From Fourier to Neural ODEs: Flow Matching for Modeling Complex Systems

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Introduction

Neural ordinary differential equations (NODEs) (Chen et al., 2018), a class of continuous-depth neural networks, have garnered substantial interest in recent years.

$$\dot{\boldsymbol{z}} = \boldsymbol{F}_{\boldsymbol{\theta}}[\boldsymbol{z}(t), t],$$

$$\boldsymbol{z}(t_1) = \text{ODEsolve}[\boldsymbol{z}(t_0), \boldsymbol{F}_{\boldsymbol{\theta}}, t_0, t_1] = \boldsymbol{z}(t_0) + \int_{t_0}^{t_1} \boldsymbol{F}_{\boldsymbol{\theta}}[\boldsymbol{z}(t), t]\mathrm{d}t.$$

However, modeling complex systems using standard NODEs often faces some essential challenges, including high computational costs and susceptibility to local optima. To address these challenges and enhance the speed and robustness of dynamic modeling, we propose a framework called **Fourier NODEs** (F-NODEs)

Contributions

★ FNODEs reduce training time by more than tenfold compared to standard NODEs.

★ Data augmentation training strategy generates more data points to improve the estimation of gradient flows, resulting in a positive feedback loop that enhances robustness and accuracy in dynamic modeling.

★ The framework can be extended to resolution-invariant modeling of PDEs by incorporating estimated higher-order spatial gradients based on Fourier analysis, expanding the capabilities of classical NODEs.

Methodology

FNODE estimates the temporal gradients and spatial gradients based on observational data

$$\hat{\boldsymbol{s}}'(t_n) = \frac{1}{N}\sum_{k=0}^{K} i\frac{2\pi k}{T}\tilde{\boldsymbol{s}}_k \mathrm{e}^{i\frac{2\pi k}{N}n} \approx \boldsymbol{s}'(t_n), \qquad \frac{\partial^{p+q}\boldsymbol{S}_t}{\partial^p x \partial^q y} = \mathscr{F}_{xy}^{-1}\left[(i\boldsymbol{k}_{\boldsymbol{x}})^p (i\boldsymbol{k}_{\boldsymbol{y}})^q \mathscr{F}_{xy}(\boldsymbol{S}_t)\right],$$

where $\boldsymbol{S}_t$ is the sampling matrix at time t. Then use a neural network $\boldsymbol{F}_{\boldsymbol{\theta}}$ to learn the underlying dynamics.

Data augmentation. The newly generated data is fed into our model for further training. Therefore, Fourier analysis (spectral analysis) and NODE (differential dynamics) techniques complement each other.

Datasets

Four parametric PDE systems: including Korteweg-de Vries (KDV) system, diffusion-reaction (DR) system, Kuramoto-Sivashinsky (KS) system, and 2-D Navier-Stokes (NS) system.

A simple 2-D parametric ODE system

A real-world polar motion system

Experiments

Prediction MSE under different methods, systems, and experimental conditions.

Models	$N_{\text{tr}} = 10$, $\sigma_{\text{sd}} = 0$				$N_{\text{tr}} = 1000$, $\sigma_{\text{sd}} = 0$				$N_{\text{tr}} = 1000$, $\sigma_{\text{sd}} = 5\%$			
	KDV	DR	KS	NS	KDV	DR	KS	NS	KDV	DR	KS	NS
NODEs	1.93	1.68	2.56	4.21	0.45	0.58	1.69	3.61	1.02	1.46	2.34	5.19
DeepONet	0.83	2.75	3.02	38.3	0.09	0.17	0.63	7.30	0.74	0.87	1.20	14.7
FNO	1.88	1.56	2.21	23.9	0.21	0.13	0.92	5.3	0.89	1.58	2.13	12.6
PDE-NET	1.64	1.38	2.32	2.09	0.11	0.27	0.78	0.92	1.34	0.97	1.73	2.30
PINN	**0.17**	**0.19**	**0.24**	**0.31**	**0.17**	**0.19**	**0.24**	**0.31**	**0.17**	**0.19**	**0.24**	**0.31**
MP-PDE	2.39	2.74	4.23	6.62	0.44	0.49	1.33	2.07	1.22	1.11	1.93	2.59
FNODEs	**0.23**	**0.16**	**0.28**	**0.29**	**0.023**	**0.016**	**0.11**	**0.083**	**0.14**	**0.12**	**0.46**	**0.11**

Comparing the training time of different methods.

Sys	NODEs	DeepONet	FNO	P-N	PINN	M-P	FNODEs
KDV	3938	751	271	398	1540	560	**130**
DR	2910	652	262	311	1532	367	**65**
KS	5120	641	241	492	1660	589	**74**
NS	21747	8484	549	1323	2430	734	**283**

Modeling and predicting 2D NS system using FNODEs Method.