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SYNTHESIS OF PHYSICS AND DATA: MACHINE LEARNING IN RADIATION TRANSPORT PROBLEMS

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Abstract

This paper reviews modern approaches to integrating Machine Learning (ML) and Artificial Intelligence (AI) methods into neutron-physical modeling tasks. The paradigm shift from purely physical models to hybrid systems is analyzed, where deep learning algorithms are used for nuclear data approximation, uncertainty quantification, and accelerating Monte Carlo convergence. Special attention is given to Physics-Informed Neural Networks (PINNs) for solving the transport equation and generating weight window maps in deep penetration problems. The issues of "black box" model interpretability and result verification in the context of nuclear safety are discussed.

Keywords

Machine Learning, Neural Networks, Nuclear Data, PINNs, Monte Carlo Method, Variance Reduction, Deep Learning, Surrogate Modeling, Gaussian Processes.

Introduction

Modern reactor physics faces a fundamental contradiction between modeling accuracy requirements and available computational resources. Numerical solution of the integro-differential Boltzmann transport equation via the Monte Carlo method ensures precision but suffers from slow convergence proportional to $1/\sqrt{N}$, where N is the number of particle histories. In tasks regarding radiation shielding, fuel depletion, and core optimization, computational costs become prohibitive.

Traditional acceleration methods, such as deterministic iterations or perturbation methods, are reaching their efficiency limits. In this context, Machine Learning (ML) methods offer an alternative path: replacing or augmenting resource-intensive physical calculations with high-precision statistical approximators. This involves not merely regression analysis, but embedding ML into the core of the computational process – from nuclear constant preparation to generating variance-optimized particle trajectories.

Machine Learning in Nuclear Data Evaluation

A fundamental problem in neutronics is the uncertainty of input data – microscopic interaction cross-sections. Traditional nuclear data evaluation relies on fitting theoretical models (optical model, liquid drop model) to experimental points. Here, ML methods, specifically

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Gaussian Processes (GP), demonstrate a significant advantage over classical least squares methods.

Gaussian Processes allow for reconstructing the cross-section dependence on energy $\sigma(E)$ not as a deterministic function, but as a probabilistic distribution of functions. This automatically solves the Uncertainty Quantification (UQ) problem. Within the Bayesian approach, GP defines a prior distribution, which is updated by experimental data:

$$f(x) \sim \mathcal{GP}(m(x), k(x, x')). \tag{1}$$

Using GP allows for identifying hidden systematic errors in experimental data and generating covariance matrices required for reactor safety margin assessment with much lower computational costs compared to the traditional Total Monte Carlo method.

Monte Carlo Acceleration and Variance Reduction

The most promising direction is the use of Deep Neural Networks (DNN) to automate Variance Reduction (VR) methods. In deep penetration problems (e.g., biological shielding calculations), the probability of a particle traversing the shield is negligible. Classical methods like CADIS (Consistent Adjoint Driven Importance Sampling) require a preliminary deterministic solution of the adjoint transport equation to obtain particle importance maps.

ML methods offer an "on-the-fly learning" approach. A neural network is trained to predict the importance map (weight windows) directly during the Monte Carlo simulation. The algorithm iteratively updates network parameters, minimizing flux estimation variance in the target region. The network inputs are phase space coordinates ($\mathbf{r}, E, \mathbf{\Omega}$), and the output is the optimal particle weight w_{target} . This approach avoids phase space discretization via meshes, replacing it with a continuous function approximated by the neural network, thereby eliminating mesh artifacts and significantly reducing memory requirements.

Surrogate Modeling and PINNs

For reactor design optimization tasks requiring thousands of iterative calculations, direct use of transport codes is unfeasible. Here, surrogate models – lightweight neural network approximators mimicking the response of complex codes – come into play. However, standard neural networks are "black boxes" and may violate fundamental conservation laws. The solution lies in Physics-Informed Neural Networks (PINNs).

In the PINN architecture, physical information is embedded directly into the loss function during training. If we aim to approximate the transport equation solution $\psi(\mathbf{r}, \mathbf{\Omega})$, the loss function $\mathcal{L}$ will consist of two terms: the error on data $\mathcal{L}_{data}$ and the physics residual $\mathcal{L}_{physics}$.

$$\mathcal{L} = \mathcal{L}_{data} + \lambda \left\| \mathbf{\Omega} \cdot \nabla \hat{\psi} + \Sigma_t \hat{\psi} - \hat{Q} \right\|^2, \tag{2}$$

where $\hat{\psi}$ is the neural network output and $\hat{Q}$ is the total source. Training such a network reduces to minimizing the Boltzmann equation residual. PINNs do not require large amounts of training data since they "know" the physics, guaranteeing that the predicted solution satisfies particle conservation laws within a specified error margin. This paves the way for ultra-fast solvers for multiphysics tasks where neutronics must be coupled with thermal-hydraulics in real-time.

Conclusion

Despite impressive results, widespread adoption of ML in nuclear engineering practice is hindered by interpretability issues. Unlike transparent Monte Carlo algorithms, neural networks are difficult for regulatory bodies to verify. There is a risk that in unexplored phase space regions (extrapolation), the ML model may produce physically incorrect results.

Nevertheless, the integration of Machine Learning into computational nuclear physics is irreversible. The development of hybrid modeling methods, where ML handles routine approximation and acceleration tasks while rigorous physical codes perform final validation, allows for overcoming the stagnation in traditional algorithm performance. The synergy between probabilistic modeling (Monte Carlo) and statistical learning (Deep Learning) forms a new class of computational tools essential for designing Generation IV reactors and fusion devices.

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