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Hypothesis testing of quantum Monte Carlo simulations¹ MARKUS WALLERBERGER, ALEXANDER GAENKO, EMANUEL GULL, University of Michigan, Ann Arbor — The large implementation complexity of modern quantum Monte Carlo solvers makes careful testing of the algorithm as well as verification of the results an imperative. Due to their deterministic nature, traditional unit tests are unsuited for verifying probabilistic results: they are prone to false positives in the case of outliers or changes to the implementation. Therefore, Monte Carlo data are often checked by visual inspection only, which is susceptible to incomplete and non-continuous test coverage. Statistical hypothesis testing provides a non-deterministic alternative: we choose an exact result (which exists for certain limits) as the null hypothesis and compute the statistical significance score for the Monte Carlo data. Rejection or too strong acceptance of the null hypothesis then amounts to a failed test, thus providing a test criterion for both the Monte Carlo estimate and its error bars. While this does not provide a binary answer, ambiguous cases can be systematically refined by lengthening the Monte Carlo run, and the procedure lends itself to automation. We develop a testing framework and illustrate the procedure for the two-dimensional Ising model as well as for Continuous-time quantum Monte Carlo data for the single impurity Anderson model.

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