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Exact recording of Metropolis-Hastings-class Monte Carlo simulations using one bit per sample

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The Metropolis-Hastings (MH) algorithm is the prototype for a class of Markov chain Monte Carlo methods that propose transitions between states and then accept or reject the proposal. These methods generate a correlated sequence of random samples that convey information about the desired probability distribution. Deciding how this information gets recorded is an important step in the practical design of MH-class algorithm implementations. Many implementations discard most of this information in order to reduce demands on storage capacity and disk writing throughput. Here, we describe how recording a bit string containing 1's for acceptance and 0's for rejection allows the full sample sequence to be recorded with no information loss, facilitating decoupling of simulation design from the constraints of data analysis. The recording uses only one bit per sample, which is an upper bound on the rate at which information about the desired distribution is acquired. We also demonstrate the method and quantify its benefits on a nontrivial colloidal system of charged particles in the canonical ensemble. The method imposes no restrictions on the system or simulation design and is compatible with descendants of the MH algorithm.

Submission history

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