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Geometric Allocation Approach for Transition Kernel of Markov Chain

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We introduce a new geometric approach that constructs a transition kernel of Markov chain. Our method always minimizes the average rejection rate and even reduce it to zero in many relevant cases, which cannot be achieved by conventional methods, such as the Metropolis-Hastings algorithm or the heat bath algorithm (Gibbs sampler). Moreover, the geometric approach makes it possible to find not only a reversible but also an irreversible solution of rejection-free transition probabilities. This is the first versatile method that can construct an irreversible transition kernel in general cases. We demonstrate that the autocorrelation time (asymptotic variance) of the Potts model becomes more than 6 times as short as that by the conventional Metropolis-Hastings algorithm. Our algorithms are applicable to almost all kinds of Markov chain Monte Carlo methods and will improve the efficiency.

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