# Geometric Allocation Approach for Transition Kernel of Markov Chain

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In the Markov Chain Monte Carlo method for a stationary distribution, the total balance, namely the invariance of distribution, is usually imposed to the transition kernel for sampling from the target distribution asymptotically. Since the invention of the method in 1953, the detailed balance, the reversibility, is used as a sufficient condition in most practical implementations, where every elementary transition is forced to balance with a corresponding inverse process. It is essential to optimize the kernel and reduce the autocorrelation of Markov chain, that is, the asymptotic variance, for the method to work in practice. However, only few algorithms to make a transition kernel have been known, such as the Metropolis-Hastings algorithm and the Gibbs sampler.

We present a new approach for constructing a transition kernel of Markov chain. Our method applies a geometric allocation of weight (measure) of configurations instead of solving the detailed balance equation algebraically. By this approach, it becomes possible to easily find many solutions that satisfy the total balance. Especially, we can certainly construct rejection-minimized transition probability, given candidate configurations. In the meanwhile, the reversibility is not a necessary condition for the invariance of distribution. A method to generally construct a nonreversible kernel, however, has not been known. By using our geometric approach, we can also find a nonreversible solution with rejection minimized. This algorithm is directly applicable to generic models with discrete variables and moreover can be extended to some models with continuous variables. Our approach is the first versatile method that generally construct a transition kernel without the detailed balance.

In the presentation, we will compare convergence of expectation values with that by other conventional methods and show that our algorithm significantly reduces autocorrelation of Markov chain in some basic models, e.g. the Potts model, the Gaussian model and quantum physical models.