Exploiting PINNs for solving complex free boundary problems

From Shape Optimization to Error Control

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Outline

Free Boundary Problems and Deep Learning

Free Boundary Problems (FBP):

- Classical challenges: expensive remeshing, geometric complexity, moving boundaries.
- Need for mesh-free and flexible methods to handle geometry changes naturally.

The Data-Driven Revolution:

- Neural Networks as universal approximators for PDEs.
- Two main phases in our research group's activity:
  1. **Supervised/Geometric approach:** Learning shape functionals from data.
  2. **Physics-Informed approach:** Solving PDEs and geometry via energy minimization.

Step 1: Learning Geometry (Supervised Approach)

Reference: *Deep Learning for the Approximation of a Shape Functional* (ArXiv:2110.02112, 2021).

The Problem:

- Approximating the **Torsional Rigidity** $T(\Omega) = \int_\Omega u \, dx$ of a planar domain.
- PDE constraint: $-\Delta u = 1$ in Ω, $u = 0$ on $\partial\Omega$.

The Method (CNN):

- **Input:** Digital images (bitmaps) of domains Ω.
- **Model:** Convolutional Neural Network (CNN) trained on FEM-generated solutions.
- **Outcome:** The network acted as a fast surrogate model to predict a complex geometric functional.

Limitation: Purely data-driven; required an external solver (FEM) for training data.

Step 2: Physics-Informed Approach (Bernoulli Problem)

Reference: *A physics-informed learning approach to Bernoulli-type free boundary problems* (CAMWA, 2022).

The Problem (Bernoulli FBP):

- Finding an unknown annular domain and potential u such that:

$$\begin{cases} u = 1 & \text{in } \Omega \\ \Delta u = 0 & \text{in } \Sigma \\ u = 0 & \text{outside } \Omega \cup \Sigma \\ |\nabla u| = Q & \text{on } \Gamma_{free} \text{ (Bernoulli condition)} \end{cases}$$

The Innovation: Variational PINNs

- Instead of supervised learning, we minimize the **Total Energy** (Dirichlet + Volume term).
- The Free Boundary emerges naturally as the shape that minimizes the energy.
- **Advantage:** No mesh generation/remeshing required. The NN solves

The Current Challenge: From Results to Rigor

The "Black Box" Issue

We showed that PINNs work for FBPs (Bernoulli). But can we guarantee the accuracy? If the Loss tends to zero, does the error $|u - \tilde{u}|$ tend to zero?

Focus of current work:

- Establishing a theoretical foundation for error control.
- Designing Loss Functions that provide sharp error bounds.
- *Ref: S. Cuomo et al., "Error Control in PINNs: The Role of Loss Function"*

Theoretical Bounds: Toy Model (ODE)

First Order ODE: $u'(t) = f(t, u(t))$.

For this simple case, the Mean Squared Error (MSE) residual $\mathcal{R}$ successfully bounds the error:

$$||u - \tilde{u}||_\infty \leq C_1 h + C_2 \mathcal{R}^{\frac{1}{2}}$$

Implication: Minimizing the standard quadratic loss guarantees convergence to the true solution for ODEs.

The Dimensional Gap: Poisson Problem

Elliptic PDE: $-\Delta u = f$ in $\Omega \subset \mathbb{R}^N$.

We derive an error estimate splitting *Discretization* vs *Model* error:

$$\max_{\Omega} |u - \tilde{u}| \leq \underbrace{Ch}_{\text{Vanishes with } h \to 0} + \underbrace{C(\Omega)||\text{Residual}||}_{\text{Model Error}}$$

Crucial Finding: In high dimensions ($N \geq 5$), the standard L^2 (MSE) norm of the residual is **not sufficient** to control the L^∞ error of the solution efficiently.

Proposing Robust Loss Functions

To strictly control the Uniform Norm (L^∞) of the error, the Loss Function must be adapted to the dimension.

Theoretical Constraint: We need $p > N/2$ for L^p loss functions to guarantee L^∞ convergence (Theorem 2.3).

Summary and Outlook

Trajectory of Research:

1. **2021:** NNs as geometric approximators (Supervised).
2. **2022:** Variational PINNs for solving Free Boundary Problems (Bernoulli) without meshes.
3. **Current:** Rigorous Error Control. We proved that "Standard MSE is not enough" in high dimensions.

Future Steps:

- Find the same type of error estimates for more complex problems, elliptic problems like for instance Bernoulli, or even evolutionary PDE.
- Work out a new type of PINNS where the Neural Network provides not only the function (solution to the PDE) but also information on the domain.

Thank you!