Spectral-Informed Neural Networks Outperform Spectral Methods in High-dimensional PDEs

Tianchi Yu[1 2], Ivan Oseledets[1 3]

[1] AXXX
[2] Applied AI Institute
[3] INM

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Solving Partial Differential Equations

Conventional solvers

- Finite difference methods
- Finite element methods
- Spectral methods

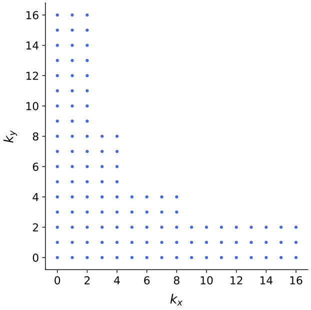
✓ Rigorous theoretical guarantees
✓ High interpretability
✓ Accurate for low-dimensional problems

PDE-informed NN solvers

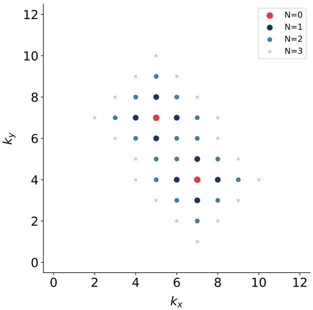
- Physics-informed NNs
- Spectral-informed NNs — **We are here**

✓ Mesh-free
✓ Easy implementation
✓ Exploitation of problem-specific structure

Motivation



(a) Hyperbolic cross sets.



(b) Stamping sets.

Spectral-Informed Neural Networks

Spectral-Informed Neural Networks (SINNs) are proposed to integrate spectral methods into neural networks. For example, consider the following Poisson's equation with periodic boundary conditions:

$$-u_{xx}(x) = f(x), \quad x \in [0, 2\pi], \tag{1}$$

The loss function of SINNs by fourier spectral basis is defined as

$$\mathcal{L}(\theta) = \sum_{k \in \mathcal{K}} \left| k^2 \hat{u}_\theta(k) - \hat{f}_k \right|^2, \tag{2}$$

where $\hat{u}_\theta(k)$ is the output of the neural network with input k, $\hat{f}_k$ is the spectral coefficient of f at frequency k and $\mathcal{K}$ is the set of frequencies used in the loss function.

Modified Spectral-Informed Neural Networks

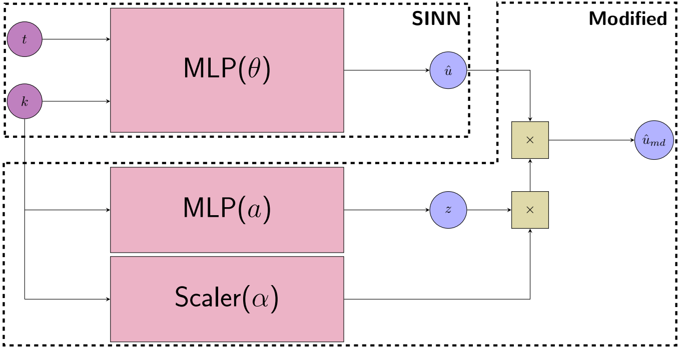


Figure: Scaler(α): coefficient decay and MLP(a): basis embedding.

Experiments

Table: High-dimensional Schrödinger equations solved by SGSM+SINN.

Metric	Dimension		
	2	5	8
SGSM ($s = 1.0$)	2.62e-7	4.42e-6	3.89e-4
N_{valid}	1.47e+3	1.91e+5	8.46e+5
SGSM ($s = 0.9$)	2.28e-3	9.37e-2	3.05e-1
+SINN	8.83e-5	1.60e-2	1.23e-3
Promotion	96.13%	82.92%	99.60%
N_{valid}	1.32e+3	1.72e+5	7.62e+5
SGSM ($s = 0.8$)	2.07e-1	2.43e-1	4.41e-1
+SINN	1.10e-3	3.74e-2	1.67e-3
Promotion	99.47%	84.61%	99.62%
N_{valid}	1.18e+3	1.53e+5	6.77e+5

Experiments

Table: Poisson's equations.

Dim	PINN	DRM	SINN
2	3.20e-4	2.48e-3	1.61e-4
5	5.54e-3	7.95e-3	2.24e-4
10	9.68e-3	1.03e-2	1.99e-4
30	1.70e-2	2.23e-2	2.76e-4
50	3.17e-2	3.20e-2	1.20e-3
100	5.50e-1	5.94e-2	7.75e-3

Table: Heat equations.

Dim	PINN	DRM	SINN
2	8.61e-4	1.12e-1	2.31e-4
5	1.41e-2	5.33e-2	2.20e-4
10	2.09e-2	3.40e-2	3.66e-4
30	3.01e-2	3.10e-2	1.46e-3
50	5.86e-2	2.02e-2	8.57e-3
100	7.39e-1	4.18e-1	3.69e-1