Incremental Fourier Neural Operator

Abstract

Recently, neural networks have proven their impressive ability to solve partial differential equations (PDEs). Among them, Fourier neural operator (FNO) has shown success in learning solution operators for highly non-linear problems such as turbulence flow. FNO is discretization-invariant, where it can be trained on low-resolution data and generalizes to problems with high-resolution. This property is related to the low-pass filters in FNO, where only a limited number of frequency modes are selected to propagate information. However, it is still a challenge to select an appropriate number of frequency modes and training resolution for different PDEs. Too few frequency modes and low-resolution data hurt generalization, while too many frequency modes and high-resolution data are computationally expensive and lead to over-fitting. To this end, we propose Incremental Fourier Neural Operator (IFNO), which augments both the frequency modes and data resolution incrementally during training. We show that IFNO achieves better generalization (around 15% reduction on testing L2 loss) while reducing the computational cost by 35%, compared to the standard FNO. In addition, we observe that IFNO follows the behavior of implicit regularization in FNO, which explains its excellent generalization ability.

1 Introduction

The use of neural networks for solving partial differential equations (PDEs) has shown impressive performance recently. One of the most promising directions is to learn the solution operator parametrized by neural operator [1,2]. The neural operator maps the input-initial conditions and boundary conditions to the output-solution functions, which also serves as a mapping between two infinite dimensional spaces.

Fourier neural operator (FNO) proposed by Li et al. [3] is a family of neural operators, which achieves state-of-the-art performance in solving PDEs. FNO has shown success in learning solution operators for highly non-linear problems such as weather forecast [4], plasticity [5], and multi-phase flow [6]. In addition, it has excellent generalization ability across different PDEs and resolutions [7]. By learning a limited set of problems, FNO can be generalized to solve a wide range of PDEs sharing the same structure. Its discretization-invariance property gives FNO the ability to train and test on different resolutions without significant performance degradation. For example, FNO can be trained on low-resolution but tested on high-resolution to achieve zero-shot super-resolution.

Unlike standard neural networks, there is an additional degree of freedom in FNO in determining its model capacity. Each layer in FNO consists of a learnable linear transform over the Fourier series. To ensure discretization invariance and good generalization, FNO truncates most high-frequency
modes in the Fourier series, such that the linear transforms are only applied to a limited number of low-frequency modes.

However, it is still a challenge to select an appropriate number of frequency modes and training resolution for FNO. Too few frequency modes and low-resolution data hurt generalization as they deliver insufficient information for learning the solution operator, resulting in under-fitting. On the other hand, too many frequency modes and high-resolution data introduce high-frequency noise and poor generalization, while being computationally expensive and prone to over-fitting. The latter has a strong impact, especially in the few-data or the no-data regime (i.e. using only the PDE loss in the physics-informed setting [9]).

Our work: we propose a novel incremental Fourier neural operator (IFNO) method to incrementally select frequency modes and data resolution during training. Specifically, IFNO starts with a small number of frequency modes and low-resolution data, and increases the frequency modes and data resolution whenever the current network tends to be converged during training. Despite its simplicity, IFNO achieves better generalization while significantly improving computational efficiency. When evaluating it on 1D Burgers’ equation and 2D Darcy Flow, IFNO reduces the testing L2 loss by 15% and the computational cost by 35%, compared to the standard FNO. In addition, we observe IFNO follows the behavior of implicit regularization in FNO, where gradient descent implicitly minimizes FNO towards low-frequency solutions, which explains the excellent generalization ability of IFNO.

2 Fourier Neural Operator

FNO proposed by Li et al. [3] serves as a family of neural operators, which are formulated as a generalization of standard deep neural networks to operator setting [9]. A neural operator learns a mapping between two infinite dimensional spaces from a finite collection of observed input-output pairs. Let \( D \subset \mathbb{R}^d \) be a bounded, open set and \( \mathcal{A} = \mathcal{A}(D; \mathbb{R}^{d_a}) \) and \( \mathcal{U} = \mathcal{U}(D; \mathbb{R}^{d_u}) \) be separable Banach spaces of function taking values in \( \mathbb{R}^{d_u} \) and \( \mathbb{R}^{d_u} \) respectively.

We want to learn a neural operator \( \mathcal{G}_\theta : \mathcal{A} \times \theta \to \mathcal{U} \) that maps any initial condition \( a \in \mathcal{A} \) to its solution \( u \in \mathcal{U} \). The neural operator \( \mathcal{G}_\theta \) composes linear integral operator \( \mathcal{K} \) with pointwise non-linear activation function \( \sigma \) to approximate highly non-linear operators.

Definition 1 (Neural operator). The neural operator \( \mathcal{G}_\theta \) is defined as follows:

\[
\mathcal{G}_\theta := Q \circ (W_L + K_L) \circ \cdots \circ \sigma (W_1 + K_1) \circ \mathcal{P}
\]

where \( \mathcal{P} : \mathbb{R}^{d_u} \to \mathbb{R}^{d_{d_1}} \), \( Q : \mathbb{R}^{d_{d_1}} \to \mathbb{R}^{d_u} \) are the pointwise neural networks that encode the lower dimension function into higher dimensional space and decode the higher dimension function back to the lower dimensional space. The model stack \( L \) layers of \( \sigma (W_i + K_i) \) where \( W_l \in \mathbb{R}^{d_{i+1} \times d_i} \) are pointwise linear operators (matrices), \( K_i : \{ D \to \mathbb{R}^{d_i} \} \to \{ D \to \mathbb{R}^{d_{i+1}} \} \) are integral kernel operators, and \( \sigma \) are fixed activation functions. The parameters \( \theta \) consists of all the parameters in \( \mathcal{P}, Q, W_i, K_i \).

Li et al. [3] proposes FNO that adopts a convolution operator for \( \mathcal{K} \), which obtains state-of-the-art results for solving PDE problems.

Definition 2 (Fourier convolution operator). Define the Fourier convolution operator \( \mathcal{K} \) as follows:

\[
(\mathcal{K}v_1)(x) = F^{-1} (R \cdot (Fv_1))(x) \quad \forall x \in D
\]

where \( R \) is a learnable transformation (a part of the parameter \( \theta \) in \( \mathcal{G}_\theta \)).

Discretization and resolution. FNO is trained using a finite collection of input-output pairs \( \{ a_i, u_i \}^N \), where \( a_i \in \mathcal{A} \) and \( u_i \in \mathcal{U} \). Since \( a_i \) and \( u_i \) are functions in general, we assume access only to point-wise evaluations to work with them numerically. Let \( \hat{D} = \{ x_1, \ldots, x_n \} \subset D \) be a \( n \)-point discretization of the domain \( D \) and assume we have observations \( a_i |_{\hat{D}} \in \mathbb{R}^{n \times d_a} \), \( u_i |_{\hat{D}} \in \mathbb{R}^{n \times d_u} \), for a finite collection of input-output pairs evaluated at any index \( i \in \{ 1, \ldots, N \} \). Since we assume that \( \hat{D} \) is uniformly sampled from \( D \), the size of the discretization \( n \) also reflects the resolution \( r \) of the training data, such that \( r = n \).

As suggested by Li et al. [3], FNO is discretization-invariant, such that the model can produce a high-quality solution for any \( x \in D \), potentially \( x \notin \hat{D} \). In other words, FNO can be trained on low-resolution \( r_{\text{low}} \) but generalizes to high-resolution \( r_{\text{high}} \) (\( r_{\text{high}} >> r_{\text{low}} \)). This property is highly desirable as it allows a transfer of solutions between different grid geometries and discretizations.
We also consider the steady-state of the 2D Darcy Flow on the unit box, which is the second order, linear, elliptic PDE
\[-\nabla \cdot (a(x) \nabla u(x)) = f(x) \quad x \in (0,1)^2 \]
\[u(x) = 0 \quad x \in \partial(0,1)^2\]
with a Dirichlet boundary where \(a\) is the diffusion coefficient and \(f\) is the forcing function. We are interested in learning the operator mapping the diffusion coefficient to the solution.

### Convolution via Fast Fourier transform.
Since \(\mathcal{K}\) is applied to a discrete set of evaluations \(\hat{D}\), the Fourier transform can be efficiently computed using the fast Fourier transform (FFT) algorithm, such that for \(\mathcal{K}\) in any layer
\[\mathcal{K}(v) = \hat{F}^{-1} \cdot R \cdot \hat{F} \cdot v,\]
where \(v \in \mathbb{R}^{n \times d_v}\) is the layer input, \(\hat{F}\) and \(\hat{F}^{-1}\) are the fast Fourier transform and its inverse, and \(R\) is a linear transform.

### Effective frequency modes.
For discrete frequency mode \(k \in \{1, ..., n\}\), we have \(\hat{F}v(k) \in \mathbb{C}^{d_v}\) and \(R(k) \in \mathbb{C}^{d_v \times d_v}\). FNO picks a finite-dimensional parameterization of tensor \(R\) by truncating the Fourier series \(\hat{F}v\) at a maximal number of modes \(k_{\text{max}}\), such that \(R\) becomes a \(k_{\text{max}} \times d_v \times d_v\) tensor. We denote the modes \(1, ..., k_{\text{max}}\) as the effective frequency modes. In the standard FNO, Li et al. [3] view \(k_{\text{max}}\) as an additional hyperparameter to be tuned for each problem.

### Algorithm 1: IFNO

#### Input: initial and maximum effective frequency modes \(k_0\) and \(k_{\text{max}}\), initial and maximum data resolution \(r_0\) and \(r_{\text{max}}\), initial tensor \(R_0\), the error difference between two iterations \(\epsilon\), error threshold \(\epsilon\).

#### Step 1: Initialize FNO with \(k_0\) frequency modes

#### For iteration \(t\) in \(0, 1, ..., T\):

- Train FNO with \(r_t\) resolution for \(m\) iterations
- If \(\epsilon < \epsilon\):
  - Increase \(k_{t+1}\) and \(r_{t+1}\) when \(k_{t+1} \leq k_{\text{max}}\) and \(r_{t+1} \leq r_{\text{max}}\)
  - Enlarge \(R_t\) to match \(k_{t+1}\), where \(R_{t+1}[0:k_{t+1}-1]=R_t\) and initialize the rest randomly
- If \(\epsilon \geq \epsilon\):
  - \(k_{t+1}=k_t\) and \(r_{t}=r_t\)

Despite its simplicity, IFNO achieves surprisingly better generalization while reducing the computational complexity compared to the standard FNO. We evaluate IFNO on the 1D Burgers’ equation, which is a non-linear PDE with various applications, including modeling the flow of a viscous fluid. The 1D Burgers’ equation takes the form:
\[
\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left( u^2(x,t) / 2 \right) = \nu \frac{\partial^2 u}{\partial x^2}, \quad x \in (0,1), t \in (0,1]
\]
\[u(x,0) = u_0(x), \quad x \in (0,1)
\]
where \(u_0\) is the initial condition and \(\nu\) is the viscosity coefficient. We aim to learn the operator \(\mathcal{G}_\theta\) mapping the initial condition to the solution.

We also consider the steady-state of the 2D Darcy Flow on the unit box, which is the second order, linear, elliptic PDE
\[-\nabla \cdot (a(x) \nabla u(x)) = f(x) \quad x \in (0,1)^2 \]
\[u(x) = 0 \quad x \in \partial(0,1)^2\]
with a Dirichlet boundary where \(a\) is the diffusion coefficient and \(f\) is the forcing function. We are interested in learning the operator mapping the diffusion coefficient to the solution.
We benchmark IFNO on both 1D Burgers’ equation and 2D Darcy Flow using reduced training datasets to test its generalization performance in an extreme case. We compare IFNO with the standard FNO and two of its variants, which fix the number of frequency modes or data resolution as \( k_{\text{max}} \) or \( r_{\text{max}} \) during training. In the 1D case the \( k_{\text{max}} = 50 \) and \( r_{\text{max}} = 4096 \) whilst in the 2D case the \( k_{\text{max}} = 50 \) and \( r_{\text{max}} = 241 \times 241 \).

We evaluate the generalization performance on super-resolution, such that the test data has a much higher resolution than the training data \( r_{\text{max}} \). As shown in Table 1 and 2, IFNO reduces the testing L2 loss on super-resolution by 15% and the computational cost by 35%, compared to the standard FNO. We note that IFNO achieves higher training but lower testing loss compared to other methods, suggesting that IFNO is more robust to overfitting.

### Table 1: Evaluation on 1D Burgers’ equation. The average training L2 loss and testing L2 loss on super-resolution are reported on 5 runs with their standard deviation.

| Method                        | Train L2 ± Standard Deviation | Test L2 (Super-Res) ± Standard Deviation | Training Time (s) ± Standard Deviation |
|-------------------------------|-------------------------------|------------------------------------------|----------------------------------------|
| IFNO                          | 0.0023 ± 0.0003               | 0.0042 ± 0.0004                           | 90.02 ± 3.64                           |
| Standard FNO                  | 0.0020 ± 0.0003               | 0.0043 ± 0.0003                           | 102.12 ± 3.40                          |
| IFNO (incremental frequency only) | 0.0021 ± 0.0004               | 0.0039 ± 0.0004                           | 108.12 ± 4.40                          |
| IFNO (incremental resolution only) | 0.0023 ± 0.0002               | 0.0048 ± 0.0002                           | 95.66 ± 2.93                           |

### Table 2: Evaluation on 2D Darcy Flow. The average training L2 loss and testing L2 loss on super-resolution are reported with their standard deviation.

| Method                        | Train L2 ± Standard Deviation | Test L2 (Super-Res) ± Standard Deviation | Training Time (s) ± Standard Deviation |
|-------------------------------|-------------------------------|------------------------------------------|----------------------------------------|
| IFNO                          | 0.0031 ± 0.0010               | 0.0636 ± 0.0022                           | 215.39 ± 13.30                          |
| Standard FNO                  | 0.0018 ± 0.0001               | 0.0668 ± 0.0032                           | 254.04 ± 39.24                          |
| IFNO (incremental frequency only) | 0.0028 ± 0.0006               | 0.0638 ± 0.0015                           | 271.16 ± 9.71                           |
| IFNO (incremental resolution only) | 0.0018 ± 0.0001               | 0.0671 ± 0.0033                           | 270.36 ± 36.29                          |

### 4 IFNO and Implicit Regularization

We observe that IFNO follows the implicit frequency regularization in the standard FNO, where gradient descent favors low-frequency components during training. This helps explain the excellent generalization ability of IFNO.

Specifically, as \( R(k) \) can be viewed as a linear transform over its frequency mode \( k \), the strength of \( R(k) \) reflects the importance of the mode \( k \) in the resulting solution. We measure each mode’s strength \( S_k \) over training as follows:

\[
S_k = \sum_i \sum_j R_{k,i,j}^2
\]

which is Frobenius norm of \( R(k) \) for each frequency mode \( k \).

As shown in Figure 1, we track the evolution of \( S_k \) for different layers over training. The evolution suggests that lower frequencies tend to be learned faster and become more important in the standard FNO, which is consistent with setting \( k_{\text{max}} \) to a small value at the initial stage of training in IFNO. We note that the evolution in certain layers (e.g., layer 4 in Figure 1) is not monotonic. We leave it as a future work to investigate the reason behind this abnormal behavior.

The evolution in Figure 1 also benefits the generalization of FNO, as it serves as an implicit spectral bias. Rahaman et al. [10] proposes implicit spectral bias, which characterizes a phenomenon where neural networks learn low-frequency functions first during training. The bias suggests that gradient descent implicitly regularizes neural networks toward simple solutions, which explains why the networks can generalize while having considerably more learnable parameters than training samples.

Our proposed IFNO not only follows the implicit spectral bias but also provides additional regularization by explicitly controlling the number of effective frequency modes \( k_{\text{max}} \). As shown in Figure 2, ...
Figure 1: Frequency evolution in FNO. The evolution of frequency modes $R(k)$ at different layers for FNO trained on 1D Burgers’ equations. Darker colors indicate lower frequency modes.

Figure 2: Frequency evolution in IFNO trained on 1D Burgers’ equations. Darker colors indicate singular vectors with higher strengths.

IFNO explicitly regularizes the frequency evolution, such that the low-frequency components are prioritized during training. This explains why IFNO achieves even better generalization than the standard FNO in Table 1 and 2.

5 Conclusion

In this work, we propose Incremental Fourier Neural Operator (IFNO) that incrementally selects frequency modes and data resolution during training. Our results suggest that IFNO achieves better generalization while significantly improving the computational efficiency compared to the standard FNO. We believe IFNO opens many new possibilities, such as solving PDEs with limited labeled data and training computationally efficient neural operators. In the future, we plan to evaluate IFNO on more complex PDEs and extend it to other changeling settings, such as training physics-informed neural operators.

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References

[1] Nikola Kovachki, Zongyi Li, Burigede Liu, Kamyar Azizzadenesheli, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. Neural operator: Learning maps between function spaces. arXiv preprint arXiv:2108.08481, 2021.

[2] 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(3):218–229, 2021.

[3] Zongyi Li, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. Fourier neural operator for parametric partial differential equations. URL http://arxiv.org/abs/2010.08895 type: article.
[4] Jaideep Pathak, Shashank Subramanian, Peter Harrington, Sanjeev Raja, Ashesh Chattopadhyay, Morteza Mardani, Thorsten Kurth, David Hall, Zongyi Li, Kamyar Azizzadenesheli, et al. Fourcastnet: A global data-driven high-resolution weather model using adaptive fourier neural operators. arXiv preprint arXiv:2202.11214, 2022.

[5] Burigede Liu, Nikola Kovachki, Zongyi Li, Kamyar Azizzadenesheli, Anima Anandkumar, Andrew M Stuart, and Kaushik Bhattacharya. A learning-based multiscale method and its application to inelastic impact problems. Journal of the Mechanics and Physics of Solids, 158:104668, 2022.

[6] Gege Wen, Zongyi Li, Kamyar Azizzadenesheli, Anima Anandkumar, and Sally M Benson. U-fno—an enhanced fourier neural operator-based deep-learning model for multiphase flow. Advances in Water Resources, 163:104180, 2022.

[7] Maarten De Hoop, Daniel Zhengyu Huang, Elizabeth Qian, and Andrew M Stuart. The cost-accuracy trade-off in operator learning with neural networks. arXiv preprint arXiv:2203.13181, 2022.

[8] Zongyi Li, Hongkai Zheng, Nikola Kovachki, David Jin, Haoxuan Chen, Burigede Liu, Kamyar Azizzadenesheli, and Anima Anandkumar. Physics-informed neural operator for learning partial differential equations,. URL http://arxiv.org/abs/2111.03794.

[9] Zongyi Li, Nikola Kovachki, Kamyar Azizzadenesheli, Burigede Liu, Kaushik Bhattacharya, Andrew Stuart, and Anima Anandkumar. Neural operator: Graph kernel network for partial differential equations,. URL http://arxiv.org/abs/2003.03485.

[10] Nasim Rahaman, Aristide Baratin, Devansh Arpit, Felix Draxler, Min Lin, Fred A. Hamprecht, Yoshua Bengio, and Aaron Courville. On the spectral bias of neural networks. URL http://arxiv.org/abs/1806.08734 type: article.