[35] Bogoliubov's model Hamiltonian $H_B(\alpha, \alpha^*)$ is obtained from (2.5) by dropping the last two terms which contain three- and four-particle operators referring to $\vec{k} \neq 0$ states; Eq. (6.1) diagonalizes this truncated Hamiltonian.

[36] It is interesting that the integral involved in (6.9) or (6.12),

$$\int_0^\infty dk k^2 v^2(k)/E_k,$$

does not converge if $v(k)$ is replaced by a constant, such as $v(0)$.

[37] A. E. Glassgold, A. Kaufman, and K. M. Watson, Phys. Rev. **120**, 660 (1960).

[38] D. Ter Haar, Elements of Statistical Mechanics

(Rinehart and Company, Inc., New York, 1954), p. 216.

[39] At $T = 0$, ΔN_0^2 should be zero because the system is in a pure state in which all the bosons are in the $\vec{k} = 0$ single-particle state. Of course, for the interacting case, $\Delta N_0^2 = O(N_0)$ at $T = 0$ (4.37) as well as for $T > 0$ (4.36). This is a consequence of the interactions, which "scatter" the particles out of the $\vec{k} = 0$ state, and give rise to the "depletion effect" $(N_0 < N)$ and to fluctuations, even at $T = 0$.

[40] The suggestion by P. Hohenberg and P. M. Platzman, Phys. Rev. **152**, 198 (1966), that N_0 can be determined by neutron scattering at high energy has recently been carried out by R. A. Cowley and A. D. B. Woods, Phys. Rev. Letters **21**, 787 (1968), with inconclusive results.

Statistical Error Due to Finite Time Averaging in Computer Experiments*

Robert Zwanzig and Narinder K. Ailawadi

University of Maryland, College Park, Maryland 20742

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In using a computer experiment to calculate the time correlation function of some dynamical variable, the ensemble average over an equilibrium distribution in phase space often is replaced by a time average over a finite interval T. It is shown here that the statistical uncertainty due to this kind of average is of the order of $1/T^{1/2}$. The coefficient of the square root is related to a characteristic relaxation time of the correlation function. If *only* time averaging is performed, the resulting statistical uncertainty in typical computer experiments may be of the order of 20%.

Recently much attention has been given to the numerical evaluation of time correlation functions by means of computer experiments.[1-3] In this article we present a theoretical estimate of one particular source of error inherent in such calculations. The error is associated with replacement of an equilibrium ensemble average by a time average over a finite time interval.

In classical statistical mechanics, the time correlation function $C_\infty(t)$ of a dynamical quantity $A(t)$ is defined as

$$C_\infty(t) = \langle A(s) A(s+t) \rangle . \tag{1}$$

Here, $A(t)$ is the numerical value of some property A of a given system at time t; it is determined by the trajectory of the system point in phase space. The average denoted by $\langle \ \rangle$ is an ensemble average over an equilibrium distribution of initial system points in phase space. Note that $C_\infty(t)$ is independent of the arbitrary time s;

this is a consequence of Liouville's theorem.

According to ergodic theory, the ensemble average can be replaced by an *infinite* time average for almost all initial system points in phase space,

$$C_\infty(t) = \lim_{T \to \infty} C_T(t), \tag{2}$$

where

$$C_T(t) = \frac{1}{T} \int_0^T ds A(s) A(s+t) \tag{3}$$

is an average over the finite time interval T for a single initial point in phase space.

In typical computer experiments it is not easy to construct an accurate ensemble average. Each member of the ensemble corresponds to a repetition of an experiment with randomly chosen initial conditions. If the ensemble contains n members (i. e., the experiment is repeated n

times), the relative error of the estimated ensemble average is of order $1/n^{1/2}$. This is a consequence of the law of large numbers. For a relative error of 1%, about 10^4 repetitions are needed.

For this reason one usually performs a time average. If the time interval T is large enough, then we expect that only a single trajectory in phase space (a single computer experiment) will suffice. However, because of the nature of computer experiments, one can average over a finite interval only. So the question arises: How large an interval T is required in order to attain some specified accuracy?

In this paper we show that the relative error in a time correlation function obtained by averaging over a single trajectory for an interval T is of the order of $1/T^{1/2}$, and we present an explicit expression for the coefficient of the square root. We give numerical estimates of the error for a typical though hypothetical case.

Our argument is based on the assumption that the quantity $A(t)$ is a Gaussian random variable. Because this is not necessarily true when $A(t)$ is a dynamical quantity, our results are expected to be plausible estimates, but not rigorous. At present we do not know of any way to correct for non-Gaussian behavior.

We want to know how well an ensemble average is approximated by a finite time average. The difference between the two averages is denoted by $\Delta(t)$,

$$\Delta(t) = C(t) - C_\infty(t). \tag{4}$$

(For simplicity the subscript T on $C_T(t)$ is omitted.)

The deviation $\Delta(t)$ is a random quantity. It depends on the initial state of the system, or equivalently, on the trajectory in phase space followed by a single system. Its statistical properties may be characterized by its first and second moments.

Since the ensemble average is invariant to displacement of the time origin, Eq. (4) may be replaced by

$$\Delta(t) = \frac{1}{T} \int_0^T ds[A(s)A(s+t) - \langle A(s)A(s+t)\rangle]. \tag{5}$$

It is clear that the first moment (taken with respect to the ensemble) vanishes,

$$\langle \Delta(t)\rangle = 0. \tag{6}$$

The second moment of the deviation is

$$\langle \Delta(t_1)\Delta(t_2)\rangle = \frac{1}{T^2} \int_0^T ds_1 \int_0^T ds_2$$
$$\times [\langle A(s_1)A(s_1+t_1)A(s_2)A(s_2+t_2)\rangle$$

$$-\langle A(s_1)A(s_1+t_1)\rangle \langle A(s_2)A(s_2+t_2)\rangle]. \tag{7}$$

Very little can be done with this expression in its general form. However, it can be reduced to a more manageable form by the assumption that $A(t)$ is a Gaussian random variable.

If $A(t)$ is Gaussian, then the average of a product of four A's can be expressed in terms of products of averages of two A's,

$$\langle A_1 A_2 A_3 A_4\rangle = \langle A_1 A_2\rangle \langle A_3 A_4\rangle$$
$$+\langle A_1 A_3\rangle \langle A_2 A_4\rangle +\langle A_1 A_4\rangle \langle A_2 A_3\rangle. \tag{8}$$

But the average of a pair of A's is just the time correlation function $C_\infty(t)$. Thus the second moment of the deviation is

$$\langle \Delta(t_1)\Delta(t_2)\rangle = \frac{1}{T^2} \int_0^T ds_1 \int_0^T ds_2$$
$$\times [C_\infty(s_2 - s_1)C_\infty(s_2 - s_1 + t_2 - t_1)$$
$$+C_\infty(s_2 - s_1 + t_2)C_\infty(s_2 - s_1 - t_1)]. \tag{9}$$

The integrals in Eq. (9) may be estimated in two ways. First, we can replace the ensemble averages $C_\infty(t)$ by the corresponding time averages, and use information about $C(t)$ obtained in computer experiments to calculate the integrals.

But a more useful and convenient estimate can be found by focussing attention on a typical limiting case. The correlation function $C_\infty(t)$ usually decays to zero within some characteristic time of order τ. In typical computer experiments, the averaging time T is much larger than τ; the ratio T/τ may be, for example, about 20. Also, we are concerned with deviations $\Delta(t)$ for times such that the correlation function is not negligibly small. This means that the times t_1 and t_2 in Eq. (9) are themselves of order τ, and are much smaller than T.

In the integrals, s_1 and s_2 both vary from 0 to T. But because the correlation functions vanish for times of order τ, the dominant contribution to the integrals comes from values of s_2 that are within a range of order τ from s_1. Further, the integrand is approximately independent of s_1 when T is large, so that one integration can be done immediately, leading to a factor T. The other integration, originally from 0 to T, may be replaced by an integration from $-\infty$ to $+\infty$ so that

$$\langle \Delta(t_1)\Delta(t_2)\rangle \simeq \frac{2}{T} \int_{-\infty}^{\infty} ds[C_\infty(s)]^2$$
$$= \frac{4}{T} \int_0^{\infty} ds[C_\infty(s)]^2. \tag{10}$$

Now we *define* a mean relaxation time τ by

$$\tau = 2 \int_0^\infty ds [C_\infty(s)]^2 / [C_\infty(0)]^2 . \tag{11}$$

[Note that if $C_\infty(t)$ decays exponentially with the relaxation time τ, then the above equation is satisfied identically. This is the main reason for defining τ as in Eq. (11).]

In this way we find that the second moment of the deviation is approximately independent of t_1 and t_2, and has the value

$$\langle \Delta(t_1)\Delta(t_2) \rangle \simeq \frac{2\tau}{T} [C_\infty(0)]^2 . \tag{12}$$

The preceding result will be used to discuss the statistical properties of two different quantities that are of interest in computer experiments,

$$I = C(t)/C_\infty(0) \tag{13}$$

and $II = C(t)/C(0) .$ (14)

The difference is in the denominator. In case I, the initial value of the ratio is not necessarily unity, because $C(t)$ is a random quantity while $C_\infty(t)$ is fixed. In case II, both numerator and denominator are random, but the initial value of the ratio is unity by definition. We will see that somewhat greater accuracy can be obtained from computer experiments in case II, as a result of cancellation of randomness for short times.

In case I, the deviation from the ensemble average is

$$\Delta_I(t) = C(t)/C_\infty(0) - C_\infty(t)/C_\infty(0) . \tag{15}$$

It is clear that the mean deviation vanishes,

$$\langle \Delta_I(t) \rangle = 0 . \tag{16}$$

The second moment of the deviation can be found from Eq. (12), and is

$$\langle [\Delta_I(t)]^2 \rangle \simeq 2\tau/T. \tag{17}$$

This holds for values of the time t that are of order τ and much smaller than T.

It is convenient to introduce the normalized ensemble averaged correlation function $R(t)$,

$$R(t) = C_\infty(t)/C_\infty(0) . \tag{18}$$

If we use one standard deviation as an indication of the error to be expected in determining $R(t)$ by computer experiments in case I, we obtain

$$R(t) = C(t)/C_\infty(0) \pm (2\tau/T)^{1/2} . \tag{19}$$

It should be noted that the error is independent of t, so that this procedure will not give even the initial value $R(0) = 1$ correctly.

In a typical computer experiment where $T/\tau = 25$, the resulting accuracy of $R(t)$ determined this way is

$$R(t) = C(t)/C_\infty(0) \pm 0.28 . \tag{19a}$$

Higher accuracy can be obtained, at least for short times, by using case II. Here we want to know how well $R(t)$ is approximated by $C(t)/C(0)$. The corresponding deviation is

$$\Delta_{II}(t) = C(t)/C(0) - R(t) . \tag{20}$$

By Eq. (4) this may be transformed to

$$\Delta_{II}(t) = \frac{\Delta(t) - R(t)\Delta(0)}{C_\infty(0) + \Delta(0)} . \tag{21}$$

On expansion of the denominator to first order, we obtain

$$\Delta_{II}(t) = \frac{1}{C_\infty(0)} [\Delta(t) - R(t)\Delta(0)]$$
$$- \frac{\Delta(0)}{[C_\infty(0)]^2} [\Delta(t) - R(t)\Delta(0)] + \cdots . \tag{22}$$

The mean value of $\Delta_{II}(t)$ does not vanish. If we use the estimate given in Eq. (12), we find

$$\langle \Delta_{II}(t) \rangle \simeq \frac{2\tau}{T} [R(t) - 1] . \tag{23}$$

It will turn out, however, that a standard deviation obtained from the second moment of $\Delta_{II}(t)$ is of order $(\tau/T)^{1/2}$. So the mean value of $\Delta_{II}(t)$ is of a smaller order of magnitude, and may be neglected.

The variance of $\Delta_{II}(t)$ is easily found from Eq. (12), and is

$$\langle [\Delta_{II}(t)]^2 \rangle - [\langle \Delta_{II}(t) \rangle]^2$$

$$\simeq \frac{2\tau}{T} (1 - \frac{2\tau}{T})[1 - R(t)]^2 \simeq \frac{2\tau}{T}[1 - R(t)]^2 . \tag{24}$$

Evidently the correction from the square of the first moment is of a smaller order of magnitude, so we omit it.

Consequently, our estimate of $R(t)$ from a computer experiment in case II is

$$R(t) = C(t)/C(0) \pm (2\tau/T)^{1/2}[1 - R(t)] . \tag{25}$$

In the error term we may replace $R(t)$ by the observed $C(t)/C(0)$ without appreciable effect. On subtracting unity from both sides, the result appears a bit simpler:

$$R(t) - 1 = \left[\frac{C(t)}{C(0)} - 1\right] \times \left[1 \pm \left(\frac{2\tau}{T}\right)^{\frac{1}{2}}\right] \ . \qquad (26)$$

As an illustration, we take a hypothetical example where $T/\tau = 25$. The following table gives "measured" values of $C(t)/C(0)$ for several times, and the resulting estimate of $R(t)$:

t (psec)	$C(t)/C(0)$	$R(t)$
0	1.0	1.0 ± 0.0
0.1	0.9	0.9 ± 0.03
0.2	0.3	0.3 ± 0.20
0.3	-0.1	-0.1 ± 0.31
1	0	0 ± 0.28

[In some computer experiments, T/τ has been as large as 100. Then the error estimates given under $R(t)$ in this table should be halved.]

It appears that only the early stages of the decay of a time correlation function can be computed with any confidence by averaging over about 25 relaxation times.

If one also performs an average over an ensemble containing n members, one can obtain an improvement in the error by a factor $1/n^{1/2}$. The reason is that this extra ensemble average is roughly equivalent to considering a single system for a time interval nT.

The preceding discussion suggests that it may not be feasible economically to achieve much greater accuracy (say, 1%) by computer experiments using only time and ensemble averaging. It should be observed, however, that greater accuracy *has* been achieved in special cases, where another kind of average is possible. An example is the calculation of the velocity correlation function

$$\sigma(t) = \langle v_1(0)v_1(t)\rangle \qquad (27)$$

of an individual particle in a liquid. If all N particles in the system are identical, then the velocity correlation function is independent of the particle number, so that

$$\sigma(t) = \frac{1}{N} \sum_{j=1}^{N} \langle v_j(0)v_j(t)\rangle \ . \qquad (28)$$

This extra averaging over particle labels is roughly equivalent to averaging over an ensemble containing N systems. When a single system contains 400 particles, and the time average is taken over 25 relaxation times, an accuracy of about 1% is expected. Useful results have been obtained in this way.[1-3]

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