PHYSTAT - Statistics meets ML



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COmoving Computer Acceleration (COCA): Correcting Emulation Errors for Trustworthy N-Body Simulations

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Neural networks are increasingly used to emulate complex simulations due to their speed and efficiency. Unfortunately, many ML algorithms, including (deep) neural networks, lack interpretability. If machines predict something humans do not understand, how can we check (and trust) the results? Even if we could identify potential mistakes, current methods lack effective mechanisms to correct them, limiting the reliability of these emulators. To address these issues, we introduce COmoving Computer Acceleration (COCA), a novel hybrid framework that integrates machine learning with traditional N-body simulators. COCA solves the correct physical equations of motion within an emulated frame of reference, inherently correcting any prediction errors. Our framework significantly reduces emulation errors in particle trajectories but also requires far fewer force evaluations compared to conventional simulations. This method effectively addresses the critical challenges of interpretability and accuracy in cosmological applications of machine learning, ensuring both speed and trustworthiness in complex simulations.

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