AI in the Sciences and Engineering 2024: Lecture 14

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What you learnt so far

- Operator learning: Given Abstract PDE: $\mathcal{D}_a(u) = f$
- Learn Solution Operator: $\mathcal{G} : \mathcal{X} \mapsto \mathcal{Y}$ with $\mathcal{G}(a, f) = u$
- Enforce Continuous-Discrete Equivalence via ReNO:

$$
\begin{tikzcd}
\mathcal{X} \arrow[r, "\mathcal{G}"] \arrow[d, bend left, "\mathcal{E}"] & \mathcal{Y} \arrow[d, bend left, "\mathcal{E}"] \\
X \arrow[r, "G"] \arrow[u, bend left, "\mathcal{R}"] & Y \arrow[u, bend left, "\mathcal{R}"]
\end{tikzcd}
$$

$$\mathcal{G} = \mathcal{R} \circ G \circ \mathcal{E}$$

- Neither CNN nor FNO are ReNOs.
- SNO/DeepONet can be ReNOs but perform poorly !!
- Challenge: Design a ReNO that works

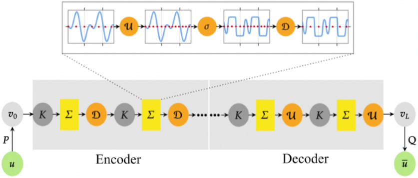
Can Convolutions be back in the reckoning ?

- Advantages of Convolution based models:
  - Variety of SOTA models in Vision etc.
  - Locality + Computational efficiency
  - CNNs closely linked with Finite difference Methods [1]
- Issue: Inconsistency in Function Space
- Plain vanilla CNNs and variants are not ReNOs

[1] Haber, Rutthoto, 2017

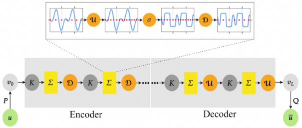
Convolutions Strike Back !!

- Convolutional Neural Operators (CNOs) of Raonic et al, 2023.



- Operator between Band-Limited Functions
- Building Blocks:
- Lifting operator: P
- Projection operator: Q

CNO Key Building Block I



- Use Continuous Convolutions on Bandlimited functions
- Convolution Kernel is still Discrete !!
- Convolution operator is a ReNO.

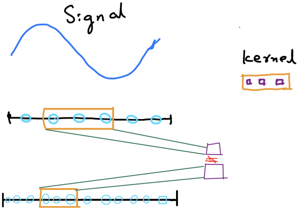
$$\begin{tikzcd} \mathcal{B}_w \arrow[r, "\mathcal{K}_w"] & \mathcal{B}_w \arrow[d, "T^*_{\Psi_w}"] \\ \ell^2(\mathbb{Z}^2) \arrow[u, "T_{\Psi_w}"] \arrow[r] & \ell^2(\mathbb{Z}^2) \end{tikzcd}$$

Contrast with CNNs

- CNNs rely on Discrete Convolutions with fixed Kernel:

$$K_c[m] = \sum_{i=-s}^{s} k_i c[m-i]$$

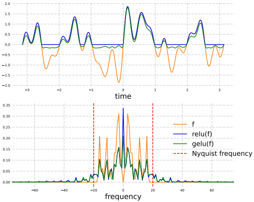
- Pointwise evaluations with Sinc basis

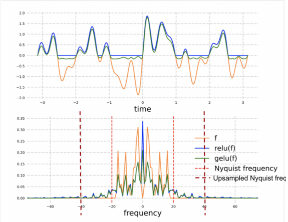


- Easy to check that CNNs are Resolution dependent as:

$$\mathcal{G}' \neq \mathcal{E}' \circ \mathcal{R} \circ \mathcal{G} \circ \mathcal{E} \circ \mathcal{R}'$$

CNO Key Building Block II: Activation Function ?

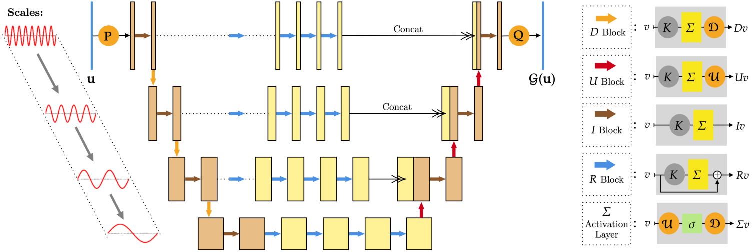




- Apply Activation as $\Sigma : B_w \mapsto B_w$ with $\Sigma = \mathcal{D}_{\bar{w},w} \circ \sigma \circ \mathcal{U}_{w,\bar{w}}$
- Upsampling: $\mathcal{U}_{w,\bar{w}} f = f$ with $w < \bar{w}$
- Downsampling: $\mathcal{D}_{\bar{w},w} f(x) = \left(\frac{\bar{w}}{w}\right)^d \int\limits_D \mathrm{sinc}(2\bar{w}(x-y)) f(y) dy$
- Activation is a ReNO if $\bar{w} >> w$:

$$\begin{tikzcd}
\mathcal{B}_w \arrow[r, hook, "P_{\mathcal{B}_{\overline{w}}(\mathbb{R}^2)}"] & \mathcal{B}_{\overline{w}} \arrow[r, "\sigma"] \arrow[d, "T^*_{\Psi_{\overline{w}}}"] & \mathcal{B}_{\overline{w}} \arrow[r, "P_{\mathcal{B}_w(\mathbb{R}^2)}"] & \mathcal{B}_w \arrow[d, "T^*_{\Psi_w}"] \\
\ell^2(\mathbb{Z}^2) \arrow[u, "T_{\Psi_w}"] \arrow[r, "\mathcal{U}_{w,\overline{w}}"] & \ell^2(\mathbb{Z}^2) \arrow[r, "\sigma"] & \ell^2(\mathbb{Z}^2) \arrow[u, "T_{\Psi_{\overline{w}}}"] \arrow[r, "\mathcal{D}_{\overline{w},w}"] & \ell^2(\mathbb{Z}^2)
\end{tikzcd}$$

CNO Architecture in Practice



- CNO instantiated as a modified Operator UNet
- Built for multiscale information processing

CNO properties

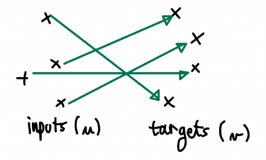
- CNO is a ReNO by construction.
- Universal Approximation Theorem:
- CNOs approximate any Continuous + operators $\mathcal{G} : H^r \mapsto H^s$
- Proof relies on building $\mathcal{G} \approx \mathcal{G}^* : \mathcal{B}_w \mapsto \mathcal{B}_{w'}$

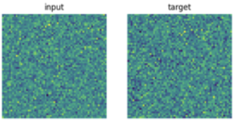
$$\begin{tikzcd}
\mathcal{B}_w \arrow[r, "\mathcal{G}^*"] \arrow[d, "T^*_{\Psi_w}"] & \mathcal{B}_{w'}, \\
\ell^2(\mathbb{Z}^2) \arrow[r, "\mathfrak{G}_{\Psi_w, \Psi_{w'}}"] & \ell^2(\mathbb{Z}^2) \arrow[u, "T_{\Psi_{w'}}"']
\end{tikzcd}$$

- Efficient PyTorch implementation with CUDA kernels.
- Code available on
  https://github.com/bogdanraonic3/ConvolutionalNeuralOperator.git

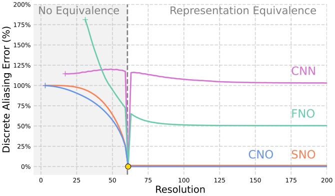
A Synthetic Example: Random Assignment

- The underlying Operator:



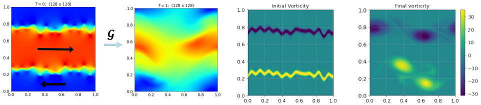


- Errors:

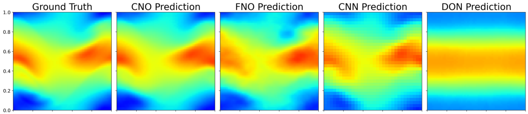


Ex 1: Navier-Stokes Eqns.

- Operator:



- Comparison:

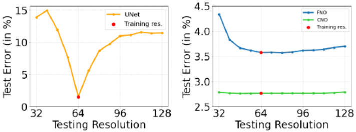


- Test Errors:

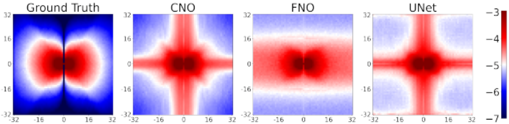
Model	FFNN	UNet	DeepONet	FNO	CNO
Error	8.05%	3.54%	11.64%	3.93%	3.01%

Further Results

- Resolution Dependence:

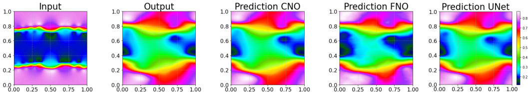


- Spectral Behavior: log spectra

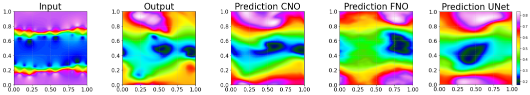


Out-of-Distribution Generalization or Zero-shot Learning

- Results for In-Distribution Testing:



- Results for Out-of-Distribution Testing:

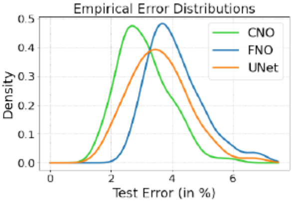


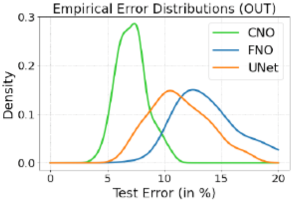
- Test Errors:

Model	FFNN	UNet	DeepONet	FNO	CNO
In	8.05%	3.54%	11.64%	3.93%	3.01%
Out	16.12%	10.93%	15.05%	13.45%	7.06%

- RunTime: 10^{-1}s on 100^2 grid for AzeBan vs 10^{-4}s for CNO

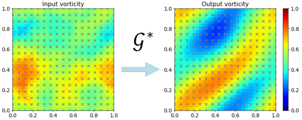
Success is a histogram, not a point !!



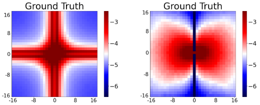


On the Choice of Benchmarks

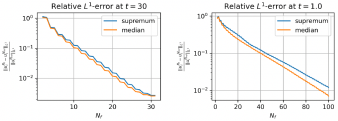
- Often used benchmark:



- Errors: 1.15% for FNO vs. 0.96% for CNO !!
- Spectral Structure is Not Rich Enough:

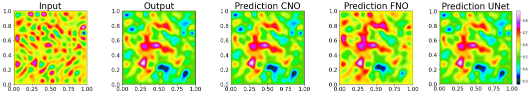


- Fast approximation with AzeBan: $< 10^{-3}$ sec

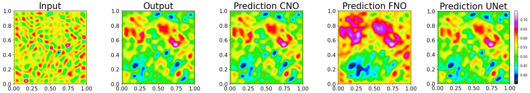


Ex 2: Poisson Eqn

- Results for In-Distribution Testing:



- Results for Out-of-Distribution Testing:

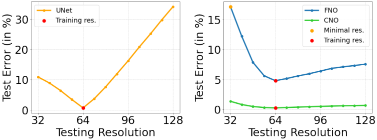


- Test Errors:

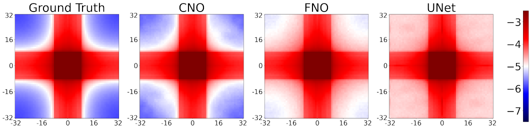
Model	FFNN	UNet	DeepONet	FNO	CNO
In	5.74%	0.71%	12.92%	4.78%	0.23%
Out	5.35%	1.27%	9.15%	8.89%	0.27%

Further Results

- Resolution Dependence:

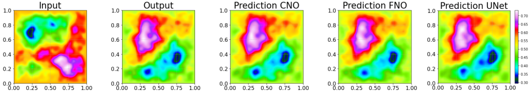


- Spectral Behavior: log spectra

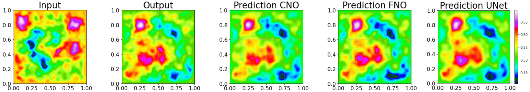


Ex 3: Wave Eqn

- Results for In-Distribution Testing:



- Results for Out-of-Distribution Testing:

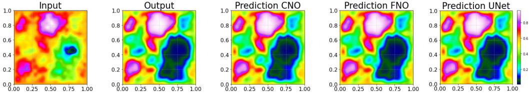


- Test Errors:

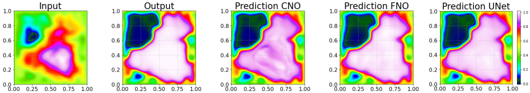
Model	FFNN	UNet	DeepONet	FNO	CNO
In	2.51%	1.51%	2.26%	1.10%	0.83%
Out	3.01%	2.03%	2.83%	1.61%	1.48%

Ex 4: Allen-Cahn Eqn

- Results for In-Distribution Testing:



- Results for Out-of-Distribution Testing:

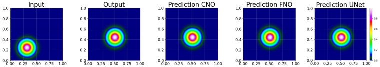


- Test Errors:

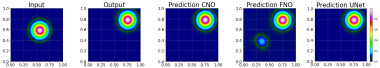
Model	FFNN	UNet	DeepONet	FNO	CNO
In	18.27%	0.82%	13.63%	0.57%	0.83%
Out	46.93%	2.18%	19.86%	2.36%	3.67%

Ex 5: Transport

- Results for In-Distribution Testing:

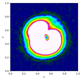


- Results for Out-of-Distribution Testing:

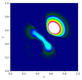


- Test Errors:

Model	FFNN	UNet	DeepONet	FNO	CNO
In	7.09%	0.49%	1.14%	0.40%	0.30%
Out	650.57%	1.28%	157.22%	13.83%	0.47%



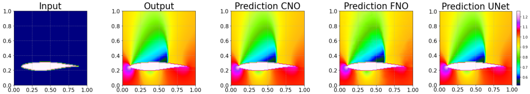
FFNN



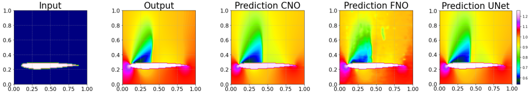
DeepONet

Ex 6: Compressible Euler Eqns

- Results for In-Distribution Testing:



- Results for Out-of-Distribution Testing:



- Test Errors:

Model	FFNN	UNet	DeepONet	FNO	CNO
In	0.78%	0.38%	1.93%	0.47%	0.35%
Out	1.34%	0.76%	2.88%	0.85%	0.62%

- RunTime: 10^2s for NuwTun vs 10^{-4}s for CNO

Similar Performance across the board !!

- Extensive Empirical evaluation on RPB benchmarks.

	In/Out	FFNN	GT	UNet	ResNet	DON	FNO	CNO
Poisson Equation	In	5.74%	2.77%	0.71%	0.43%	12.92%	4.98%	**0.21%**
	Out	5.35%	2.84%	1.27%	1.10%	9.15%	7.05%	**0.27%**
Wave Equation	In	2.51%	1,44%	1.51%	0.79%	2.26%	1.02%	**0.63%**
	Out	3.01%	1.79%	2.03%	1.36%	2.83%	1.77%	**1.17%**
Smooth Transport	In	7.09%	0.98%	0.49%	0.39%	1.14%	0.28%	**0.24%**
	Out	650.6%	875.4%	1.28%	0.96%	157.2%	3.90%	**0.46%**
Discontinuous Transport	In	13.0%	1.55%	1.31%	**1.01%**	5.78%	1.15%	**1.01%**
	Out	257.3%	22691.1%	1.35%	1.16%	117.1%	2.89%	**1.09%**
Allen-Cahn Equation	In	18.27%	0.77%	0.82%	1.40%	13.63%	**0.28%**	0.54%
	Out	46.93%	2.90%	2.18%	3.74%	19.86%	**1.10%**	2.23%
Navier-Stokes Equations	In	8.05%	4.14%	3.54%	3.69%	11.64%	3.57%	**2.76%**
	Out	16.12%	11.09%	10.93%	9.68%	15.05%	9.58%	**7.04%**
Darcy Flow	In	2.14%	0.86%	0.54%	0.42%	1.13%	0.80%	**0.38%**
	Out	2.23%	1.17%	0.64%	0.60%	1.61%	1.11%	**0.50%**
Compressible Euler	In	0.78%	2.09%	0.38%	1.70%	1.93%	0.44%	**0.35%**
	Out	1.34%	2.94%	0.76%	2.06%	2.88%	0.69%	**0.59%**

Computational Efficiency of CNO