Application of Physics-Informed Neural Networks to Inverse Problems in Material Science

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Abstract

This study explores the use of Physics-Informed Neural Networks (PINNs) for addressing inverse problems in material science. The proposed approach is applied to a pullout test, where the objective is to infer the characteristics of two materials using only a single measurement. The framework demonstrates how PINNs can simultaneously estimate unknown system parameters and solve the underlying partial differential equations, even with limited, scattered, or noisy data. By embedding the governing physical laws directly into the neural network's loss function, the method eliminates the need for conventional iterative optimization and complex mesh generation, resulting in a robust and fully mesh-free solution. The results show that inverse PINNs can accurately and efficiently identify unknown parameters, achieving significant improvements in computational speed and flexibility compared to traditional inverse modeling techniques such as the Finite Element Method (FEM) and the Finite Difference Method (FDM). Overall, the findings confirm that PINNs provide an effective framework for solving inverse problems, yielding reliable parameter estimates and accurate approximations of the pullout test response.

1 Introduction

Inverse problems play a central role in science and engineering, where the objective is to estimate unknown system parameters or inputs based on limited observational data. Such problems commonly arise in domains like geophysics, material science, and medical imaging, where direct measurements are either impractical or impossible. Traditional numerical methods, including the Finite Element Method (FEM) and the Finite Difference Method (FDM), have been widely used to address these challenges. However, these techniques often suffer from high computational costs, sensitivity to measurement noise, and the need for complex mesh generation. In contrast, Physics-Informed Neural Networks (PINNs)[Raissi et al., 2019] provide a promising alternative by embedding governing physical laws directly into the neural network's[Isaac Elias Lagaris and Fotiadis, 1998] loss function. This integration enables the model to simultaneously learn the system dynamics and infer unknown parameters, thereby alleviating the ill-posedness of inverse problems and achieving reliable solutions even with sparse or noisy data.

2 Methodology

2.1 Inverse Physics-Informed Neural Networks

An inverse PINN identifies unknown physical parameters in systems governed by differential equations by blending sparse data with physical laws. For a PDE

$$\mathcal{N}(u;\lambda) = 0, \quad x \in \Omega, \qquad \mathcal{B}(u) = 0, \tag{1}$$

2nd Conference on Applied AI and Scientific Machine Learning (CASML 2025).

where $\mathcal{B}(u)$ denotes the boundary condition. A neural network $u_\theta(x)$ approximates $u(x)$, while the unknown parameters λ are learned through the loss function:

$$\mathcal{L}(\theta, \lambda) = \frac{1}{N_d} \sum_{i=1}^{N_d} \left| u_\theta(x_i) - u_i^{obs} \right|^2 + \frac{1}{N_f} \sum_{j=1}^{N_f} \left| \mathcal{N}(u_\theta; \lambda)(x_j) \right|^2 . \tag{2}$$

2.2 Parameter Estimation

Unknown parameters are optimized jointly with network weights, ensuring the learned values satisfy both observed data and governing physics simultaneously.

3 Results

To demonstrate the capability of the proposed inverse PINN framework, we consider the classical pullout test problem[Anne Poot and Meer, 2025]. The model was trained on $N_{obs} = 10$ noisy data points sampled from the true solution (with $EA_{true} = 0.8$, $k_{true} = 70.0$) and $N_{coll} = 50$ collocation points.

The PINN successfully recovered the ground truth parameters with high accuracy. The final estimated values show minimal error, demonstrating the robustness of the method to noisy data:

- **EA Estimate:** 0.801059 (True: 0.8) 0.132% relative error
- **k Estimate:** 69.965622 (True: 70.0) 0.049% relative error

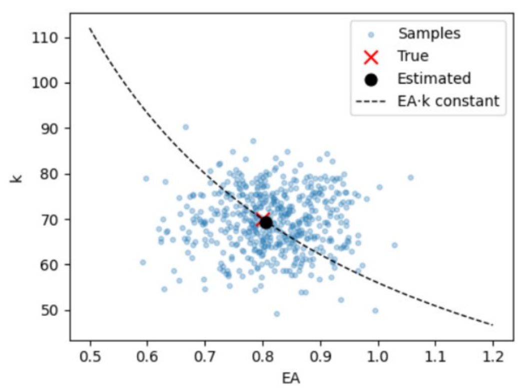

Figure 1: 1D Pullout test-PINNs solution.

4 Conclusion

This work demonstrates the effectiveness of Physics-Informed Neural Networks (PINNs) in solving inverse problems in material science. By embedding the governing physical equations directly into the loss function, the proposed PINN framework accurately identified the unknown material parameters EA and k using only ten noisy observations. The use of a hybrid Adam–L-BFGS optimization strategy enabled stable training and precise convergence, ensuring both robustness and efficiency. The results highlight the strong potential of this data-efficient and mesh-free approach for parameter identification and system discovery in complex physical systems, particularly where experimental data are limited or expensive to acquire.

5 Acknowledgements

This research was supported by the seed grant (GP-75) from Dr. B. R. Ambedkar National Institute of Technology Jalandhar to the corresponding author and a fellowship from the Ministry of Education, Government of India to the first author.

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