Parametric matrix models bridge physics and machine learning

U.S. DEPARTMENT OF ENERGY | Office of Science

NUCLEI Nuclear Computational Low-Energy Initiative

Objectives

- Researchers have introduced a new class of machine learning algorithms called parametric matrix models (PMMs).
- Unlike traditional approaches that mimic neurons or optimize generic functions, PMMs are built from matrix equations that resemble the governing equations of physical systems.
- By treating inputs as parameters for the matrix elements, PMMs capture essential structures such as smooth analytic behavior, symmetries, and conservation laws.
- PMMs are universal function approximators, able to solve general machine learning tasks while retaining strong interpretability.

Impact

- Parametric matrix models represent a paradigm shift in scientific machine learning.
- By embedding physical and mathematical structure directly into their design, PMMs produce interpretable results that adhere to known constraints, unlike many “black box” neural networks.
- This makes them especially powerful for scientific discovery, where extrapolation, efficiency, and interpretability are critical.
- PMMs can outperform state-of-the-art methods in scientific computing and compete strongly on broader machine learning tasks.

$$\begin{bmatrix} \end{bmatrix} = \begin{bmatrix} \end{bmatrix} + \theta_1 \begin{bmatrix} \end{bmatrix} + \theta_2 \begin{bmatrix} \end{bmatrix}$$

$$\begin{bmatrix} \end{bmatrix} \begin{bmatrix} \end{bmatrix} = \lambda(\theta_1, \theta_2) \begin{bmatrix} \end{bmatrix}$$

Parametric matrix models emulate physical systems through matrix equations, enabling accurate and interpretable predictions with fewer parameters than conventional machine learning methods.

Accomplishments

- “Parametric Matrix Models,” Cook, Jammooa, Hjorth-Jensen, Lee, Lee, Nat. Commun. 16, 5929 (2025).
- https://frib.msu.edu/news-center/news/researchers-develop-new-machine-learning-method