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Physics-Informed Neural Network for Deep Learning Solution of Forward and Inverse Problems Involving PDE Physical Laws

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Abstract

Physics-based AI-driven techniques integrate physical laws into neural network (NN) training. In the Physics-Informed Neural Networks (PINNs) method, a loss function includes data-driven and physics-driven components. The NN is trained to minimize this loss thereby learning solutions consistent with both observed data and the governing physical laws. In machine learning, PINNs enable the solution of ODEs and PDEs by embedding physical laws directly into the training process. PINNs incorporate the governing equation of a system as a constraint in the loss function. This method regularizes the learning process and enables robust predictions under noisy and sparse data. The nonlinear pendulum [Guckenheimer & Holmes, Springer, 1983] governed by a second-order nonlinear ODE is a canonical example of system dynamics.

For an undamped nonlinear pendulum, we have

[$\frac{d^2\theta}{dt^2}+\frac{g}{L}\sin(\theta)=0$],

where ($\theta(t)$) is the angular displacement. This presentation focuses on PDEs for modeling more complex systems in physics, engineering, and applied sciences where solutions are sought. In particular, the time-dependent Schrödinger equation (TDSE) is introduced as the foundational PDE of non-relativistic quantum mechanics governing the evolution of quantum states and giving rise to both forward and inverse problems. A forward problem predicts the system's evolution given the Hamiltonian together with initial and boundary conditions. In contrast, an inverse problem seeks to estimate unknown parameters from observed data. Inverse problems are often formulated as optimization problems like [$\underset{V}{\mathop{\min}}\,\|F(V)-\mathcal D_{\text{obs}}\|^2+\alpha R(V)$]

where ($R(V)$) is the regularization term. The TDSE for a quantum system in d spatial dimensions is [$\mathrm{i}\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=\hat{H}\Psi(\mathbf{r},t)$] where ($\Psi(\mathbf{r},t)$ is the complex-valued wavefunction.

A survey by Banerjee et al. (arXiv:240.01026, 2024) highlights growing interest in PINNs for medical image analysis. PDEs with sparse data are particulary promising for PINNs such as in hemodynamics (i.e., blood flow models) with Navier-Stokes equations, non-Newtonian blood rheology (e.g., Carreau-Yasuda, Herschel-Bulkley, Casson models), and reduced-order arterial models.