# 基于神经网络的代理模型

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# 本堂课大纲

- 卷积神经网络

- 神经算子
  - PCA-Net
  - 傅里叶神经算子
  - 深度神经算子(DeepONet)
  - Transformer

# 偏微分方程问题

- 偏微分方程问题

$$\mathcal{L}(x,u,a)=0 \quad x\in\Omega$$
$$\mathcal{B}(x,u)=0 \quad x\in\partial\Omega$$

- 代理模型(surrogate model)

两个函数空间 $\mathcal{A}=\{a:D\mapsto\mathbb{R}\}$ $\mathcal{U}=\{u:D\mapsto\mathbb{R}\}$，求解偏微分方程给出映射 $\mathcal{G}^{\dagger}:\mathcal{A}\mapsto\mathcal{U}$

降阶模型、高斯回归模型 $\mathcal{G}_\theta\approx\mathcal{G}^{\dagger}$ 是一个这样的映射的近似

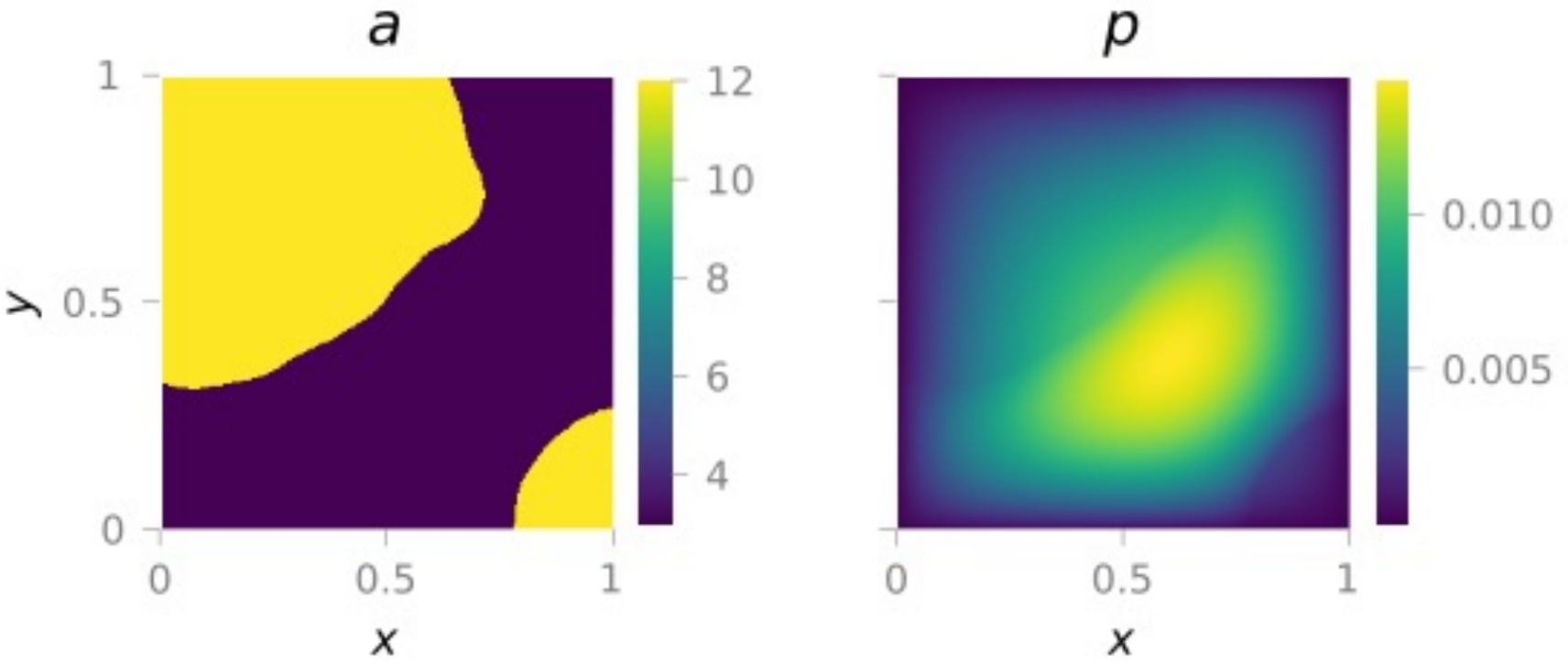
基于神经网络的代理模型 $\mathcal{G}_\theta\approx\mathcal{G}^{\dagger}$

# 卷积神经网络

- Darcy方程

$$-\nabla \cdot (a(x)\nabla p) = f(x), \qquad x \in D$$
$$p(x) = 0 \qquad\qquad x \in \partial D$$

$$\mathcal{G}^{\dagger} : a \mapsto p$$



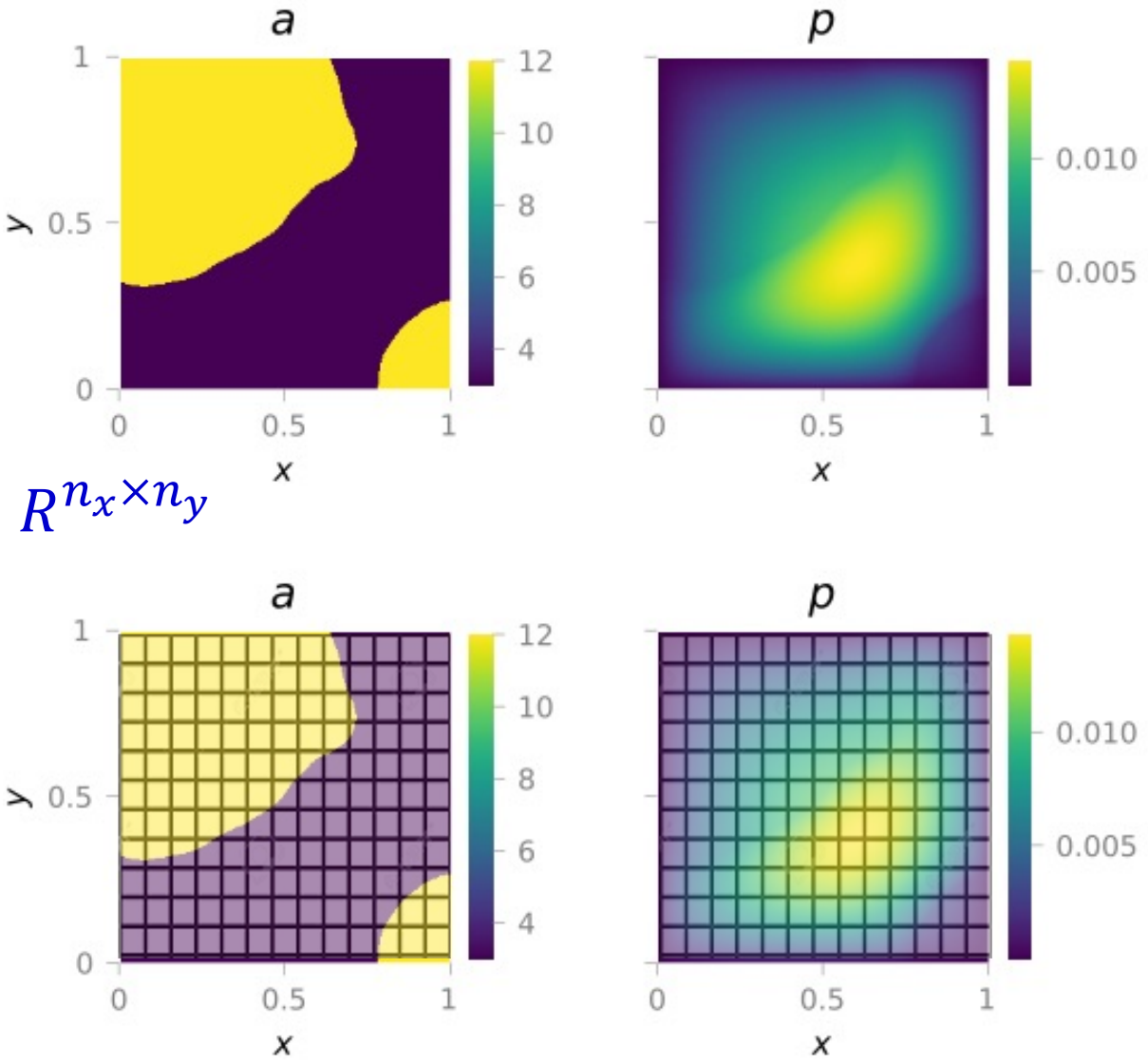
# 卷积神经网络

- 图像到图像的映射 (Zhu 2018)

$\mathcal{G}^\dagger : a \mapsto p$

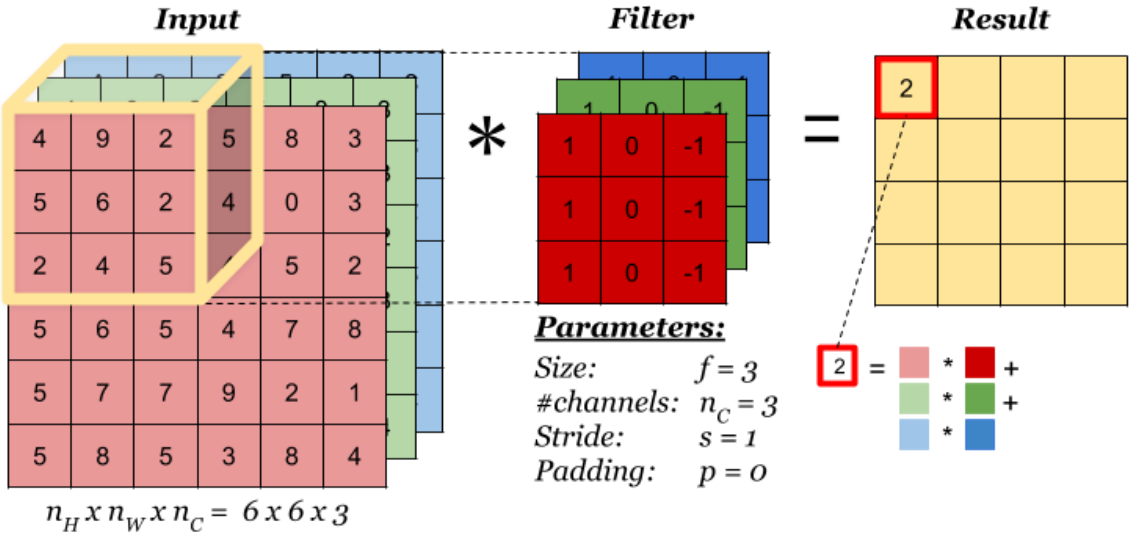
数值离散：

$f^\dagger : \tilde{a} \in R^{n_x \times n_y} \mapsto \tilde{p} \in R^{n_x \times n_y}$

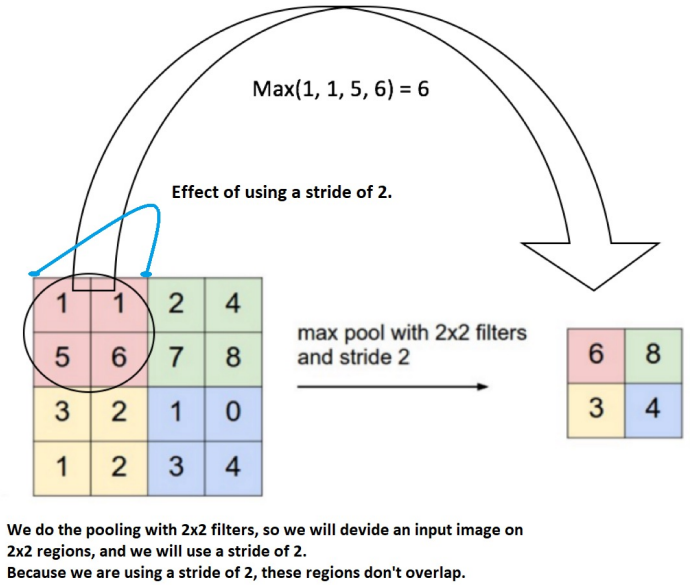


# 卷积神经网络

- 卷积模块

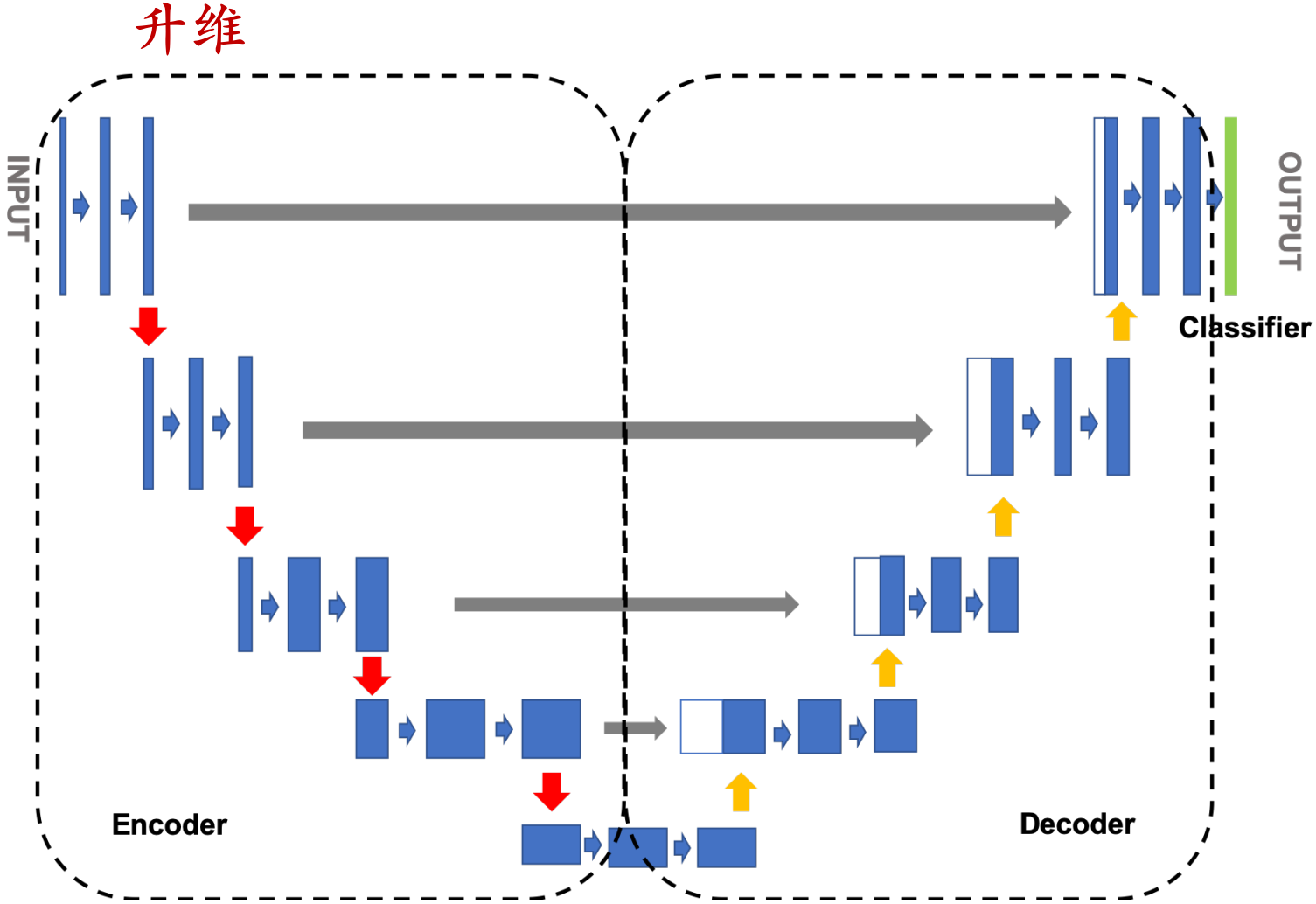



- 下采样层 (Pooling layer)



# 卷积神经网络

- U-Net (Ronneberger 2015)



# 卷积神经网络

- U-Net (Ronneberger 2015)

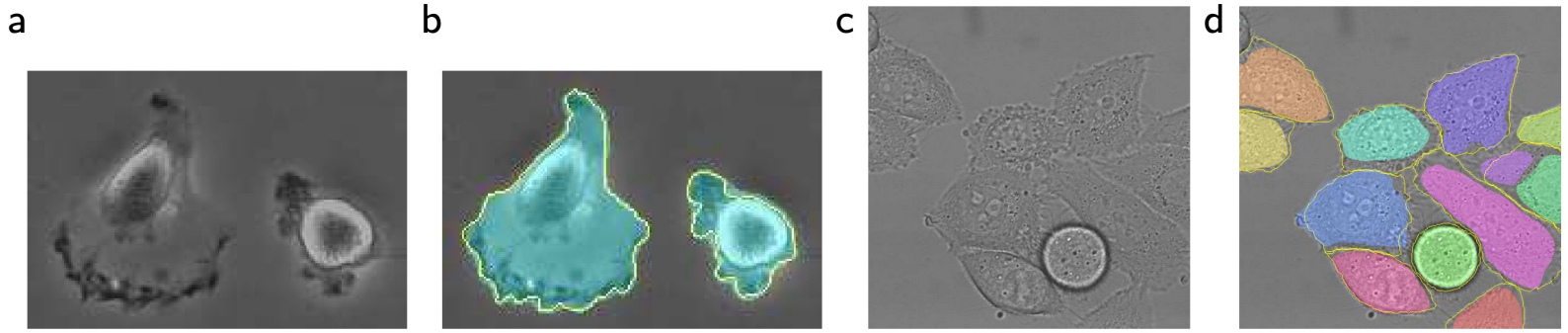


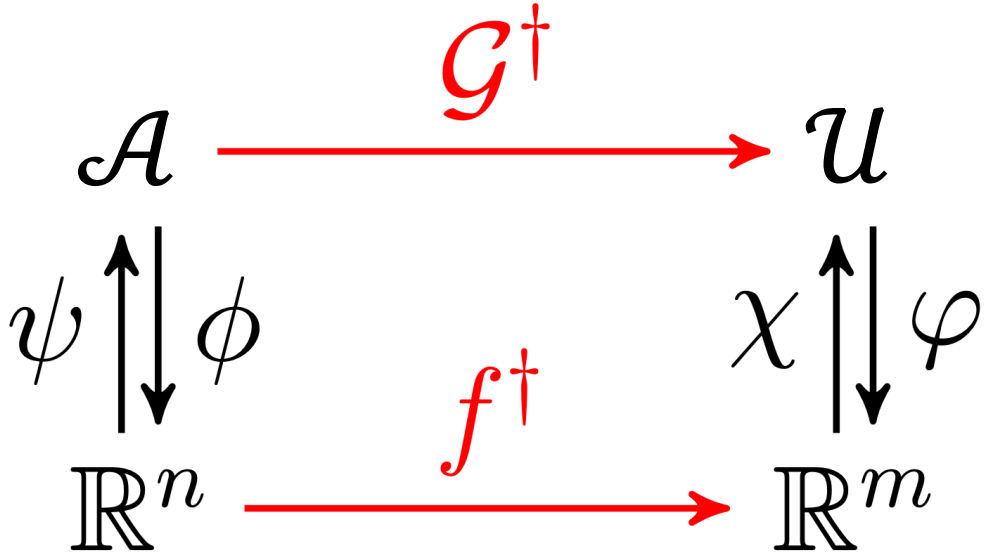

**Fig. 4.** Result on the ISBI cell tracking challenge. (**a**) part of an input image of the "PhC-U373" data set. (**b**) Segmentation result (cyan mask) with manual ground truth (yellow border) (**c**) input image of the "DIC-HeLa" data set. (**d**) Segmentation result (random colored masks) with manual ground truth (yellow border).

- Darcy方程

$$-\nabla\cdot(a(x)\nabla p)=f(x),\qquad x\in D$$
$$p(x)=0\qquad x\in\partial D$$

$$\mathcal{G}^{\dagger}:a\mapsto p$$

$$f^{\dagger}:\tilde{a}\in R^{n_x\times n_y}\mapsto\tilde{p}\in R^{n_x\times n_y}$$




直接近似$f^{\dagger}$

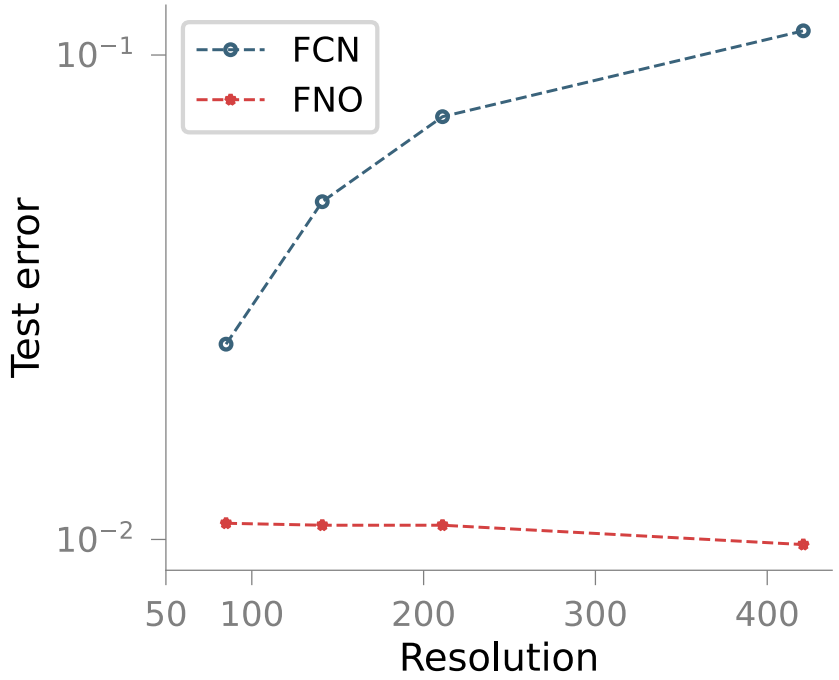
# 卷积神经网络

- Darcy方程

$$-\nabla \cdot (a(x)\nabla p) = f(x), \qquad x \in D$$
$$p(x) = 0 \qquad x \in \partial D$$

$$\mathcal{G}^{\dagger} : a \mapsto p$$

$$f^{\dagger}: \tilde{a} \in R^{n_x \times n_y} \mapsto \tilde{p} \in R^{n_x \times n_y}$$




诸如Fully Convolutional Neural Network (FCN)或者U-Net 这样先离散再近似的神经网络方法，对于不同的离散方式，如果不改变网络结构（比如卷积核尺寸）加密网格会导致测试误差将变差。

# 本堂课大纲

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  - PCA-Net
  - 傅里叶神经算子
  - 深度神经算子(DeepONet)
  - Transformer

# 神经算子

- 神经网络

函数(function)： $\mathbb{R}^n \mapsto \mathbb{R}^m$

线性函数：$x \mapsto Ax + b$

逐点激活函数：$x \mapsto \sigma(x)$

- 神经算子

算子(operator)：$\mathcal{A} \mapsto \mathcal{U}$

$$\mathcal{A} = \{a: D \mapsto \mathbb{R}\} \qquad \mathcal{U} = \{u: D \mapsto \mathbb{R}\}$$

线性算子：

$$a(x) \mapsto \int \kappa(x, y)a(y)dy + b(x), \qquad b(x) = wa(x) + b$$

逐点激活函数：$a(x) \mapsto \sigma(a(x))$

# 线性算子

- 核函数

正交基底：$\Psi = [\psi_1\ \psi_2\ \cdots\cdots\ \psi_l]$

矩阵：$A \in R^{l\times l}$

$$\kappa(x,y) = \Psi(x)A\Psi(y)^T$$

- 线性算子

$$a(x) \mapsto \int \kappa(x,y)a(y)dy + b(x)$$

$$= \int \Psi(x)A\Psi(y)^T a(y)dy + b(x)$$

计算系数

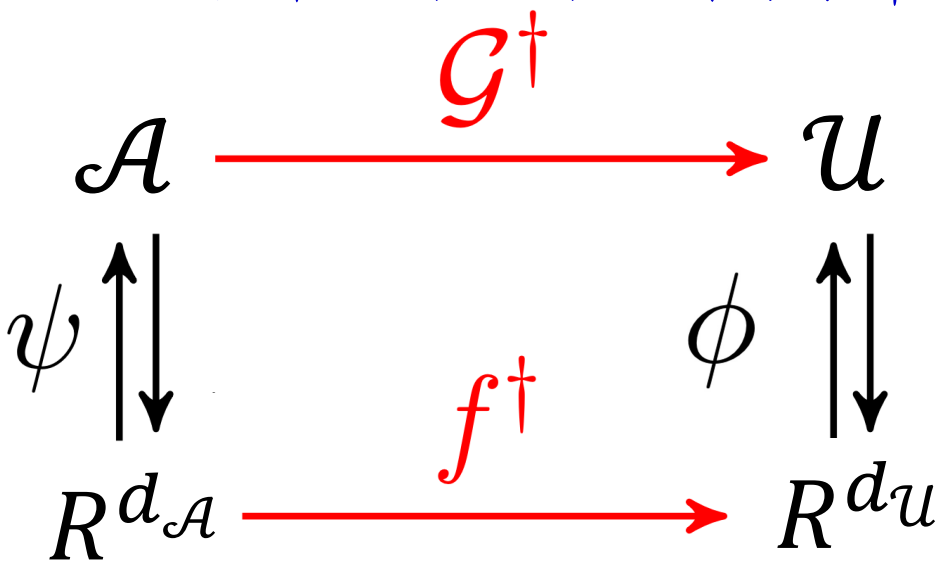
$$= \Psi(x)A\int \Psi(y)^T a(y)dy + b(x)$$

# PCA神经网络

- PCA-Net(Hesthaven 2018, Bhattachary 2021)

$$a(x) = \sum_{i=1}^{d_{\mathcal{A}}} \hat{a}_i \psi_i(x) \qquad u(x) = \sum_{i=1}^{d_{\mathcal{U}}} \hat{u}_i \phi_i(x)$$

$\{\psi_i\}_{i=1}^{d_{\mathcal{A}}}$ 和 $\{\phi_j\}_{j=1}^{d_{\mathcal{U}}}$ 分别是输入和输出函数的基底，采用本征正交分解从输入输出训练集中得到。



# PCA神经网络

**万能逼近定理(Bhattacharya 2021)**

设$\mathcal{A}$和$\mathcal{U}$为实的希尔伯特空间，设$\mu$是在$\mathcal{A}$上的概率测度，且满足$\mathbb{E}_{a\sim\mu}\|a\|^4 < \infty$。假设映射$\mathcal{G}^\dagger : \mathcal{A} \to \mathcal{U}$是全局 Lipschitz 连续。给定$d_{\mathcal{A}}$和$d_{\mathcal{U}}$，训练数据量$n$，误差参数$\epsilon > 0$，那么存在PCA神经网络$\mathcal{G}_\theta$满足：

$$\mathbb{E}_{\{a_i\}\sim\mu}\mathbb{E}_{a\sim\mu}\left\|\mathcal{G}^\dagger(a) - \mathcal{G}_\theta(a)\right\|^2$$

$$\leq C\left(\epsilon^2 + \sqrt{\frac{d_{\mathcal{A}}}{n}} + R^{\mu}(V_{d_{\mathcal{A}}}) + \sqrt{\frac{d_{\mathcal{U}}}{n}} + R^{\mathcal{G}^\dagger_{\#}\mu}(V_{d_{\mathcal{U}}})\right)$$

有限维空间的神经网络万能逼近定理

本征正交分解$\mathcal{A}$和$\mathcal{U}$空间中的投影误差

投影误差：$R^{\nu}(V) = \mathbb{E}_{\{f\}\sim\nu}\|f - \Pi_V f\|^2$

# 傅里叶神经算子

- 平移不变核函数

$$\kappa(x,y)=\kappa(x-y)$$

$$\kappa(r)=\sum \hat{\kappa}_k\, e^{2\pi ik\cdot r} \qquad (\psi_k(x)=\left[e^{2\pi ik\cdot x}\right] \quad A=\mathrm{diag}\{\hat{\kappa}_k\})$$

- 傅里叶线性算子

$$a(x)\mapsto \int \kappa(x,y)a(y)dy+b(x)$$

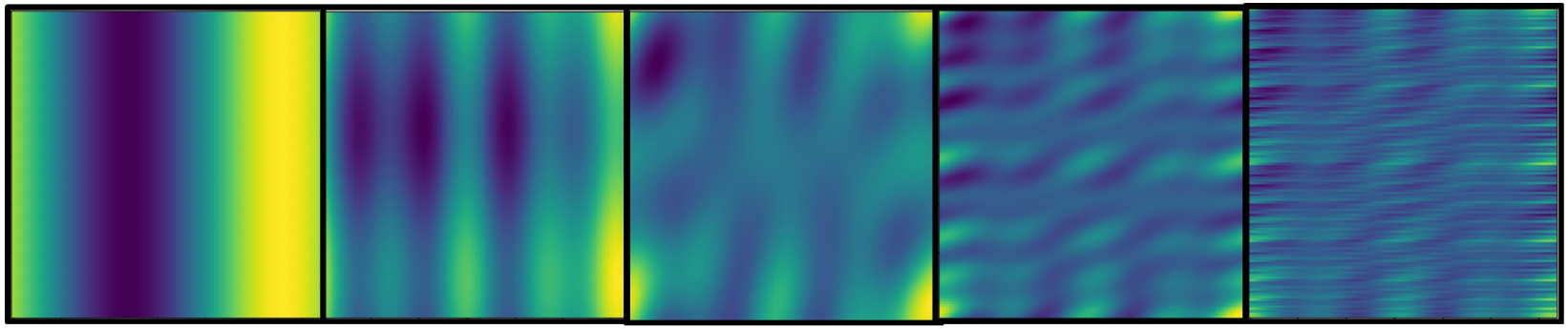
$$=\int \kappa(x-y)a(y)dy+b(x)$$

$$=\sum \hat{\kappa}_k\hat{a}_k\, e^{2\pi ikx}+b(x)$$

# 傅里叶神经算子

- 图像到图像的映射

Filters in CNN



Fourier Filters

# 傅里叶神经算子

- 傅里叶层

给定函数$a(\cdot): D \to \mathbb{R}$

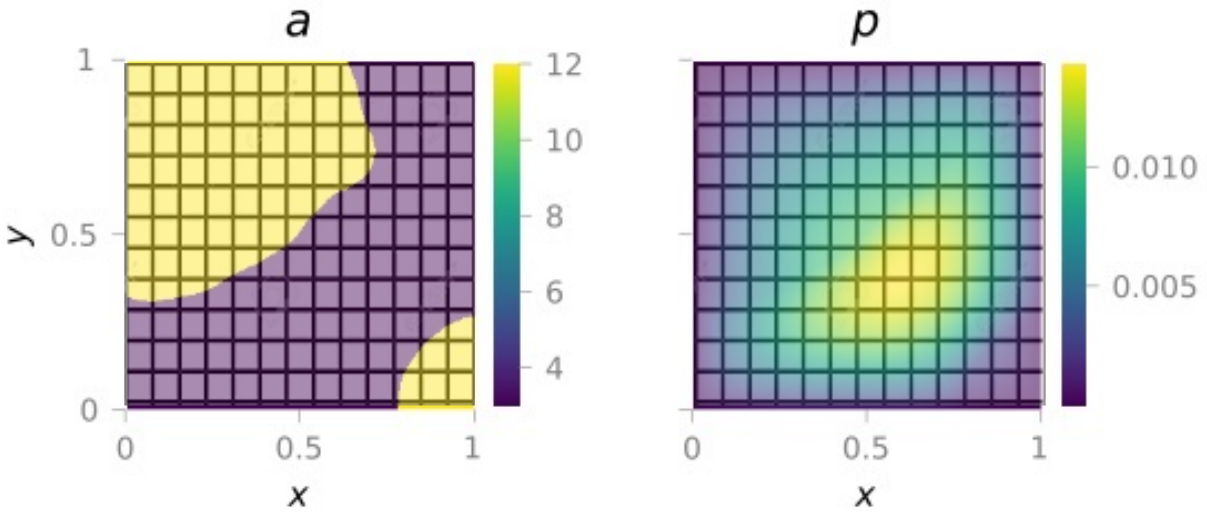
$$f(a) = h(wa + b + \mathcal{F}^{-1}A\mathcal{F}a)$$

$\mathcal{F}$和$\mathcal{F}^{-1}$为傅里叶变换和傅里叶逆变换

$w, b \in \mathbb{R}$

$A$为对角矩阵 $\mathrm{diag}\{\hat{\kappa}_k\}$

$h$为逐点的激活函数



# 傅里叶神经算子

- 傅里叶层

升维

给定函数$a(\cdot): D \to \mathbb{R}^{d_f}$

$$f(a) = h(Wa + b + \mathcal{F}^{-1}A\mathcal{F}a)$$

$\mathcal{F}$和$\mathcal{F}^{-1}$为傅里叶变换和傅里叶逆变换

$W \in \mathbb{R}^{d_f' \times d_f}, b \in \mathbb{R}^{d_f'}$

$A$为分块对角矩阵 $\mathrm{diag}\{A_i \in \mathbb{C}^{d_f' \times d_f}\}$

$h$为逐点的激活函数

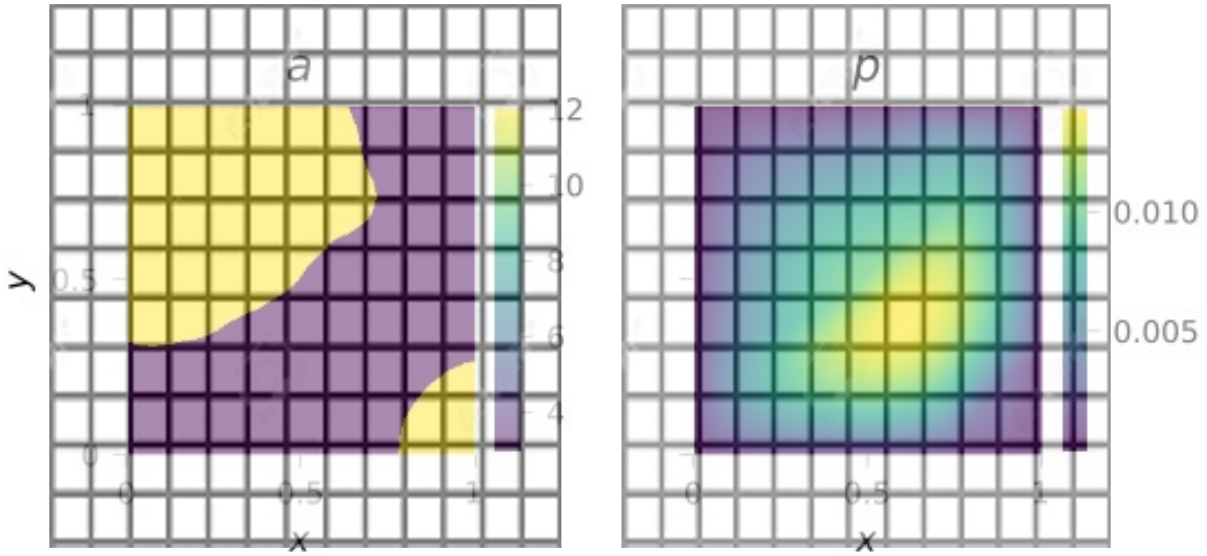
$$\mathcal{F}a_1 \Longrightarrow \begin{bmatrix} \hat{a}_1^{(1)} \\ \vdots \\ \hat{a}_{d_f}^{(1)} \end{bmatrix} \quad \begin{bmatrix} \hat{a}_1^{(2)} \\ \vdots \\ \hat{a}_{d_f}^{(2)} \end{bmatrix} \quad \cdots\cdots \quad \begin{bmatrix} \hat{a}_1^{(k_{max})} \\ \vdots \\ \hat{a}_{d_f}^{(k_{max})} \end{bmatrix}$$

$$A\mathcal{F}(\mathrm{a}(\xi)) = A_1 \begin{bmatrix} \hat{a}_1^{(1)} \\ \vdots \\ \hat{a}_{d_f}^{(1)} \end{bmatrix} \quad A_2 \begin{bmatrix} \hat{a}_1^{(2)} \\ \vdots \\ \hat{a}_{d_f}^{(2)} \end{bmatrix} \quad \cdots\cdots \quad A_{k_{max}} \begin{bmatrix} \hat{a}_1^{(k_{max})} \\ \vdots \\ \hat{a}_{d_f}^{(k_{max})} \end{bmatrix}$$

# 傅里叶神经算子

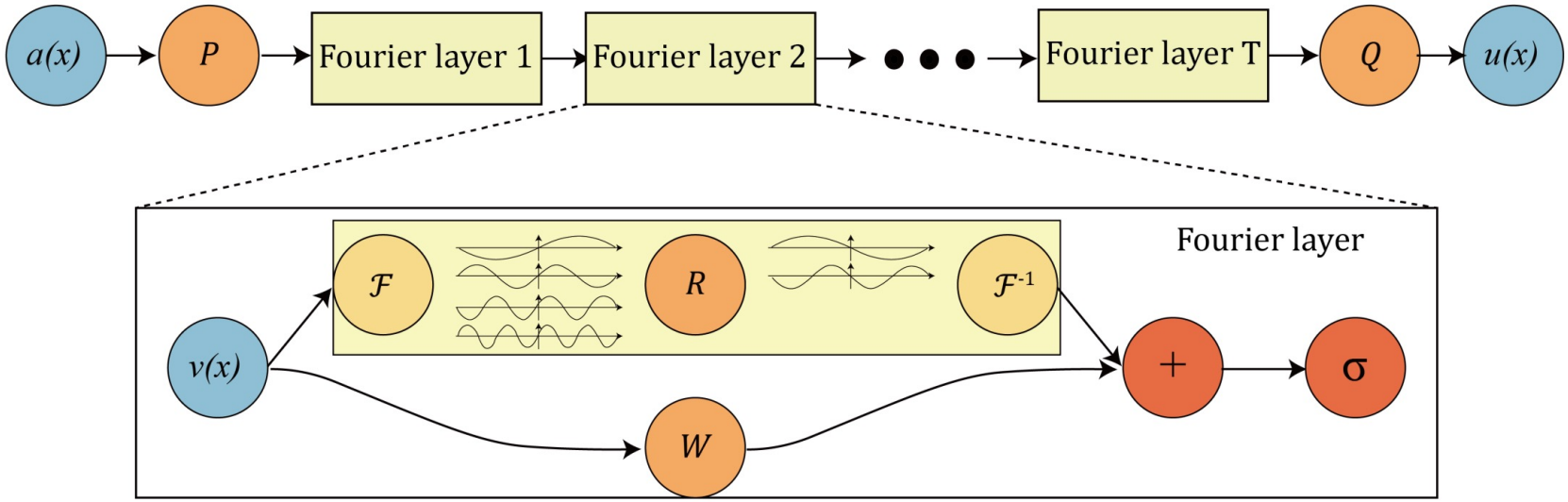
- 傅里叶层

当问题非周期时，使用补零填充(padding)



# 傅里叶神经算子

- 傅里叶神经算子




升维(lifting)算子 $P: \{D \to \mathbb{R}\} \to \{D \to \mathbb{R}^{d_f}\}$

$$P: a \to Wa + b, \qquad W \in R^{d_f \times 1}, b \in R^{d_f}$$

投影(projection)算子 $Q: \{D \to \mathbb{R}^{d_f}\} \to \{D \to \mathbb{R}\}$

$$Q: a \to W^{(2)}\sigma\left(W^{(1)}a + b^{(1)}\right) + b^{(2)},$$

$$W^{(1)} \in \mathbb{R}^{d_{out} \times d_f}, b^{(1)} \in \mathbb{R}^{d_{out}} \quad W^{(2)} \in \mathbb{R}^{1 \times d_{out}}, b^{(2)} \in \mathbb{R}$$

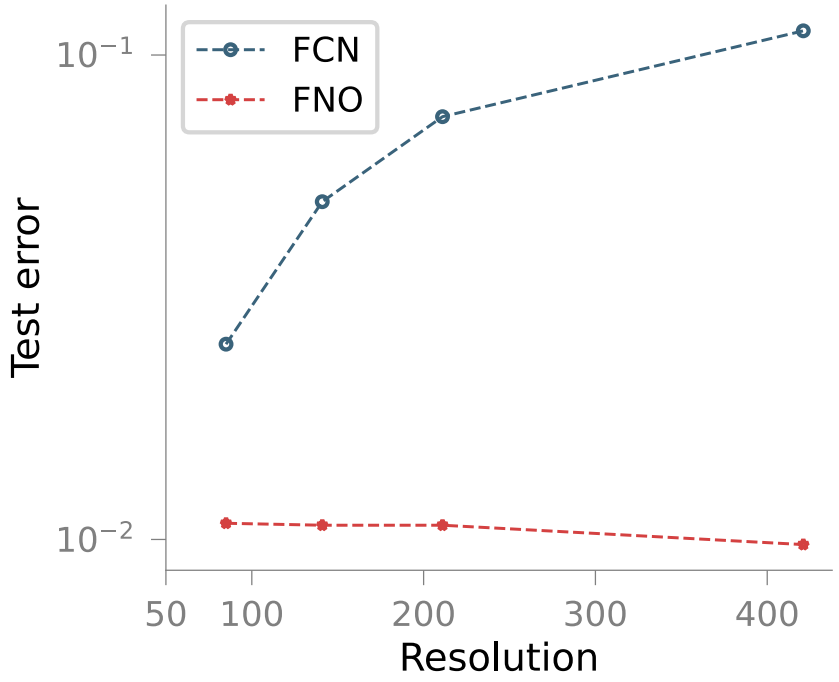
# 傅里叶神经算子

- Darcy方程

$$-\nabla \cdot (a(x)\nabla p) = f(x), \qquad x \in D$$
$$p(x) = 0 \qquad x \in \partial D$$

$$\mathcal{G}^\dagger : a \mapsto p$$

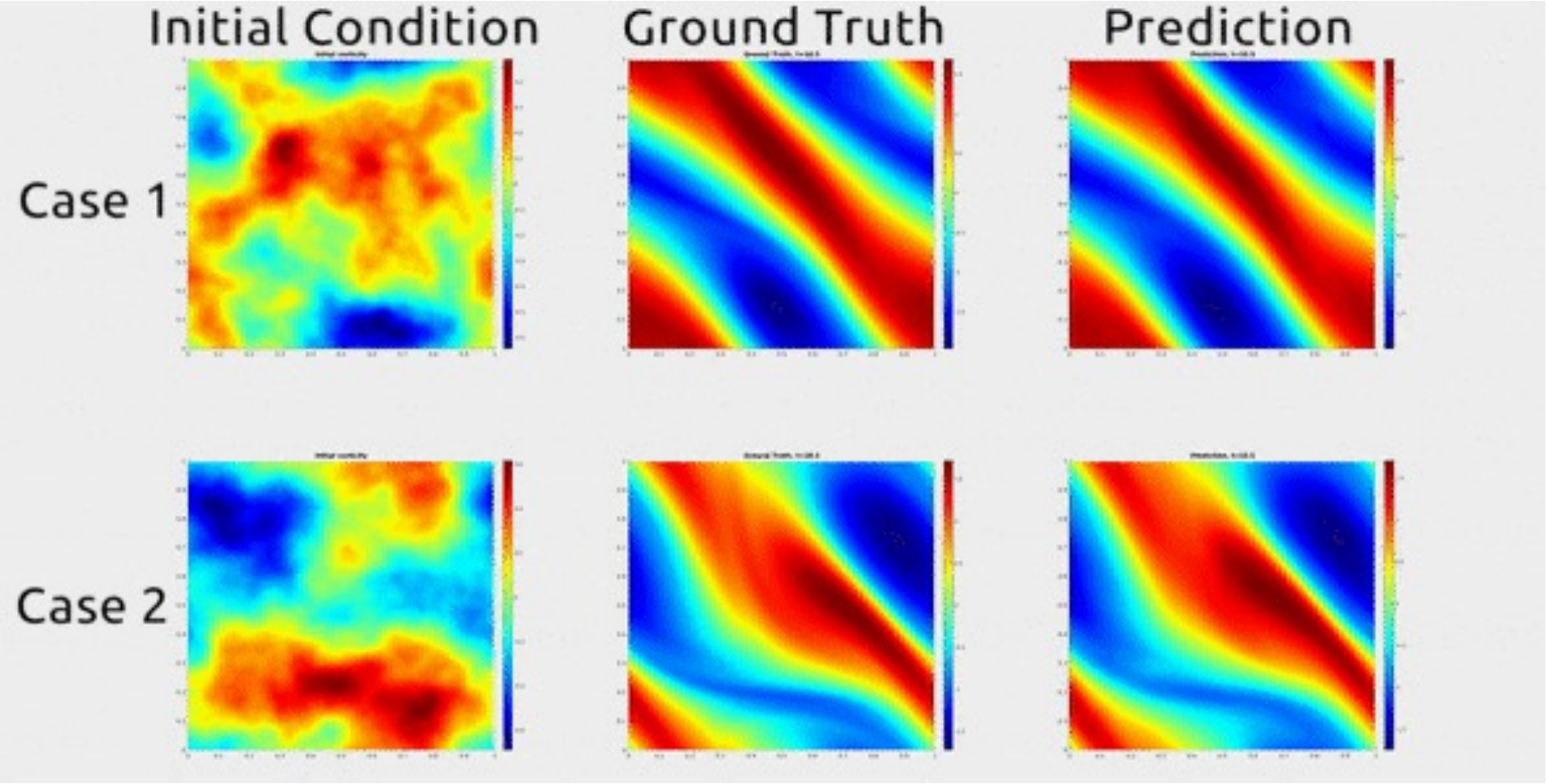
$$f^\dagger : \tilde{a} \in \mathbb{R}^{n_x \times n_y} \mapsto \tilde{p} \in \mathbb{R}^{n_x \times n_y}$$




傅里叶神经算子是函数空间上的映射，与网格离散无关，因此网格加密不会导致测试误差变差。

# 傅里叶神经算子

- 2维不可压缩Navier-Stokes方程



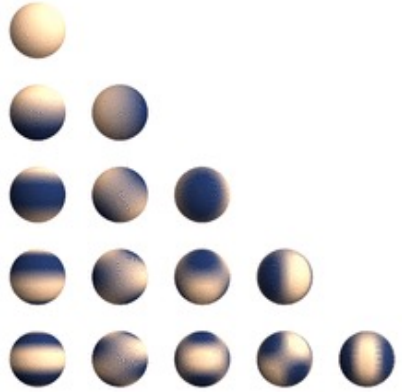
# 基底选择

- 基底函数

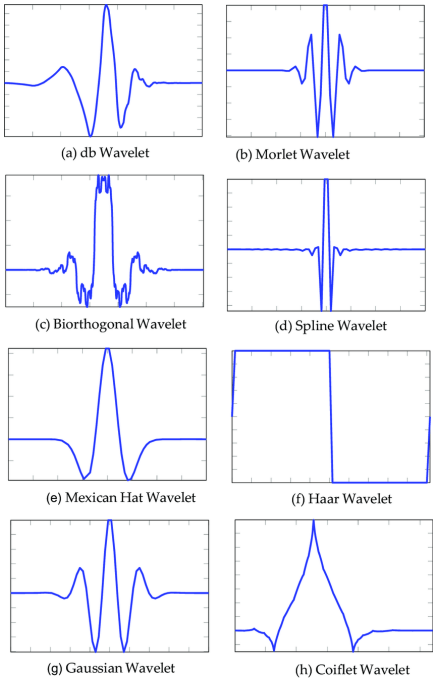
PCA基底函数

傅里叶基底函数：$e^{-2\pi ik\frac{x}{L}}$

球面上的问题：球谐函数(spherical harmonics)



多尺度问题：小波(wavelet)




从数据中学习基底函数

# 深度神经算子(DEEPONET)

- PCA-Net (Hesthaven 2018, Bhattachary 2021)

$$a(x) = \sum_{i=1}^{d_{\mathcal{A}}} \hat{a}_i \psi_i(x) \qquad u(x) = \sum_{i=1}^{d_{\mathcal{U}}} \hat{u}_i^{NN}(\hat{a}) \phi_i(x)$$

$\{\psi_i\}_{i=1}^{d_{\mathcal{A}}}$ 和 $\{\phi_j\}_{j=1}^{d_{\mathcal{U}}}$ 分别是输入和输出函数的基底，采用本征正交分解从输入输出训练集中得到。

- 深度神经算子(Deep Operator Networks)

$$a(x) = \sum_{i=1}^{d_{\mathcal{A}}} \hat{a}_i \psi_i(x) \qquad u(x) = \sum_{i=1}^{d_{\mathcal{U}}} \hat{u}_i^{NN}(\hat{a}) \phi_i^{NN}(x)$$

$\hat{u}_i^{NN}$：分支网络(branch network)

$\hat{\phi}_i^{NN}$：主干网络(trunk network)

同时从数据中进行学习

# 深度神经算子(DEEPONET)

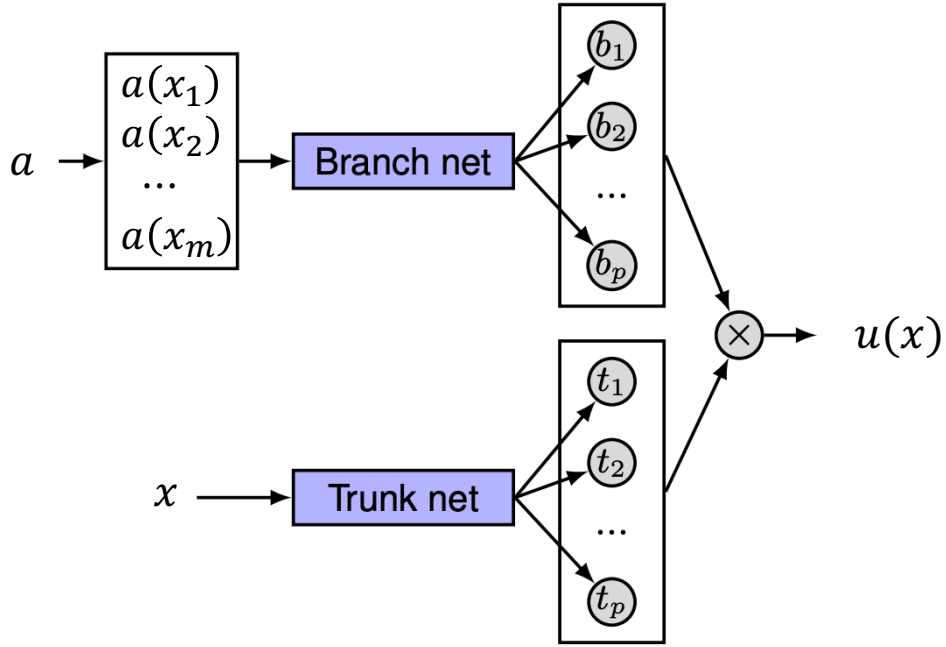
- 深度神经算子(Deep Operator Networks)

特征提取：$a(x) \to \hat{a} = [a(x_1), a(x_2), \cdots a(x_m)]$

DeepONet ：$a(\cdot) \to u(\cdot) = \sum b_i(\hat{a}) t_i(\cdot)$

$b_i$：分支网络(branch network)

$t_i$：主干网络(trunk network)



# TRANSFORMER

- 注意力机制(Attention)

编码器状态 (encoder states) $x_1, x_2, \cdots, x_n \in R^c$

解码器状态 (decoder states) $h \in R^o$

投影：

$$f = < x_1, h > x_1 + < x_2, h > x_2 + \cdots + < x_n, h > x_n$$

计算编码器状态 和解码状态的相关性:

$$\text{score}(h, x_i)$$

注意力权重：

$$a_i = \frac{\exp\big(\text{score}(h, x_i)\big)}{\sum_{i=1}^{n} \exp\big(\text{score}(h, x_i)\big)}$$

输出： $f = a_1 x_1 + a_2 x_2 + \cdots + a_n x_n$

# TRANSFORMER

- 自注意力机制(Attention)

编码器状态 (encoder states) $x_1, x_2, \cdots, x_n \in R^c$

查询 (query): $q_i = W^q x_i \ (W^q \in R^{m \times c})$

键 (key): $k_i = W^k x_i \ (W^k \in R^{m \times c})$

值 (value): $v_i = W^v x_i \ (W^v \in R^{m \times c})$

相关性(alignment\score):

$$e_{ij} = \frac{q_i \cdot k_j}{\sqrt{m}} \qquad a_{ij} = \frac{\exp(e_{ij})}{\sum_{j'=1}^{n} \exp(e_{ij'})}$$

输出：

$$\text{Attention}(q, k, v)_i = \sum_{j=1}^{n} a_{ij} v_j$$

$$= < q_i, k_1 > v_1 + < q_i, k_2 > v_2 + \cdots + < q_i, k_n > v_n$$

# TRANSFORMER

- 自注意力机制(Attention)

编码器状态 (encoder states)

$$a = [a_1, a_2, \cdots, a_c]: D \to R^c$$

查询 (query):

$$q = W^q a \ (W^q \in R^{m \times c}): D \to R^m$$

键 (key):

$$k = W^k a \ (W^k \in R^{m \times c}): D \to R^m$$

值 (value):

$$v = W^v a \ (W^v \in R^{m \times c}): D \to R^m$$

计算每个格点之间的相关性

$$a(x_i) = [a_1(x_i), a_2(x_i), \cdots, a_c(x_i)]$$
$$a(x_j) = [a_1(x_j), a_2(x_j), \cdots, a_c(x_j)]$$

# TRANSFORMER

- 自注意力机制(Attention)

相关性(alignment\score):

$$e_{ij} = \frac{q(x_i) \cdot k(x_j)}{\sqrt{m}} \qquad a_{ij} = \frac{\exp(e_{ij})}{\sum_{j'=1}^{N} \exp(e_{ij'})}$$

输出：

$$u(x_i) = \text{Attention}(q, k, v)_i = \sum_{j=1}^{N} a_{ij} v(x_j)$$

$$= < q_i, k_1 > v_1 + < q_i, k_2 > v_2 + \cdots + < q_i, k_n > v_n$$

$$u(x) = \int \frac{\exp(q(x) \cdot k(y)/\sqrt{m})}{\int \exp(q(x) \cdot k(z)/\sqrt{m}) dz} v(y) dy$$

系数　　基底

# 本堂课大纲

- 神经算子
  - 对于一些问题能够高效、精确预测
  - 需要大量数据训练
  - 超参选取
  - 预测仅限于内插（分布内数据）

# 参考文献

## 参考文献


基于卷积神经网络的代理模型：Zhu, Yinhao, and Nicholas Zabaras. "Bayesian deep convolutional encoder – decoder networks for surrogate modeling and uncertainty quantification." Journal of Computational Physics 366 (2018): 415-447.

提出U-net 的文章：Ronneberger, Olaf, Philipp Fischer, and Thomas Brox. "U-net: Convolutional networks for biomedical image segmentation." In Medical image computing and computer-assisted intervention – MICCAI 2015: 18th international conference, Munich, Germany, October 5-9, 2015, proceedings, part III 18, pp. 234-241. Springer International Publishing, 2015.

提出 PCA-Net 的文章： Hesthaven, Jan S., and Stefano Ubbiali. "Non-intrusive reduced order modeling of nonlinear problems using neural networks." Journal of Computational Physics 363 (2018): 55-78.

分析 PCA-Net 的文章：Bhattacharya, Kaushik, Bamdad Hosseini, Nikola B. Kovachki, and Andrew M. Stuart. "Model reduction and neural networks for parametric PDEs." The SMAI journal of computational mathematics 7 (2021): 121-157.

# 参考文献

## 参考文献


提出 FNO的文章： Li, Zongyi, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. "Fourier neural operator for parametric partial differential equations." arXiv preprint arXiv:2010.08895 (2020).

用球谐函数做基底的文章：Bonev, Boris, Thorsten Kurth, Christian Hundt, Jaideep Pathak, Maximilian Baust, Karthik Kashinath, and Anima Anandkumar. "Spherical fourier neural operators: Learning stable dynamics on the sphere." In International conference on machine learning, pp. 2806-2823. PMLR, 2023.

用小波做基底的文章： Gupta, Gaurav, Xiongye Xiao, and Paul Bogdan. "Multiwavelet-based operator learning for differential equations." Advances in neural information processing systems 34 (2021): 24048-24062.

提出 DeepONet的文章：Lu, Lu, Pengzhan Jin, Guofei Pang, Zhongqiang Zhang, and George Em Karniadakis. "Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators." Nature machine intelligence 3, no. 3 (2021): 218-229.