ParaFIND: Parameter Field Inference on Non-uniform Domains using Neural Network

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Abstract

Real-world physical phenomena are often governed by Partial Differential Equations (PDEs) influenced by spatially distributed properties/parameters. While many deep learning techniques offer reasonable parameter estimation results for simple cases, they struggle to generalize to irregular geometries, limiting their applicability to a narrow range of problems. To address this limitation, we propose ParaFIND a novel approach for estimating unknown PDE parameter fields distributed on non-uniform domains from scarce observations of the system's response. Our method leverages the Finite Element Method (FEM) for space discretization and learns parameters modeled as functions of space from their mesh representation. This innovative approach enables accurate parameter estimation even in complex geometrical settings. We demonstrate the robustness of our model under limited sparse data constraints using as few as 108 data samples. Our numerical simulations validate the effectiveness of ParaFIND in handling various irregularities in a given geometry, showcasing its potential for broader applications in real-world scenarios.

1 Introduction and Related Work

In recent years, deep learning informed by physics and domain knowledge has significantly advanced the understanding of complex physical phenomena. However, accurately capturing and modeling the underlying governing differential equation systems remains a challenging and time-intensive task. This difficulty often arises from the variable nature of the governing parameters in PDEs and the frequent irregularities in geometry, which present significant challenges for current data-driven methods.

Parameter estimation has been extensively studied in problems involving scalar parameters. Various methods have been employed, including finite element updating (Steenackers & Guillaume, 2006; Ebrahimian et al., 2017), Bayesian Inverse Problems (Matthies et al., 2016), least squares estimation (Ji et al., 2020), the Kalman filter (Onat, 2019; Iglesias, 2016), Gaussian processes (Zhang & Gu, 2022; Deng et al., 2020), and sparse identification (Brunton et al., 2016) and other Gradient-based Optimization Methods (Dwivedi et al., 2021). However, approaches like Bayesian methods face limitations due to the assumption that unknown parameter values adhere to a prior distribution, which can be impractical when dealing with unknown field variables. PINNs can model field parameters in certain scenarios (Yu et al., 2022; Taneja et al., 2022), where field parameters and state variables

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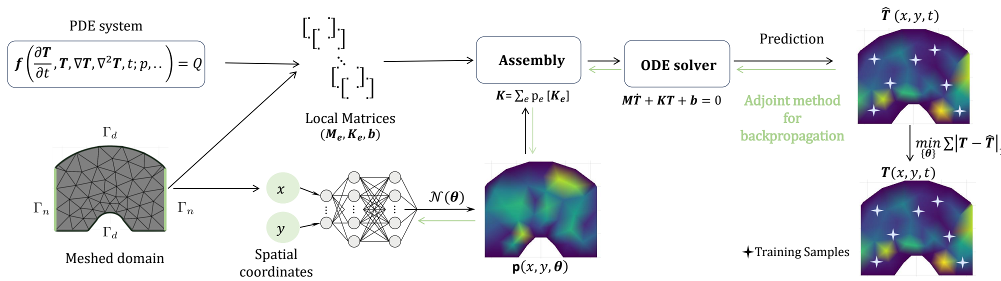

Figure 1: **Overview:** ParaFIND learns unknown field parameters through the neural network $\mathcal{N}$. The forward solution of the PDE is obtained via finite element discretization for the spatial domain and an ODE solver. The adjoint method is employed for backpropagation.

are often learned and predicted simultaneously using separate neural networks. However, achieving optimal performance with PINNs still requires substantial training data (Karniadakis et al., 2021).

Additionally, some efforts have been made to estimate field parameters using scarce data ((Li et al., 2024, 2022)). However, these methods still rely on the Finite Difference Method (FDM) for space discretization, limiting their generalization ability to arbitrary and irregular geometries. Other techniques tried to couple FEM with Neural Networks to solve inverse problems (Meethal et al., 2023), but these approaches are still validated only for 1D systems, which do not entail the modeling complexity of irregular domains.

This paper addresses the abovementioned challenges by introducing ParaFIND (see Figure 1), a field parameter estimation framework employing neural networks. ParaFIND operates assuming that the observed physics is governed by nonlinear parametric PDEs, where the unknown parameter fields characterize the physical phenomena within the computational domain. The primary goal of this work is to enable field parameter estimation on irregular geometries using only scarce response data.

We design deep neural networks to model the unknown parameter. Subsequently, the PDE system is discretized using FEM, where the system is assembled using the actual field parameters and the local stiffness matrices. Then, we solve the system using a differential equations solver. During neural network training, the spatial-temporal predictions are compared to the measured data, and the resulting errors are minimized. Once optimized, the neural network model can accurately estimate the target parameters and effectively predict the physical behavior beyond the training region (extrapolation).

2 Modeling and Discretization Approach

2.1 Finite Element Discretization

Given a first-order PDE, the discretized weak form by the finite element method gives the following equation,

$$\mathbf{M}\dot{\mathbf{T}} + \mathbf{K}\mathbf{T} = \mathbf{b} \tag{1}$$

where $\mathbf{K}$ and $\mathbf{M}$ are respectively the global assembled mass and stiffness matrices, b is the force vector. While $\mathbf{M}$ and $\mathbf{b}$ are assembled using the standard FEM techniques (Dhatt et al., 2012), the assembly of K has small differences to be able to account for the parameters prediction. We start by computing each element's local stiffness matrices $\mathbf{K_e}$.

$$\mathbf{K_e} = \int_{\Omega_e} \mathbf{B}^T \kappa(\mathbf{x}) \mathbf{B} \, d\Omega_e = \kappa_\mathbf{e} \mathbf{K_0^e} \quad , \mathbf{K_0^e} = \int_{\Omega_e} \mathbf{B}^T \mathbf{B} \, d\Omega_e \tag{2}$$

We assume that the parameter $\kappa(x)$ is constant over the element domain, which can be a reasonable assumption due to the necessity of discretization for numerical calculations. We then assemble

$$\mathbf{K} = \mathbf{assembly}([\kappa_\mathbf{e}]_{\mathbf{e}\in\mathbf{\Omega}}, [\mathbf{K^e}]_{\mathbf{e}\in\mathbf{\Omega}}) \tag{3}$$

2.2 ParaFIND Framework

The proposed ParaFIND discretizes PDEs spatially using Finite Elements (FE) discretization. This step consists of two separate steps. First, we assemble the local stiffness matrices. Second, we assemble the global stiffness matrices using the local matrices and the field parameter under consideration. (see Figure 1). The field parameter κ is modeled by a feed-forward neural network with spatial coordinates inputs x and y, which correspond to the coordinates of the element's centroid. The network in this study consists of 5 layers, each of the middle four layers containing 50 neurons and featuring skip-connections. The network parameters are denoted as $\boldsymbol{\theta}$, and the parameter is modeled as $\kappa(x, y) = \mathcal{N}(x, y, \boldsymbol{\theta})$. The estimated parameter from the neural network is inserted into differential equations for forward inference (state variable prediction). The inference is compared with available observations in mini-batches to compute the loss. We employed the $L1$ loss function as it provided superior results compared to both $L2$ and normalized $L2$ loss. The adjoint sensitivity method (Chen et al., 2018; Rackauckas et al., 2019) is utilized for backpropagation and network training.

3 Test Problem: Transient Heat Conduction Problem

In this work, we investigate the transient heat conduction problem as a benchmark to demonstrate the capabilities of the proposed framework.

3.1 Problem Setup

The heat equation characterizes the evolution of temperature $T(\mathbf{x}, t)$, where $\mathbf{x} = (x, y)$ denotes the spatial coordinates and t represents time, within the domain $\mathbf{x} \in \Omega$ over a temporal interval. Let $Q : \Omega \times (0, \tau) \to \mathbb{R}$ be the heat source. The strong form of the heat equation is expressed as:

$$c\rho\dot{T}(\mathbf{x}, t) = \nabla \cdot (\kappa(\mathbf{x})\nabla T(\mathbf{x}, t)) + Q \quad \text{in} \quad \Omega \times (0, \tau), \tag{4}$$

where c is the specific heat capacity, ρ is the density, and $\kappa(x)$ is the space-dependent thermal conductivity we aim to recover.
We assign the boundary temperature $T_d(\mathbf{x}) : \Gamma_d \times (0, \tau) \to \mathbb{R}$, and the boundary heat source $q_n(t) : \Gamma_n \times (0, \tau) \to \mathbb{R}$, where Γ_d is the domain on which the Dirichlet boundary condition is applied, Γ_n is the domain on which the Neumann boundary condition is applied, $t \in (0, \tau)$ represents the temporal domain with τ as the final time. The boundary and initial conditions are enforced by:

$$T(\mathbf{x}, t) = T_d(\mathbf{x}) \qquad \text{on} \quad \Gamma_d \times (0, \tau), \quad \nabla T(\mathbf{x}, t) \cdot \mathbf{n} \quad = q_n(t) \qquad \text{on} \quad \Gamma_n \times (0, \tau), \tag{5}$$

$$T(\mathbf{x}, 0) = 10, \qquad\qquad x \in \Omega. \tag{6}$$

where $\mathbf{n}$ is the outward normal vector. In this setup we impose the boundary heat flux to $q_n(t) = 500(1 + sin^2(\pi t))$, and $T_d(\mathbf{x}) = 0$. We perform heat conduction analysis on the domain illustrated in Figure 1. The computational mesh comprises 53 nodes and 104 triangular elements. The system under study is a steel plate, where we investigate heat diffusion from the interior toward the Γ_d boundaries of the domain, considering the influence of time-dependent heat flux originating from the Γ_n boundaries. The temperature at the Γ_d boundaries is maintained constant at a lower value.

Key parameters for the simulation include a heat source term $Q = 0$, material density $\rho = 7850\,\text{kg/m}^3$, specific heat capacity $c = 490\,\text{J/kg . C}$, and a time step $\Delta t = 1\,\text{s}$ with a total simulation time of $\tau = 300\,\text{s}$. The thermal conductivity $\kappa(x, y)$ is defined as $30 + 5 \times (5(5x + 1)^2 + 25y^2)$. This function covers the range of thermal conductivity values associated with various steel materials.

3.2 Numerical Results

We demonstrate the efficacy of ParaFIND in predicting a nonlinear field parameter distribution, achieving a mean absolute error(MAE) as low as 1.75%. We also analyze the system's response at $t = \tau$, where the response error remains below 0.8%

To provide a comprehensive comparison and emphasize the importance of modeling the parameter as a field rather than a scalar, we also present the system response based on scalar parameter prediction. In this case, a single neuron predicts the scalar parameter, which typically converges to the mean of

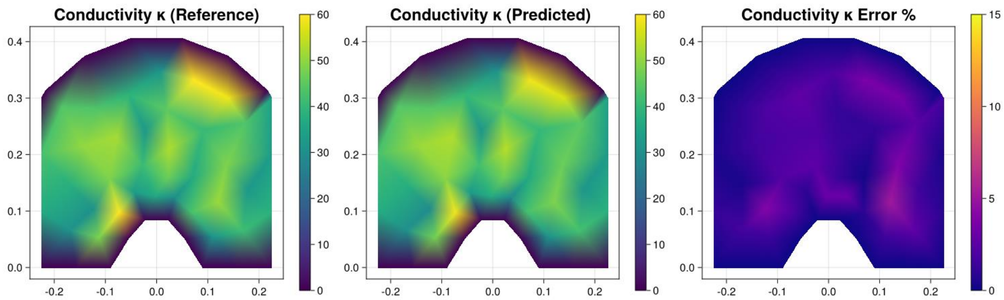

Figure 2: ParaFIND accurately estimates the field parameter κ with a MAE of 1.75%.

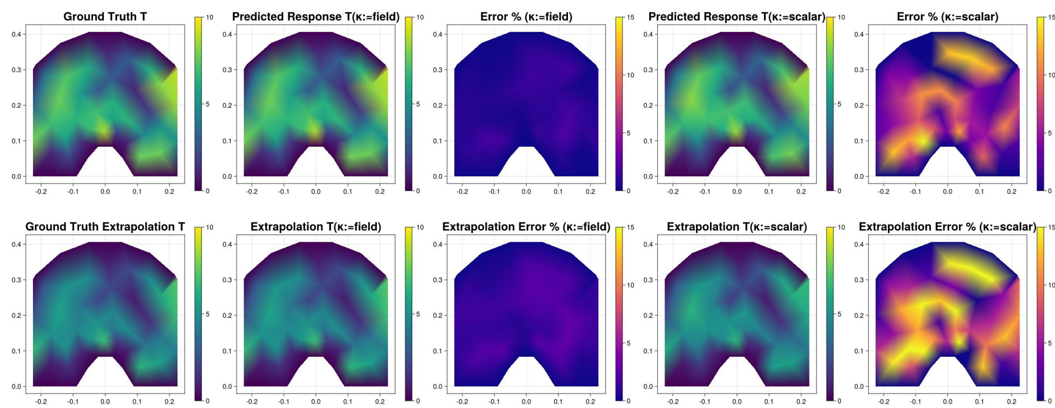

Figure 3: Forward inference using the predicted parameter. ParaFIND demonstrates robust performance in forward inference, effectively handling both interpolation and extrapolation tasks. Response of scalar parameter modeling and comparison with Ground Truth (first row), highlighting a larger MAE, of 6.27%, in forward inference compared to the field-based approach by ParaFIND (MAE 0.8%). Evaluation of ParaFIND's extrapolation performance(second row) at $t = 600s$, showing an MAE of 1.5% relative to ground truth, and a comparison with the extrapolated response of scalar parameter modeling (MAE 8.6%).

the ground truth field parameter distribution. However, this approach results in substantial errors, with a forward inference MAE of 6.27% compared to just 0.8% for the field-based approach by ParaFIND. Furthermore, we evaluate ParaFIND's extrapolation performance at $t = 600s$, where it achieves an MAE of 1.5% relative to the ground truth. In contrast, the extrapolated response using the scalar parameter model shows a significantly higher error of 8.6%. We successfully train our model using as few as 108 measurements. The training process for ParaFIND requires 140 iterations on CPU, with a total training time of $284s$.

4 Conclusion

This paper presented ParaFIND for field parameter estimation on irregular geometries. We evaluate its effectiveness in a heat conduction problem where thermal conductivity is the target parameter. Our findings demonstrate the robustness of ParaFIND across a nonlinear parameter distribution. The estimated parameter closely aligns with the reference, even with limited training data. Additionally, we highlight the importance of modeling parameters as field functions by comparing the response of scalar parameters against field parameters. We further demonstrate the capability of ParaFIND for future extrapolation. ParaFIND is expected to be highly efficient when handling multiple field parameters or multiphysics problems. Future applications could extend to PDE problems such as diffusion equations, advection, thermal runaway, and electrophysiology.

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