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ParaMonte: A high-performance parallel library for Monte Carlo optimization, sampling, and integration AMIR SHAHMORADI, FATEMEH BAGHERI, The University of Texas at Arlington — At the foundation of predictive science lies the scientific methodology, which involves multiple steps of observational data collection, developing testable hypotheses, and making predictions. Once a scientific theory is developed, it can be cast into a mathematical model whose parameters have to be fit via observational data. This leads to the formulation of a mathematical objective function for the problem at hand, which has to be then optimized to find the best-fit parameters of the model or sampled to quantify the uncertainties associated with the parameters, or integrated to assess the performance of the model. Toward this goal, a highly customizable, user-friendly high-performance parallel Monte Carlo optimizer, sampler, and integrator library is presented here which, can be used on a variety of platforms with single to many-core processors, with interfaces to popular programming languages including Python, and C/C++/Fortran. In particular, we discuss the parallel implementation of a variant of Markov Chain Monte Carlo known as Delayed Rejection Adaptive Metrolpolis (DRAM) and its scalability.

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