Reply to a Comment on
“A Comparison Between Broad Histogram and Multicanonical Methods”

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Abstract

This is a reply to the comment by M. Kastner and M. Promberger on the paper published in  
\textit{J. Stat. Phys.} 99, 691 (2000) and also in cond-mat 0002176. We show that all their criticisms do not apply.

Key words: microcanonical averages; numerical simulation.

We could find three criticisms to our work\cite{1} in the comment by M. Kastner and M. Promberger\cite{2}. First, the authors point “a signal for something fundamental going wrong”, because “computed simulation data should fluctuate statistically around the exact result”. Second, they do not like “the inappropriate title” of our paper, asserting that our comparison makes no sense and corresponds to a “mistake of conceptual kind”. Third, they criticise our assertion that the only constraint one needs to obey in measuring microcanonical averages is to sample with uniform probability the various states belonging to the same energy level. Below, we show that all these criticisms do not apply.

First criticism

The broad histogram method (BHM)\cite{3} relates the degeneracy function $g(E)$, i.e. the number of states corresponding to a given energy $E$, with the \textbf{microcanonical averages} of some quantities defined within the method itself. This relation is shown\cite{4} to be \textbf{exact and generally valid for any system}. Thus, the method consists in measuring the quoted averages as functions of $E$, \textbf{by any means}, and then obtaining the $g(E)$ at the end. Like other methods which calculate the spectral degeneracy, BHM gives $g(E)$ multiplied by an
irrelevant constant, denoted hereafter by $C$, which cancels out in performing canonical averages.

In [1], we show some of our numerical results for $g(E)$ by setting the global factor $C$ in the following way: we choose the energy $E_0$ at the center of the spectrum, and equate our numerically obtained value $Cg_{\text{numerical}}(E_0)$ with $g_{\text{exact}}(E_0)$. Then, we used this obtained value of $C$ for all other energies. We cannot know the sign of the statistical fluctuation (i.e., whether above or below of the expected value) at the particular point $E_0$ we have chosen. Nevertheless, it propagates to all other values of $E$ as well. That is why our plot in [1] does not show the local fluctuations missed by Kastner and Promberger, who claim this is the source of some “systematical deviations”. Actually it is only the trivial consequence of the true statistical fluctuation occurred at $E_0$. Anyway, it is completely irrelevant for the determination of any canonical average. The same “effect” can be seem, for instance, in figure 1 of the paper where the Entropic Sampling was first introduced [6]. There, the values of $g(E)$ are also “systematically” higher than the exact values.

Kastner and Promberger miss out in their comment our figures 3 and 4 [1], where the numerical error are shown to decrease proportionally to $\sqrt{M}$, where $M$ is the number of Monte Carlo steps taken into account. This behaviour shows that no systematic deviations are present at all.

The C code we used to calculate all the quantities present in the paper is available at: http://www.pmmh.espci.fr/~arlima

Second criticism

Kastner and Promberger correctly assert that any Monte Carlo simulation consists of two fundamental parts: SAMPLING, corresponding to the generation of a sample from configuration space by means of a Markovian process; ANALYSIS, corresponding to measure the averages of the quantities one is interested in.

For the multicanonical method (MUCA), SAMPLING corresponds to a specific random walk in the states of the system and ANALYSIS is the use of the results from SAMPLING to calculate $g(E)$. Within BHM, SAMPLING could be any dynamical rule which give good microcanonical averages and ANALYSIS is the equation defined by the method itself which calculates $g(E)$.

What we have done in [1] is: 1) to adopt the same dynamics (SAMPLING) prescribed by multicanonical methods; 2) to measure also the BHM microcanonical averages (necessary to ANALYSIS within the BHM), besides the particular quantity multicanonical prescription uses to determine $g(E)$ (ANALYSIS within MUCA). Thus, from the same Markovian set of averaging states obtained in SAMPLING, we can measure $g(E)$ twice:
first, by adopting the multicanonical prescription; second, by adopting the BHM exact relation. Then, we have compared the numerical accuracies of both methods.

Kastner and Promberger claim our work “sounds a little like comparing apples with oranges”. We compare two ANALYSIS procedures by applying them to the same set of samples (obtained with the same SAMPLING prescribed by the multicanonical method). Furthermore, this is just the main difference between both methods, and thus it is completely legitimate to compare the results. Moreover, they claim to provide “an explicit definition of these observables”, i.e. of the same BHM quantities already perfectly defined in the BHM original publication [3], five years ago. Perhaps they have contributed with the name “observables” to this definition, trying to rename BHM as “Transition Observable Method” (ref.1 of their comment).

Third criticism

Another fundamental difference between BHM and reweighting methods in general (multicanonical included) is that reweighting methods consist in measuring the number of visits to each energy level, during some previously prescribed dynamic rule. At the end, the ratio between $g(E)$ and $g(E')$ corresponding to different energy levels is obtained from the measured number of visits to these levels. BHM, on the other hand, only uses microcanonical averages obtained inside each energy level, separately, in order to determine $g(E)$. Thus, BHM does not depend on the relative number of visits to different energy levels. Only the sampling uniformity among the states within each energy level is important, no matter how the total number of visits to each level compares to others. This gives an enormous freedom to choose different and more convenient dynamic rules within BHM, as compared to reweighting methods for which the relative counting of visits is crucial. In particular, a good dynamic rule for any reweighting method is also good for BHM. However, the reverse is not true.

Kastner and Promberger also mention the possibility of including other parameters, besides the energy, for the distribution of visits being “recorded as functions of all parameters”. They quote the magnetization as an example. However, this is completely equivalent to include other terms into the Hamiltonian defining the system. Within their example, the Ising Hamiltonian would contain a magnetic field term $E_2 = \sum S_i$, besides the usual coupling $E_1 = \sum S_i S_j$. Therefore, without specifying which are the particular coupling constants $J$ and $H$ for these terms, one can walk around the space of states by visiting unitary squares on the plane $(E_1, E_2)$. Each square corresponds to a distinct energy level, and contains many different states: all of them share the same pair of values $(E_1, E_2)$. The microcanonical averages that the BHM needs in order to determine
$g(E_1, E_2)$ are performed within each such a square, again under **the only constraint of sampling with uniform probability the various states belonging to it**. This multiparametric approach was clearly formulated in [5], in spite of the “proper formulation of the method” (BHM itself!), claimed by Kastner and Promberger.

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**References**

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