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Machine Learning-Based Estimation of Cumulants of Chiral Condensate via Multi-Ensemble Reweighting with Deborah.jl

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Investigating the critical endpoint of the finite-temperature QCD phase transition requires higher-order cumulants of the chiral condensate. These, in turn, involve traces of inverse Dirac operator powers $\operatorname{Tr} M^{-n}$ (n = 1, 2, 3, 4). Because direct computation with the Conjugate Gradient method is computationally expensive, we adopted a machine-learning strategy using gradient-boosted decision tree regression with bias correction [1], trained on data from simulations with the Iwasaki gauge action and Wilson clover fermion action [2]. The labeled set was split into training and bias-correction subsets, and the trained model was applied to unlabeled data, with the resulting bias-corrected ML estimates then examined. Building on earlier progress [3], we further applied multi-ensemble reweighting and interpolation to estimate cumulants at the first-order phase transition point, investigating dependence on the fraction of labeled and training data. Using ${
m Tr}\,M^{-1}$ from original measurements both as a direct component of the cumulant calculation and as an input feature for training ML models to estimate ${\rm Tr}\,M^{-n}$ (n=2,3,4), we found that even with only 1% labeled data, susceptibility, skewness, and kurtosis agreed almost perfectly with the original, suggesting that the computational cost can be reduced to approximately 25.8% of the original. To further probe avenues for reducing computational cost, we also incorporated the Plaquette and Rectangle loops as input features. Using these, we performed bias-corrected ML estimation for all four $\operatorname{Tr} M^{-n}$ in a single workflow and then carried out multi-ensemble reweighting. Unlike our main methodology, where original Tr M^{-1} is directly used and its statistical fluctuations naturally propagate through the analysis, this setup relies solely on correlations between the features and target. This also allowed us to investigate, in detail, the sensitivity of cumulant estimates to the presence or absence of bias correction.

- [1] B. Yoon et al., Phys. Rev. D 100, 014504 (2019), arXiv:1807.05971 [hep-lat].
- [2] H. Ohno et al., PoS LATTICE2018, 174 (2018), arXiv:1812.01318 [hep-lat].
- [3] B. J. Choi et al., PoS LATTICE2024, 033 (2024), arXiv:2411.18170 [hep-lat].

Parallel Session (for talks only)

Algorithms and artificial intelligence

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