Discretization Invariant Operator Learning

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Outline

Operator Learning

Learn a map between function spaces.

- Denote $\mathcal{X}$ and $\mathcal{Y}$ as appropriate function spaces.
- E.g., $\mathbb{R}$-valued functions over $\Omega \subset \mathbb{R}^d$.
- Suppose that $\Psi : \mathcal{X} \to \mathcal{Y}$ denotes a mapping between $\mathcal{X}$ and $\mathcal{Y}$.

The objective of operator learning is to learn the underlying mapping Ψ.

Example

Consider the Burgers Equation given by

$$\begin{aligned} \partial_t u(x,t) + \partial_x(u^2(x,t)/2) &= \nu \partial_{xx} u(x,t), \qquad x \in (0,1), t \in (0,1] \\ u(x,0) &= u_0(x) \end{aligned}$$

with periodic boundary conditions, and ν representing the viscosity. An example of operator learning is to learn the mapping $\Psi : u_0(\cdot, 0) \to u(\cdot, 1)$.

Why Operator Learning

Broad Applications:

- Predictive Modelling.
- Solving parametric PDEs.
- Solving Inverse Problems.
- Image Processing.
- Signal Processing.

Deep Neural Network

$$y = \Psi^n(x;\theta) = \sigma \circ T \circ h^L \circ h^{L-1} \circ \cdots \circ h^1(x)$$

- $h^i(x) = \sigma({W^i}^T x + b^i)$
- σ is an activation function, e.g., $ReLU(x) = \max\{0, x\}$.
- $T(x) = V^T x$.
- $\theta = \{W^1, \cdots, W^L, b^1, \cdots, b^L, V\}$.

Approach: Learn $\Psi : \mathcal{X} \to \mathcal{Y}$.

- Use deep neural network $\Psi^n(\cdot;\theta)$ to parameterize Ψ.
- Learn Ψ^n via supervised learning, given samples $\{(f_i, g_i)\}_{i=1}^n$, $f_i \in \mathcal{X}$ and $g_i \in \mathcal{Y}$.

Why Data Driven

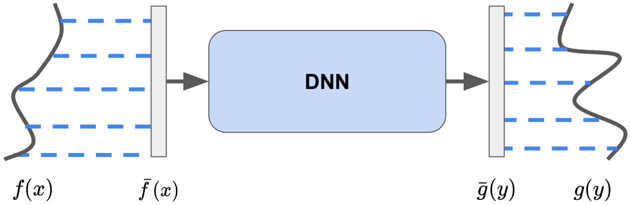
Conventional Methods

- Years of design needed to develop methods.
- Accurate but maybe slow.

Data Driven Methods

- Learn to solve from data.
- After model is trained, evaluation is fast.

Discretization Invariance



NNs were originally proposed to learn mappings between a vector space $X \subset \mathbb{R}^{d_x}$ to another vector space $Y \subset \mathbb{R}^{d_y}$.

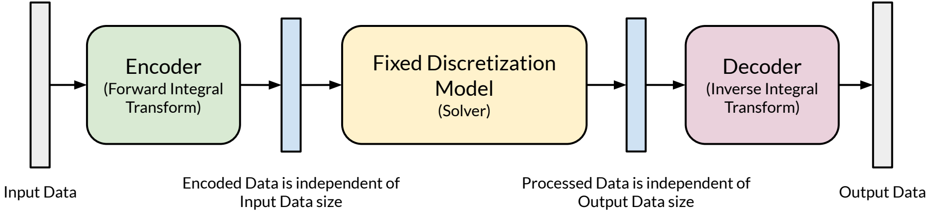
- $\bar{f} \in X$ and $\bar{g} \in Y$ comes from the discretization of functions $f \in \mathcal{X}$ and $g \in \mathcal{Y}$.
- We cannot apply a NN trained on X and Y to other discrete spaces.

Why Discretization Invariance

- Apply trained model to other resolutions.
- Expensive re-training is required to retrain a new NN for different discretization formats.
- Difficult to obtain training samples from certain discrete formats, e.g., high resolution.

Integral Autoencoder (IAE)

(Ong, Shen, Y., 2022)



Map between an Input/Output Data of arbitrary discretization to a representation of a fixed discretization.

- **Data-driven integral transforms**
- Captures intrinsic dimension (sparsity).

Y. Z. Ong, Z. Shen, and H. Yang. IAE-Net: Integral Autoencoders for Discretization-Invariant Learning (2022).

Integral Transform

(Ong, Shen, Y., 2022)
A non-linear integral transform:

$$(Tf)(z) = \int_{\Omega_x} K(f(x), x, z) f(x) dx, \qquad z \in \Omega_z.$$

- f function defined on Ω_x.
- K kernel function.
- Tf function on Ω_z, independent of Ω_x.

Idea: Design K as a NN $\phi_1(\cdot; \theta_{\phi_1})$.

$$v(z) = \int_{\Omega_x} \phi_1(f(x), x, z; \theta_{\phi_1}) f(x) dx, \qquad z \in \Omega_z.$$

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Backward Integral Transform

(Ong, Shen, Y., 2022)
Backward integral transform:

$$g(y) = \int_{\Omega_z} \phi_2(u(z), x, z; \theta_{\phi_2}) u(z) dz, \qquad y \in \Omega_y.$$

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Backward Integral Transform

(Ong, Shen, Y., 2022)
Backward integral transform:

$$g(y) = \int_{\Omega_z} \phi_2(u(z), x, z; \theta_{\phi_2}) u(z) dz, \qquad y \in \Omega_y.$$

Introduce ϕ_0 to map $v(z)$ to $u(z)$.

$$f(x) \xrightarrow{\phi_1} v(z) \xrightarrow{\phi_0} u(z) \xrightarrow{\phi_2} g(y)$$

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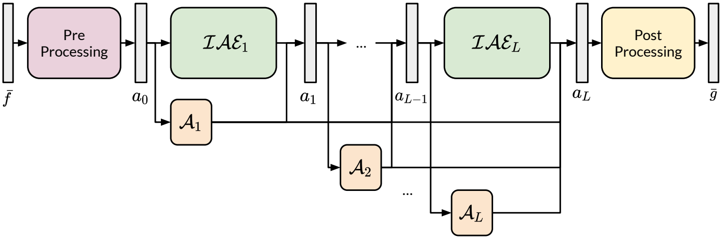
Multi-Layer Structure

(Ong, Shen, Y., 2022)



- Compose consecutive $\mathcal{IAE}$-Blocks, each containing an IAE.
- $\mathcal{IAE}_i$ takes as input $a_0, \ldots, a_{i-1}$ from previous $\mathcal{IAE}$-Blocks.
- Pre and Post Processing handle dimensions.
- $\mathcal{A}_i$ are pointwise affine transforms performing rescaling.

Y. Z. Ong, Z. Shen, and H. Yang. IAE-Net: Integral Autoencoders for Discretization-Invariant Learning (2022).

Why Multiple Layers

(Ong, Shen, Y., 2022)

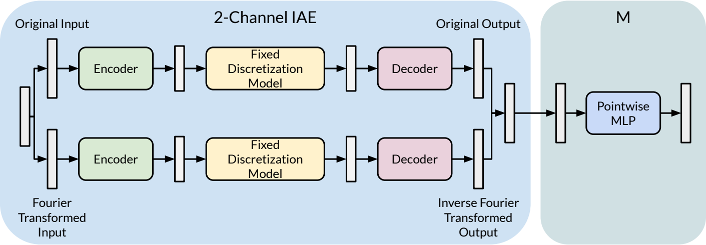
$$\bar{f} \xrightarrow{\text{Pre Process}} a_0 \xrightarrow{\mathcal{IAE}_1} a_1 \xrightarrow{\mathcal{IAE}_2} \dots \xrightarrow{\mathcal{IAE}_L} a_L \xrightarrow{\text{Post Process}} \bar{g}.$$

- Multi-layer structure incorporates multiple encoders.
- Each focus on specific features.
- Use previous approximations $a_0, \dots, a_{i-1}$ to learn a_i.

Y. Z. Ong, Z. Shen, and H. Yang. IAE-Net: Integral Autoencoders for Discretization-Invariant Learning (2022).

Multi-Channel Structure

(Ong, Shen, Y., 2022)



- Multiple IAEs are assembled in parallel, using known integral transforms as a guide.
- Different features are captured in different domains.

Y. Z. Ong, Z. Shen, and H. Yang. IAE-Net: Integral Autoencoders for Discretization-Invariant Learning (2022).

Data Augmentation

(Ong, Shen, Y., 2022)

- IAE-Net uses data-driven integral kernels.
- Does not assume any known structure in the data.

Question: How do we guide IAE-Net to learn to encode data from different resolutions?

Data Augmentation!

$$\min_{\theta_{\Psi^n}} \mathbb{E}_{(\bar{f},\bar{g})\sim p_{data}} \mathbb{E}_{I_T\sim\mathcal{I}}[L(\Psi^n(\bar{f};\theta_{\Psi^n}),\bar{g}) + \lambda \mathbf{L}(\boldsymbol{\Psi}^{\mathbf{n}}(\mathbf{I_T}(\bar{\mathbf{f}});\theta_{\boldsymbol{\Psi}^{\mathbf{n}}}),\mathbf{I_T}(\bar{\mathbf{g}}))],$$

$I_T \sim \mathcal{I}$ denotes a randomly sampled interpolation operator from a set of interpolator functions $\mathcal{I}$.

Y. Z. Ong, Z. Shen, and H. Yang. IAE-Net: Integral Autoencoders for Discretization-Invariant Learning (2022).

Baseline Models

- UNet (Ronneberger et al., 2015)
- DeepONet (Lu et al., 2019)
- Fourier Neural Operator (FNO) (Li et al., 2020)
- Fourier Transformer (FT), Galerkin Transformer (GT) (S. Cao, 2021)

UNet: O. Ronneberger, P. Fischer, T. Brox. U-net: Convolutional networks for biomedical image segmentation (2015).
DeepONet: L. Lu, P. Jin, G. E. Karniadakis. Deeponet: Learning nonlinear operators by neural networks with arbitrary activation functions and its application to dynamical systems (2019).
Fourier Neural Operator (FNO): Z. Li, N. B. Kovachki, K. Azizzadenesheli, B. Liu, K. Bhattacharya, A. M. Stuart, A. Anandkumar. Fourier neural operator for parametric partial differential equations (2020).
Fourier Transformer (FT), Galerkin Transformer (GT): S. Cao. Choose a transformer: Fourier or galerkin (2021).

Predictive Modelling

Example 1: Burgers Equation

$$\partial_t u(x,t) + \partial_x(u^2(x,t)/2) = \nu \partial_{xx} u(x,t), \quad x \in (0,1), t \in (0,1]$$
$$u(x,0) = u_0(x)$$

- Periodic Boundary Condition.
- ν denotes a given viscosity coefficient.
- **Operator:** Mapping from $u(x,0) \to u(x,1)$.

Predictive Modelling

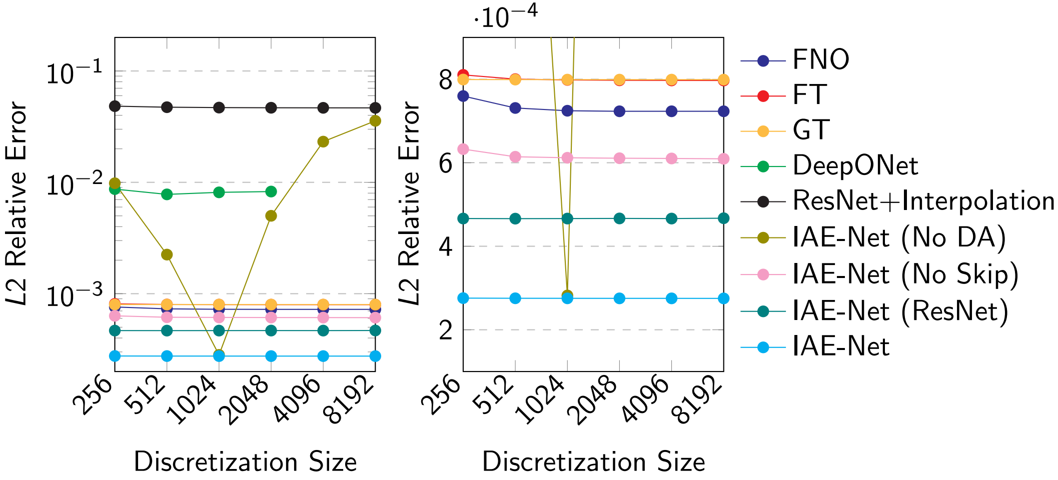


Figure: $L2$ relative error on the Burgers data set with $\nu = 1e^{-1}$ (Left) and its closeup (Right). Models are trained with $s = 1024$ and tested on the other resolutions.

Forward Problem

Example 2: Darcy Flow

$$
\begin{aligned}
-\nabla \cdot (a(x)\nabla u(x)) = f(x), \quad x \in (0,1)^2 \\
u(x) = 0, \quad x \in \partial(0,1)^2,
\end{aligned}
$$

- $f(x)$ denotes a given forcing function.
- **Operator:** Mapping from $a(x) \to u(x)$.

Forward Problem

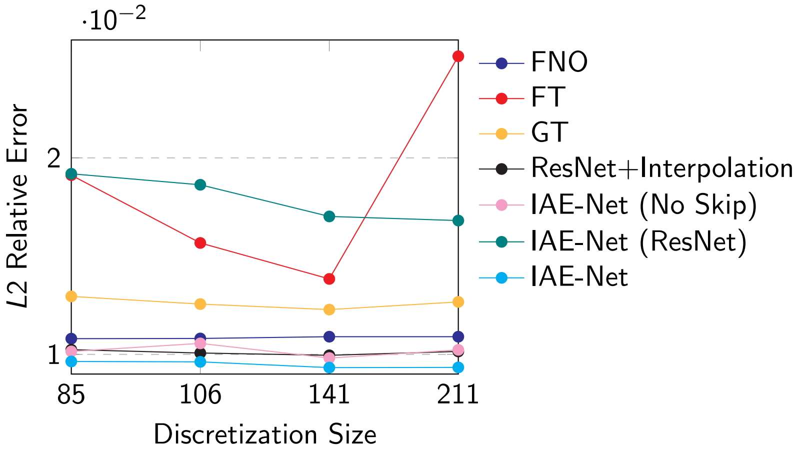


Figure: $L2$ relative error on the benchmark Darcy data set. Models are trained with $s = 141$ size training data and tested on the other resolutions.

Inverse Problem

Example 3: Scattering Problem
Helmholtz Equation

$$(-\Delta - \frac{\omega^2}{c^2(x)})u = 0$$

In most applications, a known background velocity $c_0(x)$ exists. Introduce

$$\frac{\omega^2}{c(x)^2} = \frac{\omega^2}{c_0(x)^2} + \eta(x) \qquad L_0 = -\Delta - \frac{\omega^2}{c_0^2(x)}$$

Parametric PDE

$$(L_0 - \eta(x))u(x) = 0$$

- **Operator:** Mapping between $u(x)$ and $\eta(x)$.

Inverse Problem

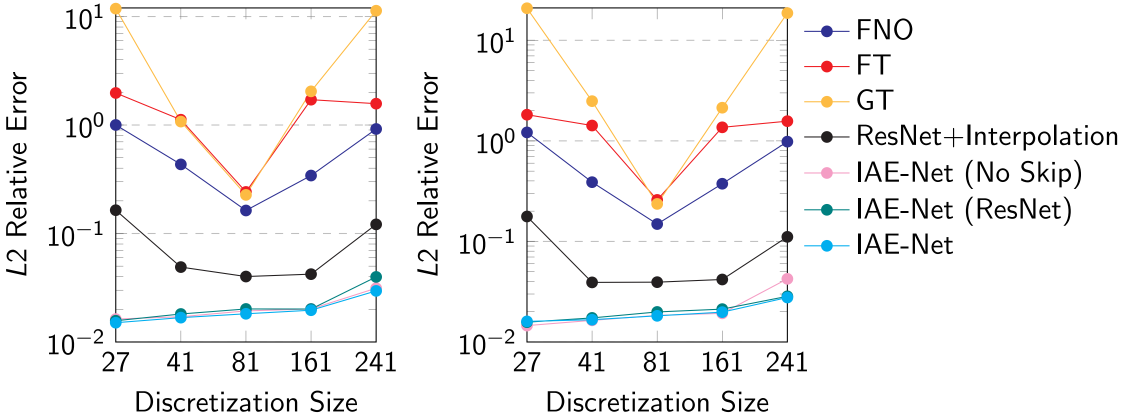


Figure: $L2$ relative error on the scattering data set for the forward (Left) and inverse (Right) problem. Model is trained with $s = 81$ and tested on different resolutions.

Example 4: ECG Signal Separation

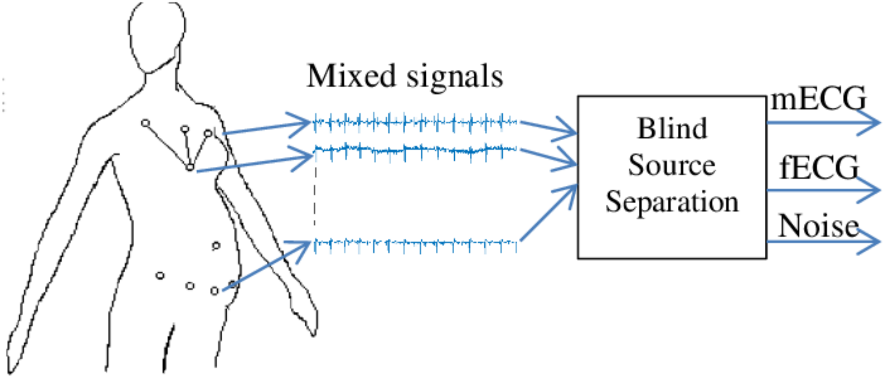


Image From: K. Bensafia, A. Mansour, S. Haddab. Blind Source Subspace Separation and Classification of ECG Signals (2017).

Signal Processing

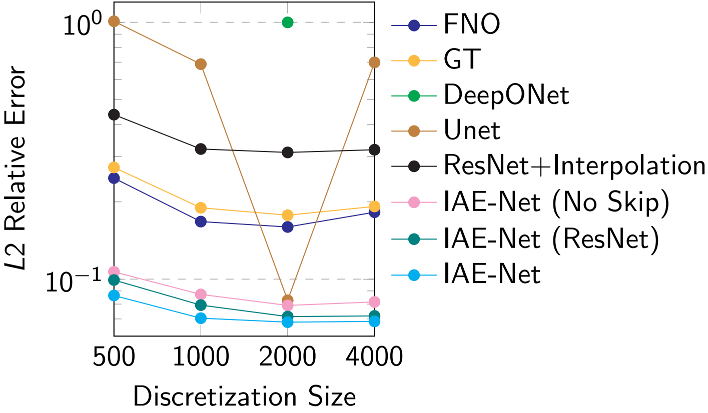


Figure: $L2$ relative error on the fecgsyndb data set. Model is trained with s=2000 and tested on different resolutions.

Summary

Proposed IAE-Net for Discretization Invariant Operator Learning.

- Learn a **data-driven kernel** function using DL and **Data Augmentation** to achieve discretization invariance.
- **Multi-Layer**, **Multi-Channel** helps improve the learning process.

Numerically, we show that

- Discretization invariance is achievable for mathematically well-posed problems even with simple interpolation techniques, but IAE-Net achieves state-of-the-art accuracy.
- Existing methods fail to achieve discretization invariance for ill-posed and highly oscillatory problems, while IAE-Net succeeds with reasonably good accuracy.

Paper: `https://arxiv.org/abs/2203.05142`
Code: `https://github.com/IAE-Net/iae_net`
Email: e0011814@u.nus.edu

Thank you for your attention!