

The standard paradigm in Monte Carlo integration is to estimate a ratio. In the prototypical scenario, a simulation is used to obtain the fraction of randomly sampled points which lie within an encompassing reference region. The integrand of interest is then estimated by multiplying this fraction with the known reference area.

More sophisticated algorithms retain the feature that they estimate ratios of normalizing constants [1] or partition functions [2]. Furthermore, the efficiency of all these integration techniques depend on the degree of overlap between the target integrands. Hence, much effort has been devoted to obtaining intermediate functions which bridge the integrands of interest.

Recently, Adib introduced a class of theorems, which he dubbed the replica gas identities, that can be used to estimate absolute integrals [3]. These identities are based on the simple physical idea of measuring the volume of a container by filling it with a specified density of ideal gas, and then counting the number of particles. Similarly, an integrand can be estimated by creating multiple non-interacting copies (or replicas) of a system that fill a region with a specified density, and then counting the number of replicas. Adib also described a complementary and more abstract identity relevant to simulations with a fixed number of replicas. A variant of this latter identity, which is particularly applicable to existing parallel tempering (a.k.a. replica exchange) simulations, will be the focus of the present work.

In this work, we shall consider integrals of the form,

$$Z = \int_{\Omega} dx \pi(x), \tag{1}$$

where Ω is the support of the integral and $\pi(x)$ is a positive-definite function of a d -dimensional vector x (see Ref. [3] for a generalization to non-positive definite integrands). The function $\pi(x)$ can be regarded as an unnormalized probability density. For many equilibrated physical systems with the energy function $E(x)$, $\pi(x) = e^{-E(x)}$ describes the relative probability of observing x , and Z is the partition function. Discrete integrals can be treated analogously.

Suppose that we have multiple replicas of a system on the same support, each independently sampling from their own respective distributions. The replica gas identities couple these copies together by means of transition functions, $T(x'|x)$, which are normalized conditional probability distributions that one can sample from and evaluate. Appropriate transition functions include candidate-generating functions routinely used in Markov Chain