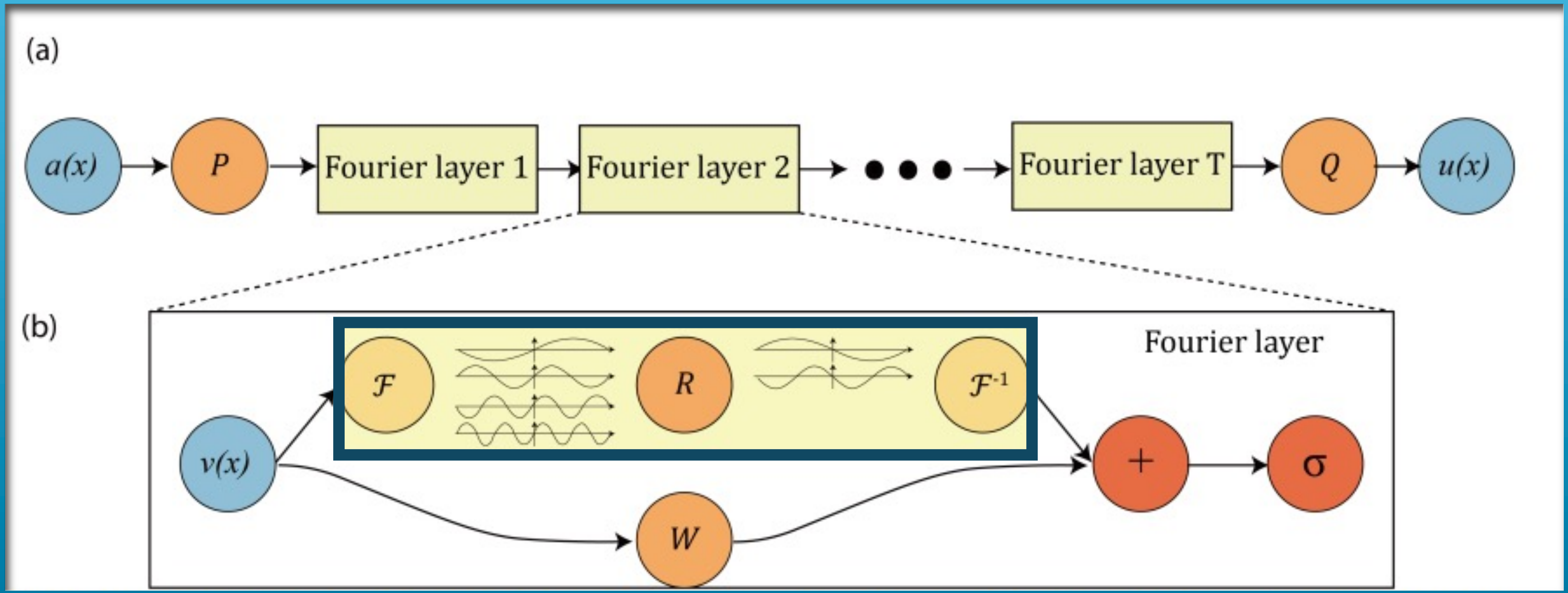

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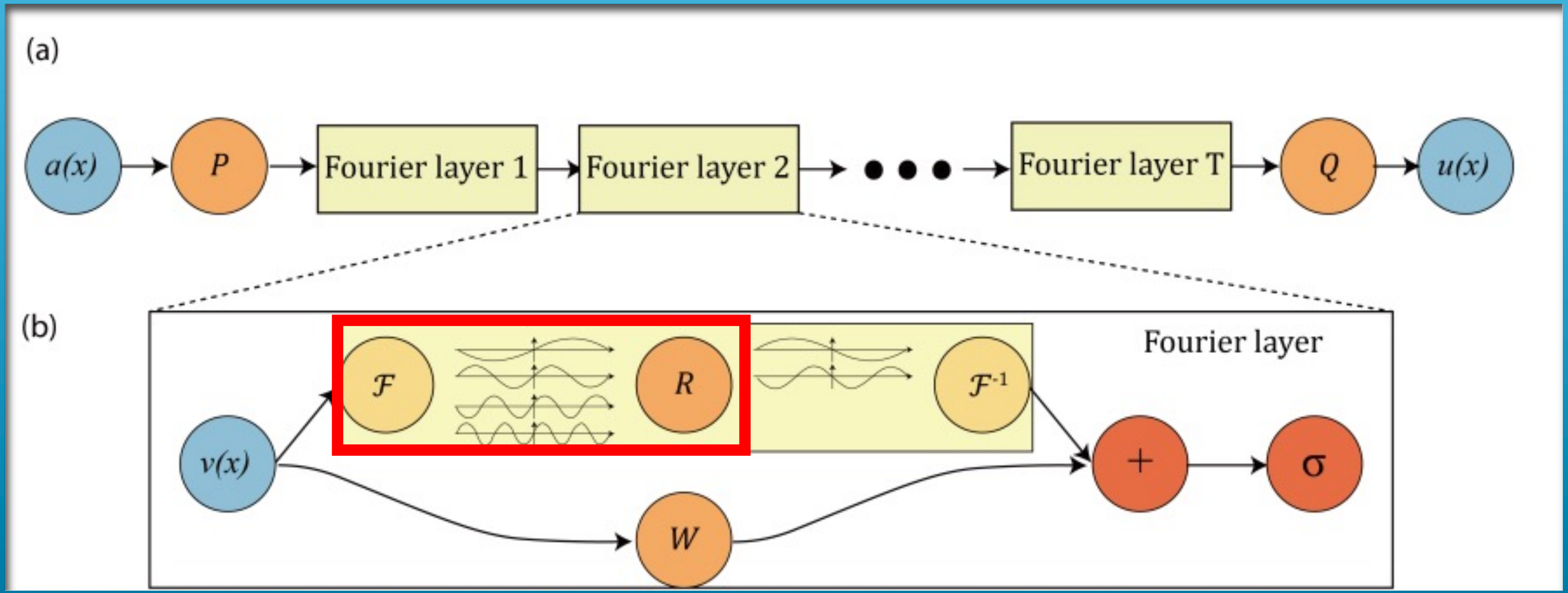

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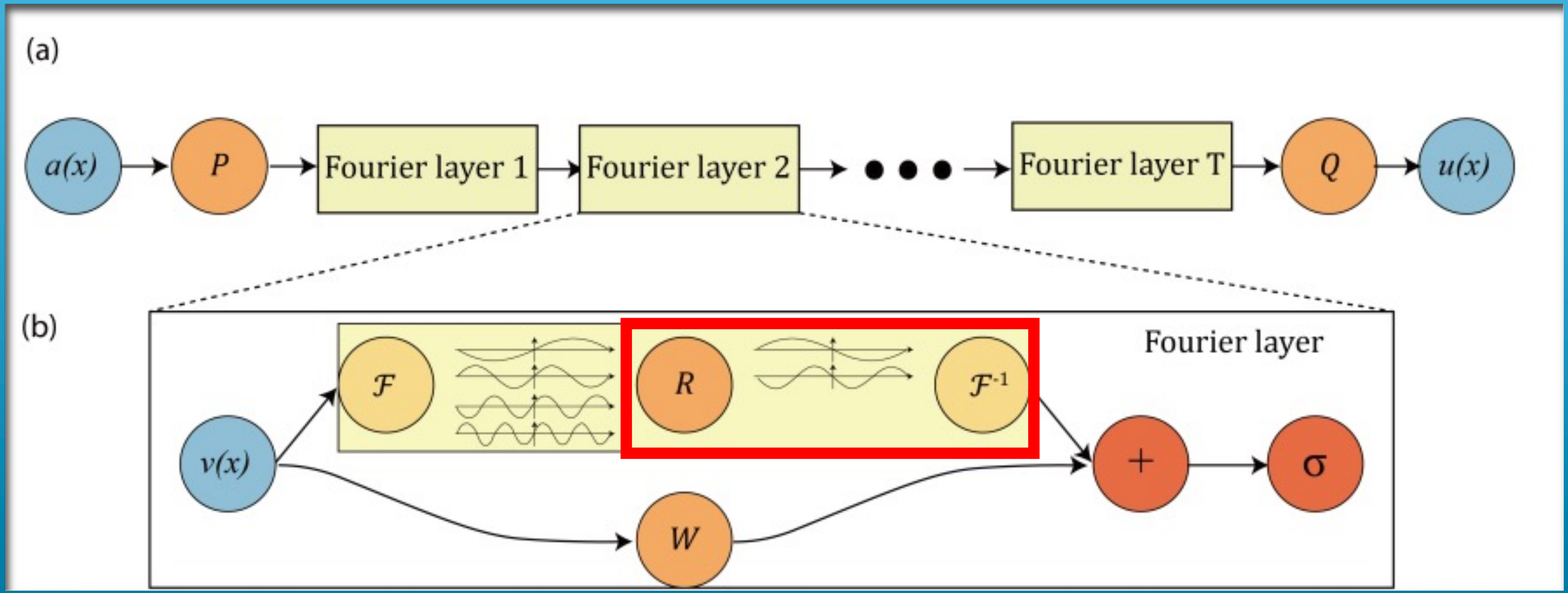

FOURIER INTEGRAL OPERATOR

$$(\mathcal{K}(a;\phi)v_t)(x) = \mathcal{F}^{-1}(\mathcal{F}(\mathcal{k}_\phi)\cdot\mathcal{F}(v_t))(x)$$

$$\downarrow$$

$$(\mathcal{K}(a;\phi)v_t)(x) = \mathcal{F}^{-1}(R_\phi\cdot\mathcal{F}(v_t))(x)$$

FOURIER INTEGRAL OPERATOR

$$(\mathcal{K}(a;\phi)v_t)(x) = \mathcal{F}^{-1}(\mathcal{F}(\textcolor{red}{\mathscr{k}_\phi}) \cdot \mathcal{F}(v_t))(x)$$
$$\downarrow$$
$$(\mathcal{K}(a;\phi)v_t)(x) = \mathcal{F}^{-1}(R_\phi \cdot \mathcal{F}(v_t))(x)$$

Assumed $\mathscr{k}_\phi$ periodic

FOURIER INTEGRAL OPERATOR

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$$(\mathcal{F}f)_j(k) = \int_D f_j(x)e^{-2i\pi\langle x,k\rangle}\,dx$$

$$\downarrow$$

Fourier series expansion

$$\downarrow$$

Work with the discrete modes $\mathscr{k}_\phi \in \mathbb{Z}^d$

FOURIER INTEGRAL OPERATOR

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R_ϕ Fourier transform of periodic function κ

Finite-dimensional parameterization ➔ Truncating at k_{max}

SO FAR

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Finite-dimensional parameterization ➔ Truncating at k_{max}

DISCRETE FOURIER TRANSFORM

$$(\mathcal{K}(a;\phi)v_t)(x) = \mathcal{F}^{-1}(\mathcal{F}(\mathscr{k}_\phi) \cdot \mathcal{F}(v_t))(x)$$

$\downarrow$

$$(\mathcal{K}(a;\phi)v_t)(x) = \mathcal{F}^{-1}(R_\phi \cdot \mathcal{F}(v_t))(x)$$

$\downarrow$

Finite-dimensional parameterization ➔ Truncating at k_{max}

$$R_\phi \cdot \mathcal{F}(v_t)$$

$\downarrow$

Point-wise multiplication

$+$

Lying in different dimensions

$\downarrow$

Truncate higher modes of $\mathcal{F}(v_t)$

$\downarrow$

$$(R \cdot (\mathcal{F}_{v_t}))_{k,l} = \sum_{j=1}^{d_v} R_{k,l,j} (\mathcal{F}_{v_t})_{k,l}$$

DISCRETE FOURIER TRANSFORM

$$(\mathcal{F}f)_j(k) = \int_D f_j(x) e^{-2i\pi\langle x,k\rangle}\, dx$$

$$\downarrow$$

$$(\mathcal{F}f)_j[k] = \sum_{x=0}^{n-1} f_j[x] e^{-2i\pi\frac{\langle x,k\rangle}{n}}$$

$$where: k \in \left[-{}^{k_{max}}/_{2}, \dots, {}^{k_{max}}/_{2}\right]$$

FAST FOURIER TRANSFORM

$$(\mathcal{F}f)_j(k) = \int_D f_j(x) e^{-2i\pi\langle x,k\rangle}\, dx$$

$$\downarrow$$

$$(\mathcal{F}f)_j[k] = \sum_{x=0}^{n-1} f_j[x] e^{-2i\pi\frac{\langle x,k\rangle}{n}}$$

$$where: k \in \left[-{}^{k_{max}}/_{2}, \ldots, {}^{k_{max}}/_{2}\right]$$

$$(\hat{\mathcal{F}}f)_l(k) = \sum_{x_1}^{s_1} \ldots \sum_{x_d}^{s_d-1} f_l(x_1, \ldots, x_d) e^{-2i\pi \sum_{j=1}^{d} x_j k_j}$$

$$where: l = 1, \ldots, d_v$$

INVARIANCE TO DISCRETIZATION

- The Fourier layers are discretization-invariant

INVARIANCE TO DISCRETIZATION

- The Fourier layers are discretization-invariant

Parameters learned in Fourier space

$\downarrow$

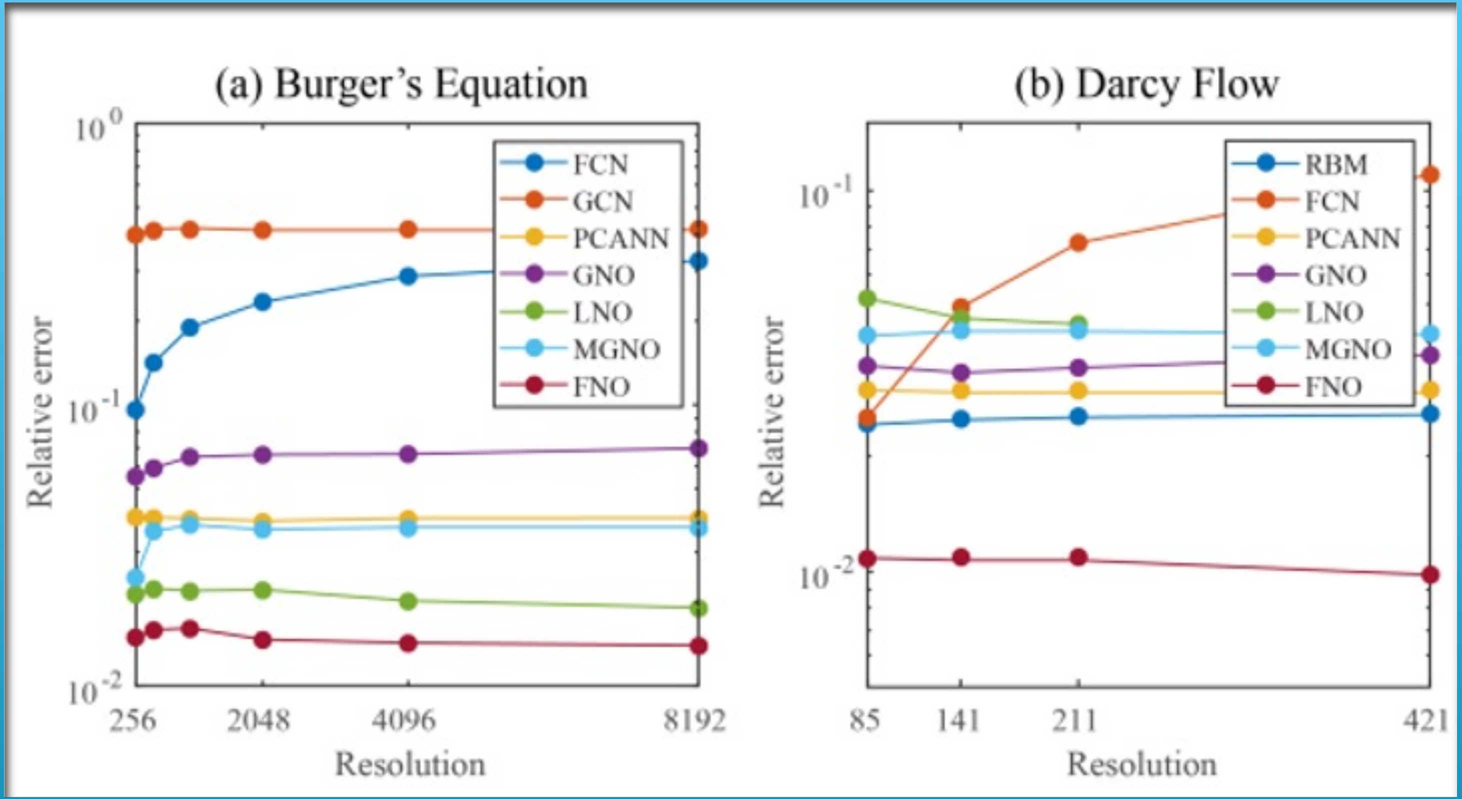
Projecting on the basis $e^{2\pi i\langle x,k\rangle}$

$\rightarrow$ Physical space

$\downarrow$

Well-defined everywhere on $\mathbb{R}^d$ + Consistent error at any resolution

INVARIANCE TO DISCRETIZATION



RUNTIME

- Inner multiplication has complexity $O(k_{max})$
- Fourier transforms have complexity $O(nk_{max})$

RUNTIME

- Inner multiplication has complexity O(k_{max})
- Fourier transforms have complexity O($\mathrm{n}k_{max}$)

FFT has complexity O($nlog(n)$)

↓

Uniform discretization is required

NUMERICAL EXPERIMENTS

THE MODEL

- 4 Fourier layers

+ ReLU

+ Batch normalization

- 500 epochs
- Learning rate: 0.001, halved every 100 epochs

TESTS

- 1-d Burgers' equation
- 2-d Darcy Flow problem
- 2-d Navier-Stokes equation
- Bayesian Inverse Problem

SIMULATION

- Compared against other popular solvers

SIMULATION

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- Two different Fourier Neural Operators:
  - ❖ FNO-2D learns spatial relation between time steps to predict next step

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2DConv

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  - ❖ FNO-3D learns full space-time relation of whole interval

2DConv

SIMULATION

- Compared against other popular solvers
- Two different Fourier Neural Operators:
  - ❖ FNO-2D learns spatial relation between time steps to predict next step
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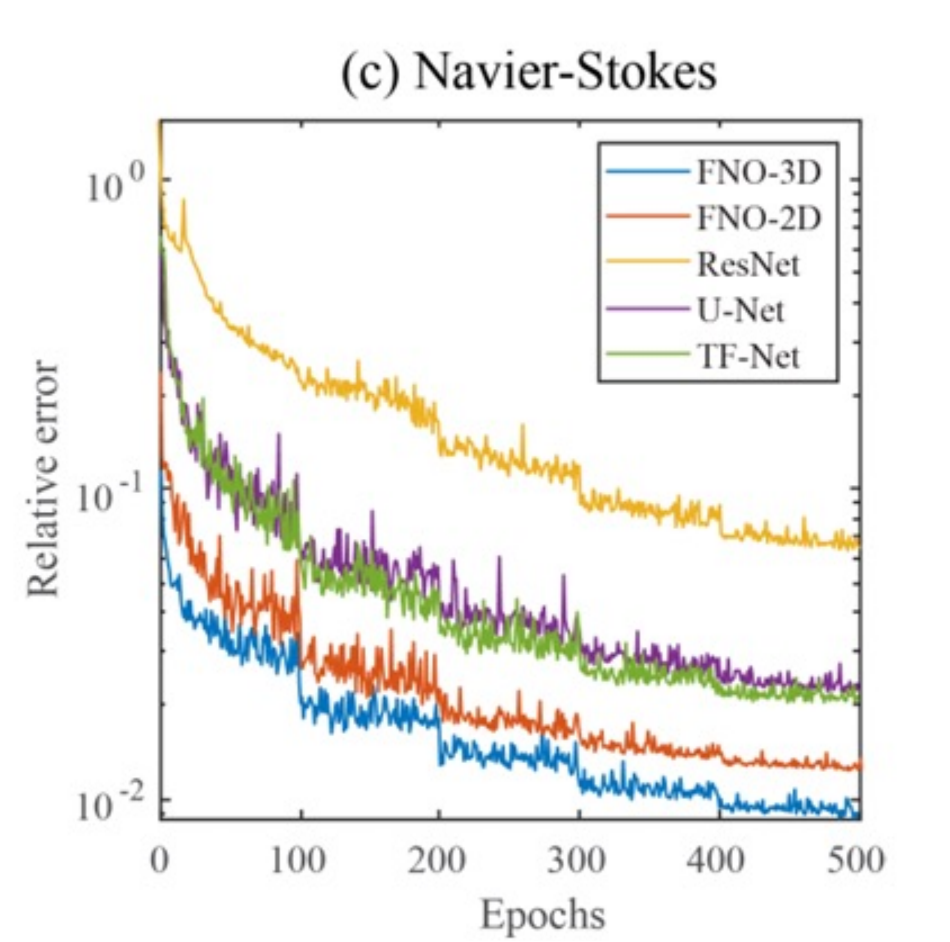
2DConv

3DConv

SIMULATION



Config	Parameters	Time per epoch	$\nu = 1e{-3}$ $T = 50$ $N = 1000$	$\nu = 1e{-4}$ $T = 30$ $N = 1000$	$\nu = 1e{-4}$ $T = 30$ $N = 10000$	$\nu = 1e{-5}$ $T = 20$ $N = 1000$
FNO-3D	6,558,537	38.99s	**0.0086**	0.1918	**0.0820**	0.1893
FNO-2D	414,517	127.80s	0.0128	**0.1559**	0.0834	**0.1556**
U-Net	24,950,491	48.67s	0.0245	0.2051	0.1190	0.1982
TF-Net	7,451,724	47.21s	0.0225	0.2253	0.1168	0.2268
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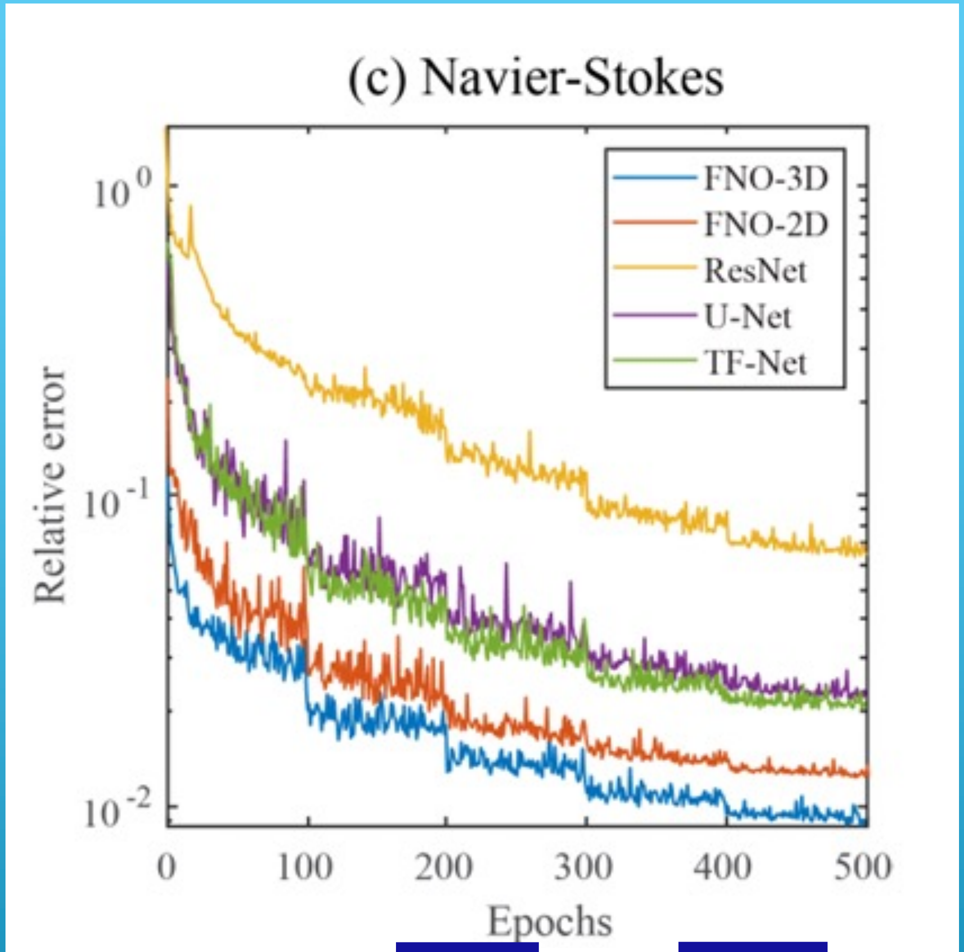
- With sufficient data:

SIMULATION



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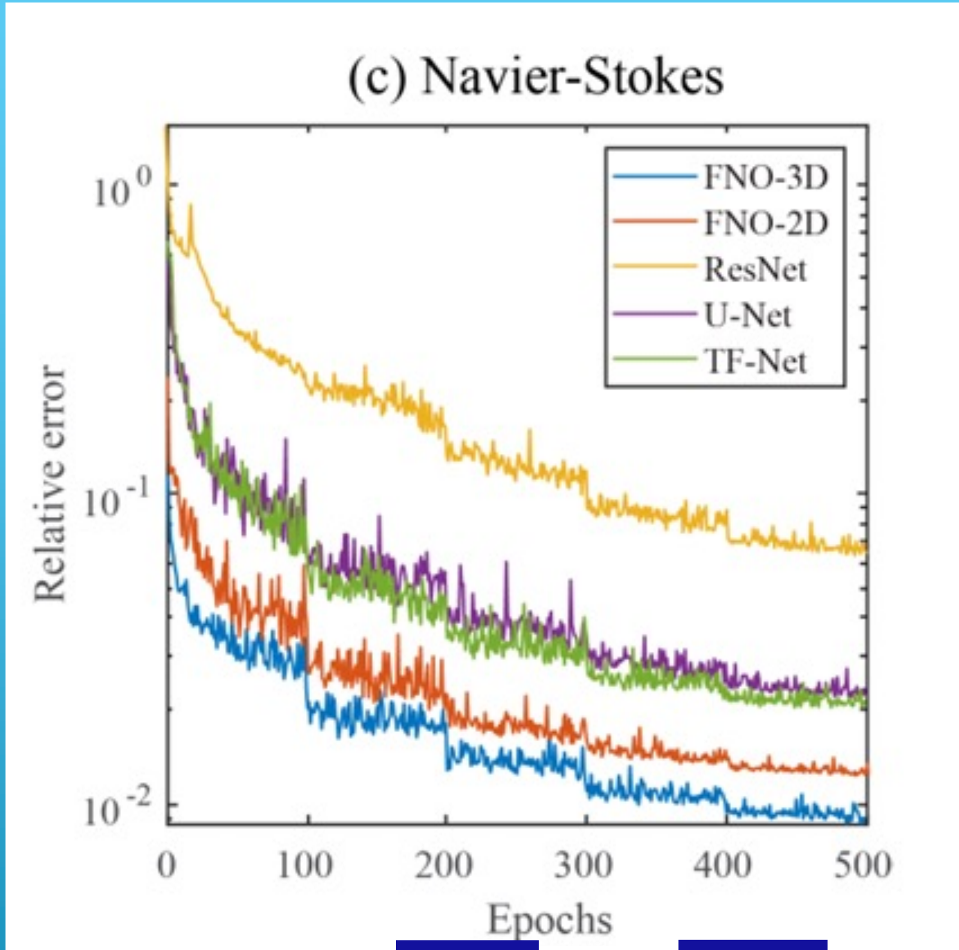
SIMULATION



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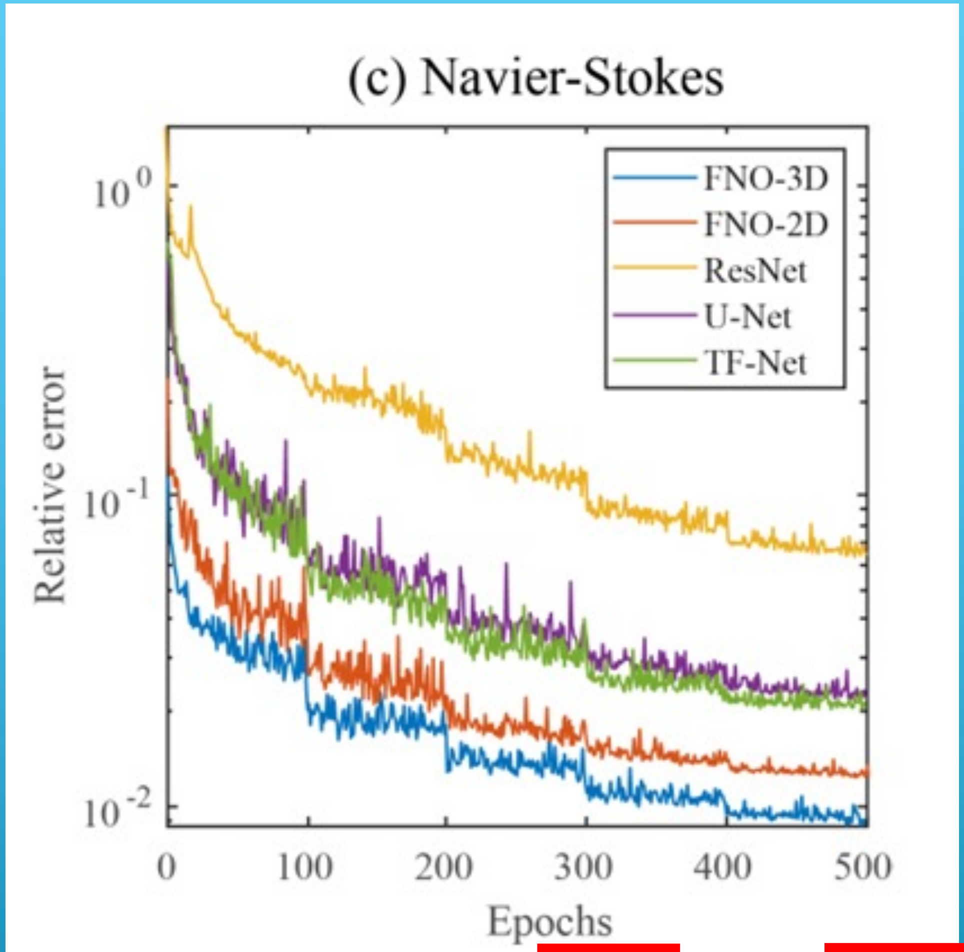

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FNO-3D

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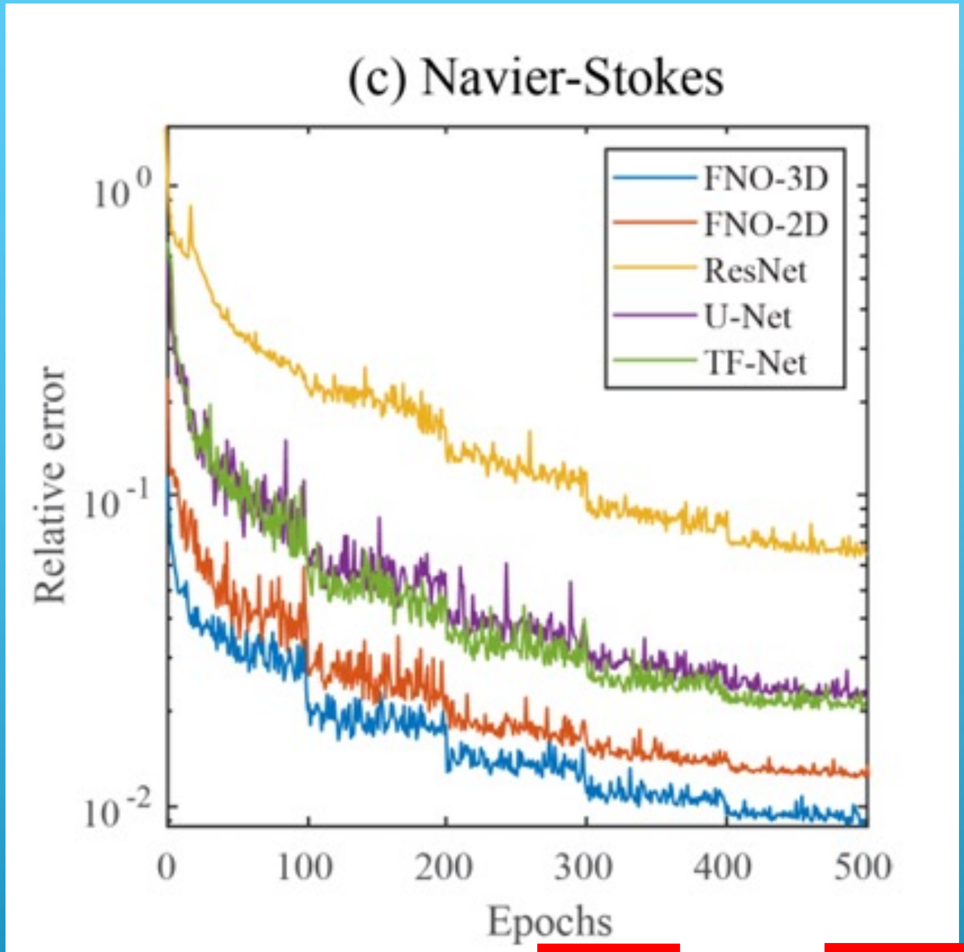
SIMULATION



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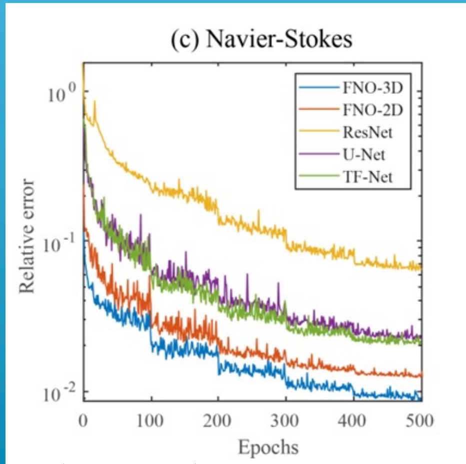
SIMULATION

FOURIER NEURAL OPERATOR WINS!



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KEY FEATURES

Speed and Accuracy:

- Speedy & no accuracy degradation
- Effective in downstream applications

Approximates:

- Highly non-linear operators with high frequency modes and slow energy decay

KEY FEATURES

Resolution-Invariant Solution Operator:

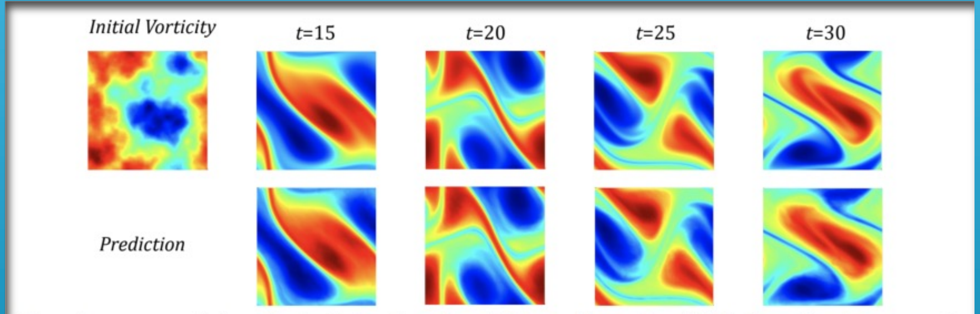
- First for Navier-Stokes equations in the turbulent regime

Shared Parameters:

- Maintains same learned network parameters

Capable of zero-shot super-resolution:

- Training lower resolution ➔ Evaluated higher resolution



Zero-shot super-resolution: Navier-Stokes Equation with Reynolds number 10000; Ground truth on top and prediction on bottom; trained on $64 \times 64 \times 20$ dataset; evaluated on $256 \times 256 \times 80$ (see Section 5.4).

Figure 1: **top:** The architecture of the Fourier layer; **bottom:** Example flow from Navier-Stokes.

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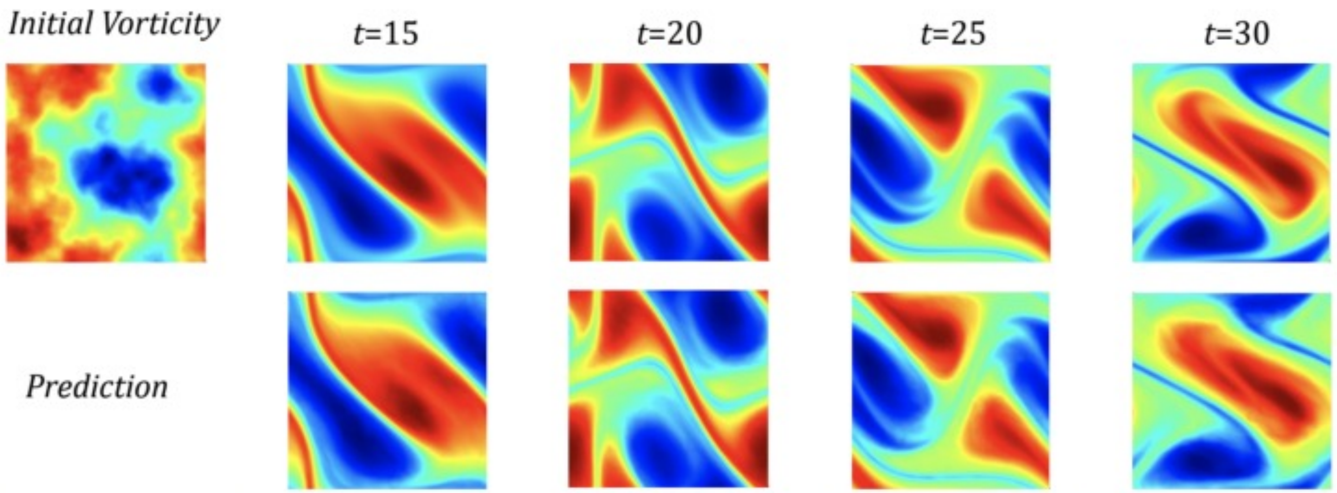

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