

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

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This is a reply to the comment by M. Kastner and M. Promberger on the paper published in *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⁽¹⁾ in the comment by M. Kastner and M. Promberger.⁽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)⁽³⁾ relates the degeneracy function $g(E)$, i.e. the number of states corresponding to a given energy E , with the

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microcanonical averages of some quantities defined within the method itself. This relation is shown⁽⁴⁾ to be **exact and generally valid for any system**. Thus, the method consists in measuring the quoted averages as functions of E , **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 ref. 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 ref. 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 seen, for instance, in Fig. 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 Figs. 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 ref. 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 micro-canonical 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 ref. 5, in spite of the “proper formulation of the method” (BHM itself!), claimed by Kastner and Promberger.

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NOTE ADDED AFTER COMMENT'S SECOND VERSION

We could find two minor differences between the first and second versions of the comment by M. Kastner and M. Promberger.⁽²⁾ First, the authors re-formulated their criticism concerning what they call “systematical deviations,” in our Monte Carlo data, Fig. 1.⁽¹⁾ Now they focus into the “gradient of the entropy,” i.e. the slope of our plot. Before, they blamed the absence of fluctuations. In our case, these supposed deviations, sys-

tematic or not, with or without fluctuations, cannot be blamed to come neither from the method itself (which is shown to be exact) nor from the multicanonical dynamic rule adopted (extensively studied by many people). Anyway, contrary to their claim concerning their own numerical work, **any** Monte Carlo simulation also presents systematic deviations, besides statistical fluctuations. There are many reasons for that, among them, for instance, the influence of different random number generators as shown by Ferrenberg *et al*, PRL **69**:3382 (1992). The purpose of our paper was to compare the performance of two methods, showing why one presents **intrinsically** larger accuracy than the other, also presenting numerical evidence for that. All deviations, systematic or not, come from **the same** sampled states for both methods. That is why we “do not seem to worry about that” (expression now missing in their second version). Kastner and Promberger can pursue a better accuracy than our modest figure of 10^{-3} (10^{-4} in Fig. 4), by using better random number generators, by measuring and improving residual correlations along the Markovian chain, etc. We are not interested in this line of research, but perhaps it can lead to what they think to be the correct way. They can start from our *C* program quoted above.

The second difference we found in their comment's new version is the absence of the former final phrase, where they claim themselves to have “a proper mathematical formulation” for our Broad Histogram Method. Why did they erase this claim? On the other hand, the former title of their work published in PRE (2000), where they tried to re-name our method, is still quoted in their first reference. Why did they change the title?