



Physics-Informed Machine Learning: A survey on Problems, Methods and Applications

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Content

- Introduction—why and how PIML
- Problem Formulation
- Neural Simulation
 - Neural Solver
 - Neural Operator
 - Theory
- Inverse Problem (Inverse Design)
- Computer Vision & Reinforcement Learning

Introduction



- Limitations of Statistical ML models
 - Not robust
 - Lack interpretability
 - Violate physical constraints
- Current statistic learning are not aware of the internal physical mechanism that generates the data

Introduction



■ Concept of Machine Learning

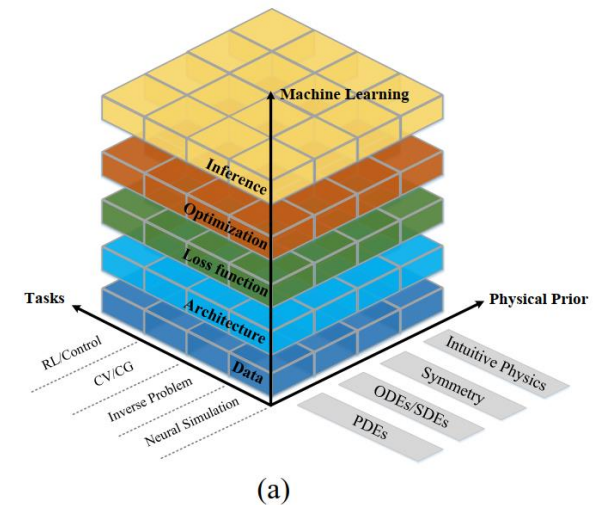
- *build models that leverage empirical data to improve performance on some set of tasks*

■ Concept of Physics-Informed Machine Learning

- *build models that leverage empirical data **and available physical prior knowledge** to improve performance on a set of tasks that **involve a physical mechanism***

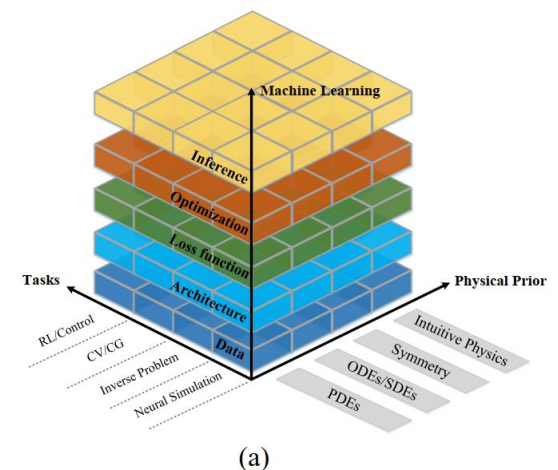
Introduction

- Representation of physical prior
 - PDEs/ODEs/SDEs
 - Symmetry
 - Intuitive physics
- How to encode physical prior
 - Data
 - Architecture
 - Loss functions
 - Optimizer
 - Inference



Introduction

- Tasks of PIML
 - Neural Simulation
 - Neural Solver (PINN...)
 - Neural Operator (DeepONet, FNO...)
 - Inverse Problem
 - Computer Vision/Computer Graphics
 - Reinforcement Learning/Control

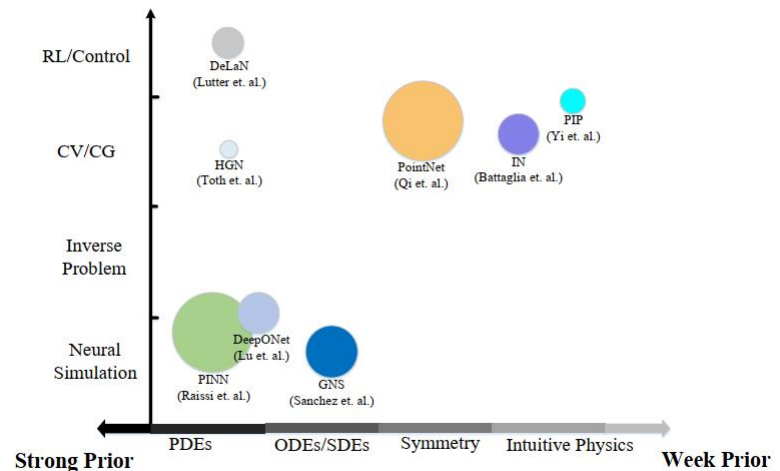
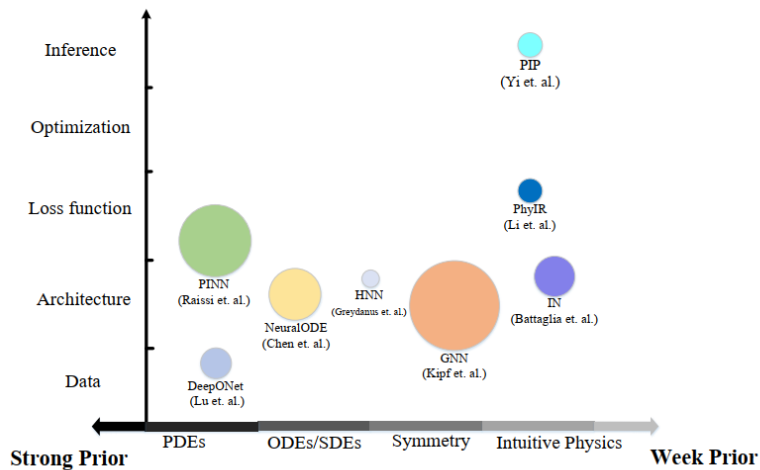


Introduction



■ Representative works

- Methods for incorporating physical prior (left)
- Works for solving different tasks (right)



Problem Formulation

- Problem formulation

- View ML as an optimization problem

$$\min_{f \in \mathcal{H}} \mathcal{L}(f; \mathcal{D}) + \Omega(f; \mathcal{D}).$$

- The root of physical prior is data is physical

$$\mathcal{F}(\mathcal{D}) = 0,$$

- Data $\mathcal{D}_p = P(\mathcal{D})$
- Architecture $f \in \mathcal{H}_p \subseteq \mathcal{H}$.
- Loss/Reg $\mathcal{L}_p(f; \mathcal{D})$ or $\Omega_p(f; \mathcal{D})$
- Optimization OPT_p
- Inference $g_p(x, f(\mathbf{x}))$

Neural Simulation



■ Notations and Problem Formulation

□ PDEs

$$\mathcal{F}\left(u, \frac{\partial u}{\partial x_1}, \dots, \frac{\partial u}{\partial x_d}, \frac{\partial^2 u}{\partial x_1^2}, \frac{\partial^2 u}{\partial x_1 \partial x_2}, \dots, \frac{\partial^2 u}{\partial x_d^2}, \dots; \theta\right)(x_i, t) = 0,$$

$$\mathcal{I}\left(u, \frac{\partial u}{\partial x_1}, \dots, \frac{\partial u}{\partial x_d}, \frac{\partial^2 u}{\partial x_1^2}, \frac{\partial^2 u}{\partial x_1 \partial x_2}, \dots, \frac{\partial^2 u}{\partial x_d^2}, \dots; \theta\right)(x_i, t_0) = 0,$$

$$\mathcal{B}\left(u, \frac{\partial u}{\partial x_1}, \dots, \frac{\partial u}{\partial x_d}, \frac{\partial^2 u}{\partial x_1^2}, \frac{\partial^2 u}{\partial x_1 \partial x_2}, \dots, \frac{\partial^2 u}{\partial x_d^2}, \dots; \theta\right)(x_i, t) = 0.$$

□ Neural Solver

$$\min_{w \in W} \|u_w(\mathbf{x}) - \tilde{u}(\mathbf{x})\|,$$

□ Neural Operator

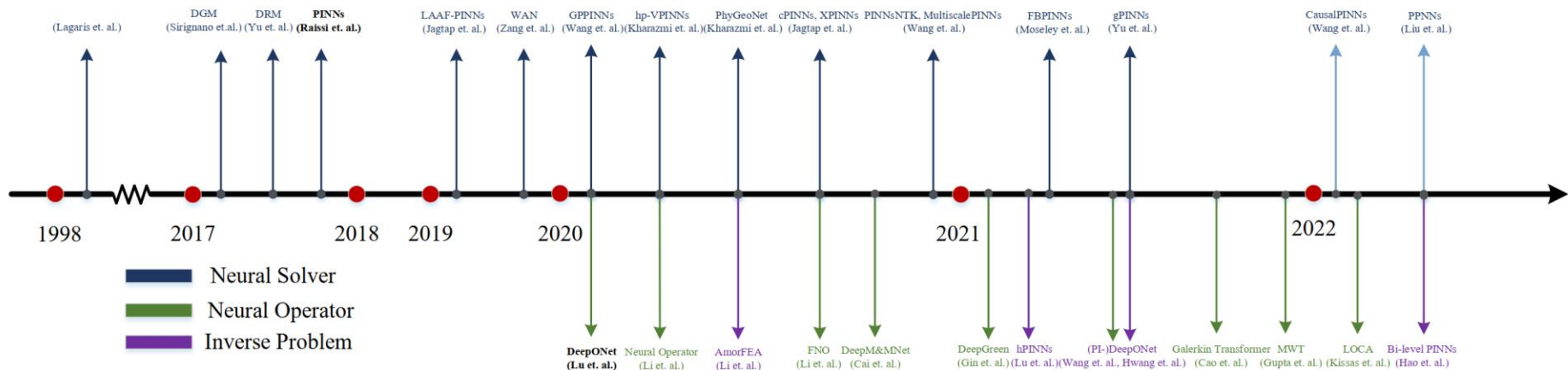
$$\min_{w \in W} \|G_w(\theta)(\mathbf{x}) - \tilde{G}(\theta)(\mathbf{x})\|,$$

Neural Simulation



■ Chronological overview

- Neural Solver: DGM[1]/DRM[2]/PINN[3]...
- Neural Operator: DeepONet[4]/FNO[5]...
- Inverse Design: PINNs/DeepONets/AmorFEA[6]...



Neural Solver

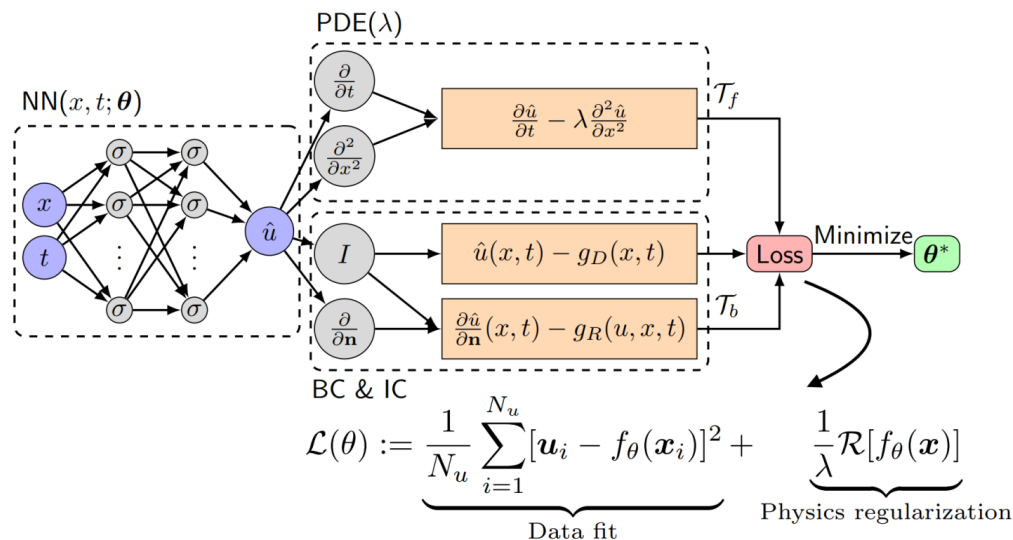


Basic PINNs

- Parametrize solution with NNs and optimize following loss

$$\mathcal{L} = \frac{\lambda_r}{|\Omega|} \int_{\Omega} \|\mathcal{F}(u_w; \theta)(\mathbf{x})\|^2 d\mathbf{x} + \frac{\lambda_i}{|\Omega_0|} \int_{\Omega_0} \|\mathcal{I}(u_w; \theta)(\mathbf{x})\|^2 d\mathbf{x} + \frac{\lambda_b}{|\partial\Omega|} \int_{\partial\Omega} \|\mathcal{B}(u_w; \theta)(\mathbf{x})\|^2 d\mathbf{x} + \frac{\lambda_d}{N} \sum_{i=1}^N \|u_w(\mathbf{x}_i) - u(\mathbf{x}_i)\|^2,$$

- Graphical illustration of PINNs



Neural Solver



- Variants of PINNs
 - Loss Reweighting and Data Resampling
 - Novel optimization targets
 - Numerical Differentiation
 - Variational Formulation
 - Regularization terms
 - Novel Neural Architectures
 - Activation functions
 - Feature preprocessing (embedding)
 - Boundary Encoding
 - Sequential Architecture/Convolutional Architecture
 - Domain Decomposition

Neural Solver



■ Loss Reweighting

- Balance learning rates by gradient norms [7]

$$\hat{\lambda}_i = \frac{\max\{\|\nabla_w \mathcal{L}_r(w_n)\|\}}{\|\nabla_w \mathcal{L}_i(w_n)\|}.$$

$$\lambda_i \leftarrow (1 - \alpha)\lambda_i + \alpha\hat{\lambda}_i,$$

- NTK reweighting
- Variance reweighting
- ...

■ Data Sampling

- Sample points with higher error with IS [8]

$$\mathcal{L}_r = \mathbb{E}_{\mathbf{x} \sim q} \left[\frac{p(\mathbf{x})}{q(\mathbf{x})} \|\mathcal{F}(u)(\mathbf{x})\|^2 \right]$$

$$q(\mathbf{x}_i) = \frac{\|\nabla_w l_r(w, \mathbf{x}_i)\|}{\sum_j \|\nabla_w l_r(w, \mathbf{x}_j)\|} \approx \frac{l_r(w, \mathbf{x}_i)}{\sum_j l_r(w, \mathbf{x}_j)}$$

Neural Solver



■ Novel Optimization Targets--Variational Formulation

- For the following problem

$$\begin{aligned}\Delta u &= f(\mathbf{x}), x \in \Omega, \\ \frac{\partial u}{\partial n} &= 0, x \in \partial\Omega.\end{aligned}$$

- PINN optimizes

$$\mathcal{L}(w) = \frac{\lambda_r}{|\Omega|} \int_{\Omega} \|\Delta u_w - f(\mathbf{x})\|^2 d\mathbf{x} + \frac{\lambda_b}{|\partial\Omega|} \int_{\partial\Omega} \left\| \frac{\partial u_w}{\partial n} \right\|^2 d\mathbf{x}$$

- Deep Ritz Method [2] optimizes

$$\mathcal{J}(w) = \int_{\Omega} \left(\frac{1}{2} |\nabla u_w(\mathbf{x})|^2 - f(\mathbf{x})u_w(\mathbf{x}) \right) d\mathbf{x}.$$

- VPINNs [9] choose a set of test functions

$$\mathcal{J}(w) = \frac{1}{K} \sum_{k=1}^K |\langle \mathcal{F}(u_w), v \rangle_{\Omega}|^2 + \lambda_b \frac{1}{N_b} \sum_{i=1}^{N_b} |u_w(\mathbf{x}_i) - g(\mathbf{x}_i)|^2.$$

Neural Solver

- Novel Optimization Targets—Regularization terms
 - Gradient-enhanced PINNs [10]
 - For PDEs, we penalize itself as well as its derivatives

$$f\left(\mathbf{x}; \frac{\partial u}{\partial x_1}, \dots, \frac{\partial u}{\partial x_d}; \frac{\partial^2 u}{\partial x_1 \partial x_1}, \dots, \frac{\partial^2 u}{\partial x_1 \partial x_d}; \dots; \boldsymbol{\lambda}\right) = 0, \quad \mathbf{x} = (x_1, \dots, x_d) \in \Omega,$$

- Loss function of gPINNs

$$\mathcal{L} = w_f \mathcal{L}_f + w_b \mathcal{L}_b + w_i \mathcal{L}_i + \sum_{i=1}^d w_{g_i} \mathcal{L}_{g_i}(\boldsymbol{\theta}; \mathcal{T}_{g_i}),$$

$$\mathcal{L}_{g_i}(\boldsymbol{\theta}; \mathcal{T}_{g_i}) = \frac{1}{|\mathcal{T}_{g_i}|} \sum_{\mathbf{x} \in \mathcal{T}_{g_i}} \left| \frac{\partial f}{\partial x_i} \right|^2$$

Neural Solver



■ Novel Architectures

- Boundary encoding [11] (use hard boundary constraints)

$$\begin{aligned} \mathcal{F}(u)(\mathbf{x}) &= 0, x \in \Omega, \\ u(\mathbf{x}) &= g(\mathbf{x}), x \in \partial\Omega. \end{aligned} \quad \longrightarrow \quad \begin{aligned} u(\mathbf{x}) &= v(\mathbf{x}) + D(\mathbf{x})y(\mathbf{x}). \\ D(\mathbf{x}) &= 0, x \in \partial\Omega. \end{aligned}$$

- Feature Embedding [12] (e.g. Fourier features)

$$\gamma(\mathbf{x}) = (\sin(2\pi\mathbf{b}_1^T \cdot \mathbf{x}), \cos(2\pi\mathbf{b}_1^T \cdot \mathbf{x}), \dots, \sin(2\pi\mathbf{b}_m^T \cdot \mathbf{x}), \cos(2\pi\mathbf{b}_m^T \cdot \mathbf{x})).$$

- Adaptive activation functions [13]...

Neural Solver



- Novel Architectures

- Sequential Architectures [14]

- Solves time-dependent PDEs and uses LSTM architectures

$$\mathcal{L}_{\text{reg}} = \left\| \frac{u_{i+1} - u_i}{\Delta t} - F \left(u_i, \frac{\partial u_i}{\partial x_1}, \dots, \frac{\partial u}{\partial x_d}, \dots, \theta \right) \right\|^2$$

- Convolutional Architectures [14]

- Replace spatial differentiation with numerical ones and use CNNs

$$D_1 \approx \frac{1}{h^2} \begin{pmatrix} 1 & -2 & 1 \end{pmatrix}$$



$$\Delta u(x, y) \approx D_2 * U$$

$$D_2 \approx \frac{1}{h^2} \begin{pmatrix} 0 & 1 & 0 \\ 1 & -4 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$



Neural Solver

- Novel Architectures—Domain Decomposition

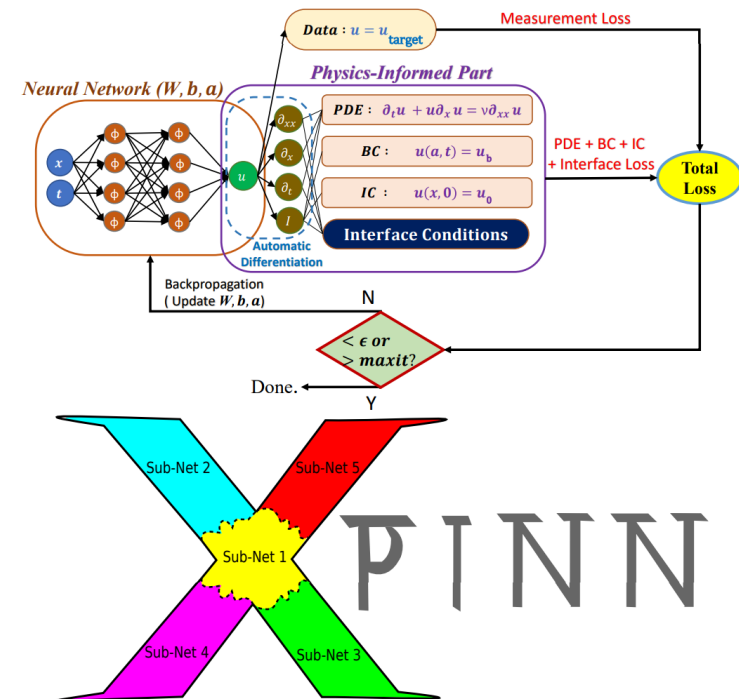
- XPINNs [15]: use K subnets for K subdomains

- Loss functions:

$$\mathcal{L} = \sum_{k=1}^K (\lambda_r^k \mathcal{L}_r^k + \lambda_b^k \mathcal{L}_b^k + \lambda_i^k \mathcal{L}_i^k) + \sum_{m=1}^M \lambda_I^m \mathcal{L}_I^m.$$

- \mathcal{L}_I^m : Interface condition

- Continuity of physical quantities
 - Conservation/continuity of other variables flow or gradients



Neural Solver



■ Summary of existing methods for neural solver

	Method	Description	Representatives
Neural Solver	Loss Reweighting	Grad Norm NTK Reweighting Variance Reweighting	GradientPathologiesPINNs [43] PINNsNTK [44] Inverse-Dirichlet PINNs [45]
	Novel Optimization Targets	Numerical Differentiation Variational Formulation Regularization	DGM [46], CAN-PINN [47], cvPINNs [48] vPINN [49], hp-PINN [50], VarNet [51], WAN [52] gPINNs [53], Sobolev Training [54]
	Novel Architectures	Adaptive Activation Feature Preprocessing Boundary Encoding Sequential Architecture Convolutional Architecture Domain Decomposition	LAAF-PINNs [55], [56], SReLU [57] Fourier Embedding [58], Prior Dictionary Embedding [59] TFC-based [60], CENN [61], PFNN [62], HCNet [63] PhyCRNet [64], PhyLSTM [65] AR-DenseED [66], HNN [67], HGN [68] PhyGeoNet [69], PhyCRNet [64], PPNN [70] XPINNs [71], cPINNs [72], FBPINNs [73], Shukla et al. [74]
	Other Learning Paradigms	Transfer Learning Meta-Learning	Desai et al. [75], MF-PIDNN [76] Psaros et al. [77], NRPINNs [78]

TABLE 2: An overview of variants of PINNs. Variants of PINNs include loss reweighting, novel optimization targets, novel architectures and other techniques such as meta-learning.



Neural Operator

- Learning an operator $\tilde{G}: \Theta \times \Omega \rightarrow \mathbb{R}^m$

$$\min_{w \in W} \|G_w(\theta)(\mathbf{x}) - \tilde{G}(\theta)(\mathbf{x})\|$$

where $\theta \in \Theta$ is control/design parameters, G_w is the trained neural model.

- Training dataset

- Data points: $\{\tilde{G}(\theta_i)(\mathbf{x}_j)\}$

- Collocation points: $\{(\theta_i, \mathbf{x}_j)\}$ (physics-informed loss)

- Categories

- Direct Methods, Green's Function learning, Grid-based Operator Learning, Graph-based Operator Learning.

Direct Methods

- Directly parameterize $\tilde{G}: \Theta \times \Omega \rightarrow \mathbb{R}^m$ as a neural network, following the format in *Universal Approximation Theorem of Operator*

Category & Formulation	Representative	Description
Direct Methods $G_w(\theta)(\mathbf{x}) = b_0 + \sum_{k=1}^p b_k(\theta)t_k(\mathbf{x})$	DeepONet [153]	Parameterize b_k and t_k with neural networks, which are trained with supervised data.
	Physics-informed DeepONet [154]	Train DeepONet with a combination of data and physics-informed losses.
	Improved Architectures for DeepONet [155], [156]	Including modified network structures (see Eq. (99)), input transformation ($\mathbf{x} \mapsto (\mathbf{x}, \sin(\mathbf{x}), \cos(\mathbf{x}), \dots)$), POD-DeepONet (see Eq. (101)), and output transformation (see Eq. (102) and Eq. (103)).
	Multiple-input DeepONet [157]	A variant of DeepONet taking multiple various parameters as input, i.e., $\tilde{G}: \Theta_1 \times \Theta_2 \times \dots \times \Theta_n \rightarrow Y$.
	Pre-trained DeepONet for Multi-physics [158], [159]	Model a multi-physics system with several pre-trained DeepONets serving as building blocks.
	Other Variants	Including Bayesian DeepONet [160], multi-fidelity DeepONet [161], and MultiAuto-DeepONet [162].

Green's Function learning

- We are interested when θ is a *function* ($\tilde{G}: f \mapsto u$)

$$\mathcal{F}_L[u] = f, \quad \mathbf{x} \in \Omega$$

$$\mathcal{B}_L[u] = g, \quad \mathbf{x} \in \partial\Omega$$

where \mathcal{F}_L and \mathcal{B}_L are two linear operators

- Represent the solution via Green's function

$$u(\mathbf{x}) = \int_{\Omega} \mathcal{G}(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) d\mathbf{y} + u_{\text{homo}}(\mathbf{x})$$

where $\mathcal{G}(\mathbf{x}, \mathbf{y})$ is parameterized by NN (**double dimension**)

Green's Function Learning $G_w(\theta)(\mathbf{x}) = \int_{\Omega} \mathcal{G}(\mathbf{x}, \mathbf{y}) \theta(\mathbf{y}) d\mathbf{y} + u_{\text{homo}}(\mathbf{x})$, where θ is a function $\theta = v(\mathbf{x})$	Methods for Linear Operators [163], [164]	Parameterize \mathcal{G} and u_{homo} with neural networks, which are trained with supervised data (and possibly physics-informed losses).
	Methods for Nonlinear Operators [165]	Discretize the PDEs and use trainable mappings to linearize the target operator, where Green's function formula is subsequently applied to construct the approximation.

Grid/Graph-based Methods



- Grid-based operator learning (image-to-image)

$$\tilde{G}: \{u(\mathbf{x}_i)\} \mapsto \{v(\mathbf{x}_i)\}$$

- Graph-based Methods (graph-to-graph)

$$\tilde{G}: \text{node features} \mapsto \text{node features}$$

Grid-based Operator Learning $G_w(\theta) = \{u(\mathbf{x}_i)\}_{i=1}^N$, where $\{u(\mathbf{x}_i)\}_{i=1}^N$ and $\theta = \{v(\mathbf{x}_i)\}_{i=1}^N$ are discretizations of input and output functions in some grids	Convolutional Neural Network [69], [166]	A convolutional neural network is utilized to approximate such an image-to-image mapping, where the loss function is based on supervised data (and possibly physics-informed losses).
	Fourier Neural Operator [167]	Several Fourier convolutional kernels are incorporated into the network structure, to better learn the features in the frequency domain.
	Neural Operator with Attention Mechanism [168], [169], [170]	The attention mechanism is introduced to the design of the network structure, to improve the abstraction ability of the model.
Graph-based Operator Learning $G_w(\theta) = \{u(\mathbf{x}_i)\}_{i=1}^N$, where $\{u(\mathbf{x}_i)\}_{i=1}^N$ and $\theta = \{v(\mathbf{x}_i)\}_{i=1}^N$ are discretizations of input and output functions in some graphs	Graph Kernel Network [171]	A graph kernel network is employed to learn such a graph-based mapping.
	Multipole Graph Neural Operator [172]	The graph kernel is decomposed into several multi-level sub-kernels, to capture multi-level neighboring interactions.
	Graph Neural Operator with Autogressive Methods [173]	Extend graph neural operators to time-dependent PDEs.



Neural Operator



■ Open Challenges

- Incorporating physical priors
 - Generalizability \uparrow , Data Demand \downarrow
 - Close integration of physics knowledge and models, in addition to *physics-informed loss functions*
- Reducing the cost of gathering datasets (**major**)
 - Large design space Θ , complex geometry Ω
 - High cost of data generating
- Developing large pre-trained models
- Modeling real-world physical systems

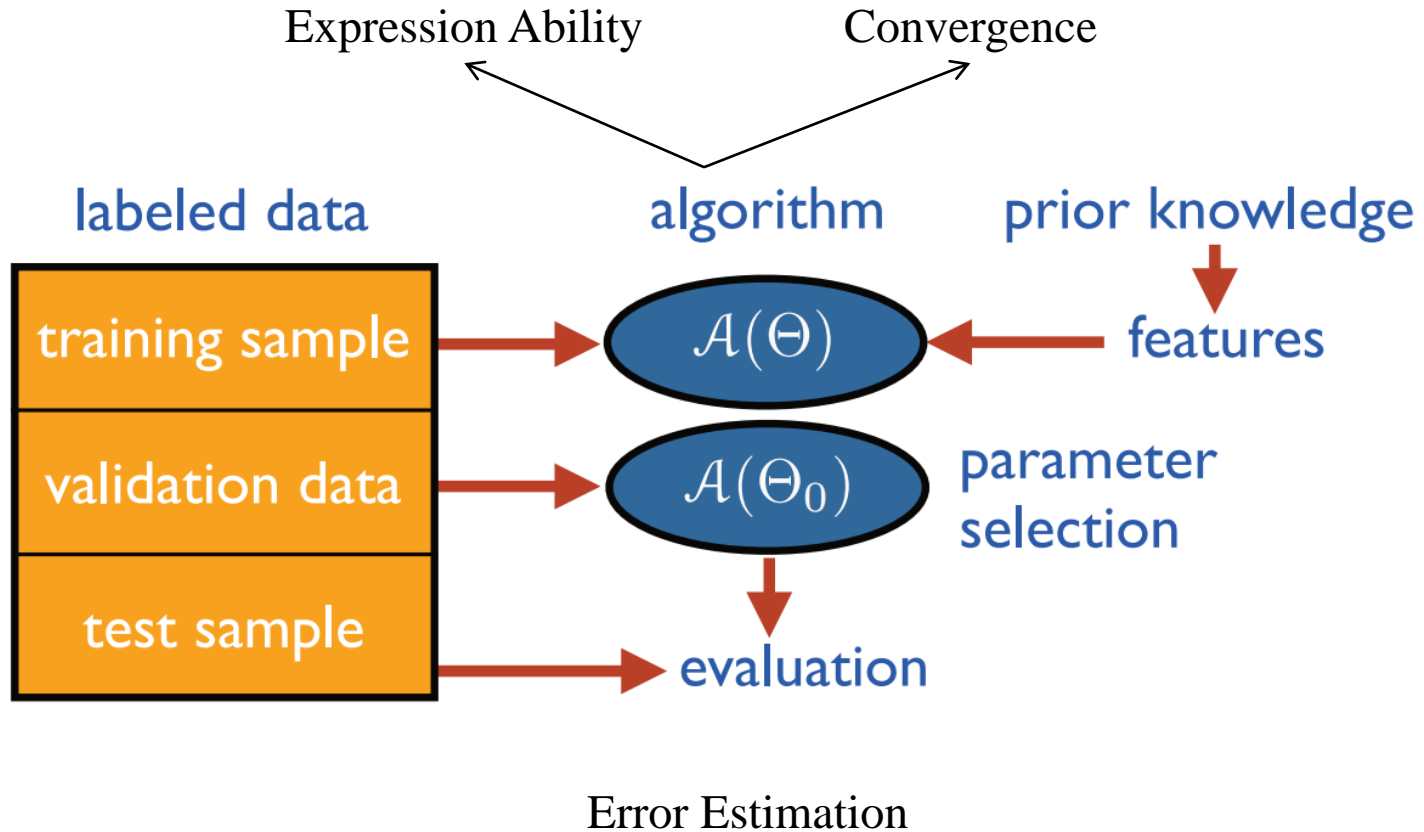
Neural Operator



■ Open Challenges

- Incorporating physical priors
- Reducing the cost of gathering datasets (**major**)
- Developing large pre-trained models
 - Handle so many downstream tasks
 - A possible to reduce data cost and training overhead
- Modeling real-world physical systems
 - From idealized experiments to real-world ones
 - It may be helpful to borrow from the field of numerical computing
 - Efficiently employed in industrial scenarios, e.g., optimization, simulation, etc.

Theory in PIML



Expression Ability

- It is well known that multi-layer neural networks are **universal approximators**, i.e., they can approximate any measurable function to arbitrary accuracy.
- A major concern in PIML is to approximate neural operator.
- **One-layer neural networks** can approximate any operators [16, 17]. (DeepONet)
- Next question: how many nodes do we need?
- **Wide, shallow** neural networks may need exponentially many neurons to obtain similar expression ability with **deep, narrow** ones [18].

Expression Ability

- [18] takes a first step for providing an upper bound of the width of the deeper neural networks for approximating operators.
- **Future work:**
- design more effective architecture to approximate operators with fewer nodes is significant for designing more stable and effective algorithms
- analyze the expression ability of other architectures

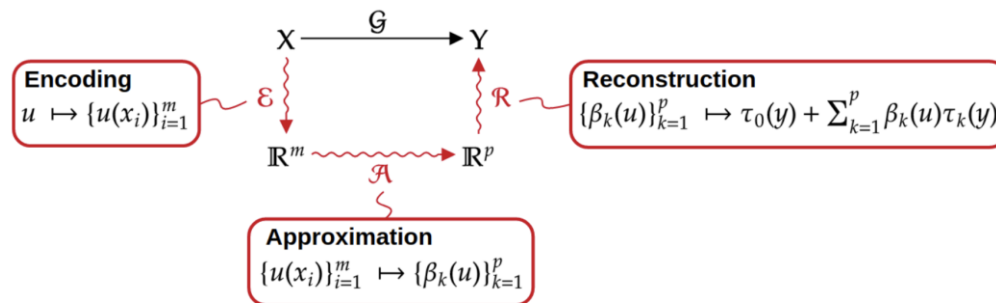
Convergence

- evaluate the algorithm: **whether it converges** and **its convergence speed**
- combine optimization and PDEs
- current with little research: PINNs [19], neural operator [20], deep ritz methods [21]

Error Estimation



- There are different kinds of error: **approximation error** (the target loss), **generalization error** (generalize to unseen samples) ...
- [22] first analyzes the approximation error and generalization error of DeepONet



Theory in PIML



- **Future work:**
- design more effective architecture to approximate operators with fewer nodes is significant for designing more stable and effective algorithms
- analyze the expression ability of other architectures
- analyze the convergence of PINNs for different kinds of PDEs for designing more efficient architectures and algorithms

Inverse Problem (Inverse Design)

- To optimize or discover unknown parameters of a physical system, including scientific discovery, shape optimization, optimal control, etc.

$$\begin{aligned} & \min_{\theta \in \Theta} \mathcal{J}(u(\mathbf{x}; \theta), \theta), \\ & \text{s.t. } \mathcal{P}(u; \theta)(\mathbf{x}) = 0. \end{aligned}$$

- Traditional methods
 - SQP, Adjoint PDE
 - infeasible in large-scale problems
 - heavy computational cost
 - non-differentiable physical process

Inverse Design



- Solving inverse design usually involves multiple steps
 - e.g., simulation, evaluation, configuration
- System Simulation & Evaluation
 - Neural Surrogates
 - PINN, Neural Operator, Neural Simulator
- Neural Representation
- Design Prediction
- Data Generation
- ...

Neural Surrogates



With PINN

- Directly extend PINN to inverse design[26]

$$\mathcal{L} = \lambda_p \mathcal{L}_{PINN} + \lambda_d \mathcal{J}$$

- imbalance training objectives

- PINN with hard constraints (h-PINN)[23]

- imposing hard constraints with the penalty method and the augmented Lagrangian method

- Bi-level optimization framework[24]

$$\begin{aligned} \min_{\theta} \quad & \mathcal{J}(w^*, \theta) \\ \text{s.t.} \quad & w^* = \arg \min_w \mathcal{L}_{PINN}(w, \theta). \end{aligned}$$

Neural Surrogates

With Neural Operator

- Trained differentiable neural operator predicting the state variables[25]

$$w^* = \arg \min_{w \in W} \mathcal{L}_{operator},$$
$$\min_{\alpha} \mathcal{J}(G_{w^*}(\theta_{\alpha})(\mathbf{x}), \theta_{\alpha}),$$

- using various models, e.g., DeepONet[27], Autoencoder[28]

With Neural Simulators

- Differentiable simulators mapping parameters to the values of interest to avoid numerical simulations[29]

Other Methods



- Neural Representation
 - parameterize the parameters/configurations with neural network to achieve more highly-detailed and continuous representations[30]
- Design Prediction
 - map the desired targets to the design parameters[31]
- Data Generation
 - generate novel samples with superior performance using generative models like VAE[32]

Open Problems and Challenges



- Neural Surrogate Modeling
 - balance of multiple loss terms and training convergence for physics-informed methods
 - large demand of data for operator and simulator training
- Large Scale Application
 - potential challenges like curse of dimensions, computational complexity in large scale scenarios
- Other Directions
 - using neural networks in other steps of inverse design besides simulation

Computer Vision and Graphics



- Traditional Visual Tasks (Classification & Detection)
 - knowledge of symmetry, such as equivariance to rotation[33]
- Motion and Pose Analysis/Physical Scene Understanding
 - knowledge of mechanics and kinematics, such as motion constraints[34], Hamiltonian canonical equations[35]
- Computer graphics
 - knowledge of rendering, such as classical volume rendering equations[36]

Reinforcement Learning



- Goal
 - to interact with an unknown world to maximize reward, with/without the learning of world models
- Policy Training
 - use knowledge to design rewards for specific goals, such as adaptive mesh refinement[37]
- Model Training
 - use knowledge to learn a better world model, such as equations of continuous dynamics[38]
- Exploration Guiding
 - use knowledge to restrict exploration to safe regions, such as logical sandboxes[39]

Open Problems and Challenges

- Better Description of Physical World
 - to learn meaningful representations from visual observations
 - to find formulated representations of intuitive physics
- Generic Modeling of Physical Tasks
 - to deal with new tasks from proper expert knowledge instead of case-by-case design
- Solving High-Dimensional Problems in RL
- Guaranteeing Safety in Complex, Uncertain Environments

Conclusions

- Open challenges
- From methodological perspective
 - Standardized dataset
 - Better algorithms for inference and optimization
 - Scalable algorithms for intuitive physics in real world
- From tasks perspective
 - Better methods for neural simulation
 - Inverse problems
 - More applications in real world CV/RL



Thank you!

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