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Self-Learning Monte Carlo Method¹ JUNWEI LIU, YANG QI, Department of physics, Massachusetts Institute of Technology, ZI YANG MENG, Institute of Physics, Chinese Academy of Sciences, LIANG FU, Department of physics, Massachusetts Institute of Technology — Monte Carlo simulation is an unbiased numerical tool for studying classical and quantum many-body systems. One of its bottlenecks is the lack of general and efficient update algorithm for large size systems close to phase transition or with strong frustrations, for which local updates perform badly. In this work, we propose a new general-purpose Monte Carlo method[1], dubbed self-learning Monte Carlo (SLMC), in which an efficient update algorithm is first learned from the training data generated in trial simulations and then used to speed up the actual simulation. We demonstrate the efficiency of SLMC in a spin model at the phase transition point, achieving a 10-20 times speedup. [1]J. Liu, et al. arXiv:1610.03137 (2016)

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