Error estimates on averages of correlated data

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We describe how the true statistical error on an average of correlated data can be obtained with ease and efficiency by a renormalization group method. The method is illustrated with numerical and analytical examples, having finite as well as infinite range correlations.

I. INTRODUCTION

Computer simulations of physical systems by Monte Carlo methods or molecular dynamics typically produce raw data in the form of finite time series of *correlated* data. In the wide class of cases, where *stationary* states are investigated, the first step in the data analysis consists in computing time averages. Since such averages are over *finite* times, they are *fluctuating* quantities: another simulation of the same system will typically give a different value for the same quantity. So the next step in the data analysis consists in estimating the *variance* of finite time averages. A mixed practice has developed around this problem.

A popular estimator for the error on a time average of correlated data is based on the correlation function for these data. There is actually a whole family of such estimators, all being approximations to one of two original estimators. They are reviewed in Sec. III of this paper with some attention paid to the approximations, subjective choices, and computational effort involved. That should make the reader appreciate the alternative, the "blocking," or "bunching," method, described in Sec. IV. In our opinion this method combines maximum rigor with minimum computation and reflection. It involves no approximations for subjective choices, automatically gives the correct answer, when it is available from the time series being analyzed, and warns the user, when this is not the case. We also give some—hopefully illustrative—examples, analytical ones (Secs. V and VI) as well as numerical ones (Secs. VII and VIII). In Sec. IX we describe situations in which the blocking method cannot be used. The reader, who wants just a recipe for the blocking method, needs only read Secs. II, IV, and IX, and a few equations in Sec. III.

The "blocking" method was not invented by us. It is part of the verbal tradition in a part of the simulation community. It may have been invented by K. Wilson.[1] This seems plausible, since it is essentially a real space renormalization group technique applied in the one-dimensional, discrete space of simulation time. The method is briefly described by Whitmer[2] and Gottlieb *et al.*[3] Recently, we were made aware that the method is unknown in parts of the simulation community, and it is upon request that we describe it in some detail here.

II. NOTATION

Let $x_1, x_2, ..., x_n$ be the result of n consecutive measurements of some fluctuating quantity. Typically the x_i's may be the result of a Monte Carlo simulation in "thermal" equilibrium, i being related to the Monte Carlo time. Or the x_i's may be the result of a molecular dynamics simulation of a system in "equilibrium," i being related to the physical time of the system. Let $\langle \cdots \rangle$ denote the expectation value with respect to the exact, but unknown, probability distribution $p(x)$ according to which x_i is distributed. p does not depend on i, since we are considering a system in equilibrium. Let $\overline{\cdots}$ denote averages over the set $\{x_1, ..., x_n\}$.

$$\langle f \rangle \equiv \int dx\, p(x) f(x), \tag{1}$$

$$\bar{f} \equiv \frac{1}{n} \sum_{i=1}^{n} f(x_i), \tag{2}$$

$\langle \cdots \rangle$ is good for theoretical considerations; $\overline{\cdots}$ is something we can compute in practice. We assume ergodicity; hence the ensemble average $\langle f \rangle$ is equal to the time average $\lim_{n\to\infty} \bar{f}$. In practice we compute finite time averages like Eq. (2), and use them as estimates for ensemble averages like Eq. (1). A finite time average is a fluctuating quantity, so we need also an estimate for the *variance* of this quantity to have a complete result. To be specific, we estimate the expectation value $\mu \equiv \langle x \rangle$ by the average value

$$m \equiv \bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i \tag{3}$$

and need an estimator for the variance of m

$$\sigma^2(m) = \langle m^2 \rangle - \langle m \rangle^2. \tag{4}$$

Inserting Eq. (3) into Eq. (4) we find

$$\sigma^2(m) = \frac{1}{n^2} \sum_{i,j=1}^{n} \gamma_{i,j} = \frac{1}{n}\left[\gamma_0 + 2 \sum_{t=1}^{n-1} \left(1 - \frac{t}{n}\right)\gamma_t\right], \tag{5}$$

where we have introduced the correlated function

$$\gamma_{i,j} \equiv \langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle \tag{6}$$

and used its invariance under time translations to define

$$\gamma_t \equiv \gamma_{i,j} \quad t = |i - j|. \tag{7}$$

III. ESTIMATORS BASED ON THE CORRELATION FUNCTIONS

$\sigma^2(m)$ is often estimated using Eq. (5) with an estimate for γ_t in γ_t's place. Doing so requires some care and consideration, since the most obvious estimator for γ_t,

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$$c_t \equiv \frac{1}{n-t}\sum_{k=1}^{n-t}(x_k-\bar{x})(x_{k+t}-\bar{x}), \tag{8}$$

is a *biased* estimator; its expectation value is *not* γ_t, but

$$\langle c_t\rangle = \gamma_t - \sigma^2(m) + \Delta_t, \tag{9}$$

where

$$\Delta_t = 2\left(\frac{1}{n}\sum_{i=1}^{n} - \frac{1}{n-t}\sum_{i=1}^{n-t}\right)\frac{1}{n}\sum_{j=1}^{n}\gamma_{i,j}. \tag{10}$$

However, if the largest correlation time in γ_t is finite, call it τ, then Eq. (5) reads

$$\sigma^2(m) = \frac{1}{n}\left[\gamma_0 + 2\sum_{t=1}^{T}\left(1-\frac{t}{n}\right)\gamma_t\right] + \mathcal{O}\left[\frac{\tau}{n}\exp(-T/\tau)\right], \tag{11}$$

where T is a cutoff parameter in the sum. For $\exp(-T/\tau) \ll 1$ the explicitly written terms in Eq. (8) clearly give a very good approximation to $\sigma^2(m) \sim \mathcal{O}(\tau/n)$. Furthermore, assuming $n \gg \tau$,

$$\Delta_t = \mathcal{O}\left(\frac{t\tau}{n^2}\right) \quad \text{for } t \ll \tau, \tag{12a}$$

growing to

$$\Delta_t = \mathcal{O}\left(\frac{\tau^2}{n^2}\right) \quad \text{for } t \gg \tau. \tag{12b}$$

So we may neglect Δ_t in Eq. (9), since it is at least a factor τ/n smaller than the term $\sigma^2(m) = \mathcal{O}(\tau/n)$. Doing that, and using Eq. (9) to eliminate γ_t from Eq. (5), we find

$$\sigma^2(m) = \frac{1}{n}\left[\langle c_0\rangle + 2\sum_{t=1}^{T}\left(1-\frac{t}{n}\right)\langle c_t\rangle\right] + \sigma^2(m)\left(\frac{1+2T}{n} - \frac{T(T+1)}{n^2}\right). \tag{13}$$

Solving for $\sigma^2(m)$ we find

$$\sigma^2(m) \approx \left\langle \frac{c_0 + 2\Sigma_{t=1}^{T}(1-\frac{t}{n})c_t}{n-2T-1+\frac{T(T+1)}{n}} \right\rangle, \tag{14}$$

where the "$\approx$" is due to the truncation of the sum over t and the neglect of Δ_t. The expression inside the angular brackets in Eq. (14) is an estimator for $\sigma^2(m)$. This estimator is unbiased within the approximations done, as Eq. (14) shows.

Notice that with Eq. (14) we have not assumed anything about T's relation with n, except $T \leqslant n$. The truncated sum in Eq. (11) clearly approximates $\sigma^2(m)$ better the larger T is, and is exact for $T = n-1$. The same is not true in Eq. (14). For $T = n-1$ the denominator vanishes, and the numerator is $\mathcal{O}(n\Delta_t) = \mathcal{O}(\tau^2/n)$. For T close to $n-1$, the right-hand side (RHS) of Eq. (14) is the ratio of small numbers, one of which fluctuates, when $\langle c_t\rangle$ is estimated with c_t. This makes the expression inside the angular brackets in Eq. (14) a very bad estimator for $\sigma^2(m)$ for T close to $n-1$. If instead one can choose T such that $\tau \ll T \ll n$, then the approximation in Eq. (11) is good, and so is that in Eq. (14). Thus T should at the same time be chosen much smaller than n and several times larger than the maximal correlation time in γ_t, assuming this quantity exists, and can be determined at least approximately from c_t. See Sec. VII for an example for which this is the case.

Alternatively one may monitor the estimate for $\sigma^2(m)$ based on Eq. (14) as a function of T, and hope to demonstrate that it is independent of T for T larger than a certain value. This makes evaluation of c_t necessary for all values of t between 0 and $T_{\max}$, the maximal value for T considered. That requires $\mathcal{O}(nT_{\max})$ numerical operations, and easily becomes a time consuming affair. For this reason one would like to choose $T_{\max}$ small. On the other hand, $T_{\max}$ can in principle only be chosen appropriately *after* $\sigma^2(m)$ has been inspected. So the choice of $T_{\max}$ cannot be automatized. This lack of automatization, and the computational effort involved are serious disadvantages of the method just described. In the next section we explain how the blocking method yields the desired result with only $\mathcal{O}(2n)$ numerical operations, and in a way that can be fully automatized.

The estimator given by Binder [Ref. 4, Eq. (2.46) and Refs. 5 and 6] is essentially Eq. (14), except the denominator is approximated by n.

Daniell *et al.* [Ref. 7, Eq. (23)] use the approximation

$$\sigma^2(m) \approx \left\langle \frac{c_0 + 2\Sigma_{t=1}^{T}c_t}{n-2T-1} \right\rangle. \tag{15}$$

One also sees the approximation

$$\sigma^2(\mathrm{m}) \approx \left\langle \frac{c_0 + 2\Sigma_{t=1}^{T}c_t}{n} \right\rangle. \tag{16}$$

All these variants of Eq. (14) are equally good when T/n is sufficiently small. There is no reason *not* to use Eq. (14) itself, though, when any of the formulas are appropriate. It is as easy to compute as any of its approximations.

A variant of Eq. (8) in use is

$$c_t \equiv \frac{1}{n-t}\sum_{k=1}^{n-t}\left(x_k - \frac{1}{n-t}\sum_{k=1}^{n-t}x_k\right) \times \left(x_{k+t} - \frac{1}{n-t}\sum_{k=1}^{n-t}x_{k+t}\right). \tag{17}$$

Like Eq. (8), Eq. (17) is a biased estimator for γ_t since

$$\langle c_t\rangle = \gamma_t - \sigma^2(m) + \tilde{\Delta}_t, \tag{18}$$

where

$$\tilde{\Delta}_t = \left(\frac{1}{n^2}\sum_{i,j=1}^{n} - \frac{1}{(n-t)^2}\sum_{i=1}^{n-t}\sum_{j=t+1}^{n}\right), \qquad \gamma_{i,j} = \mathcal{O}\left(\frac{\tau t^2}{n^3}\right). \tag{19}$$

Neglecting $\tilde{\Delta}_t$ relatively to $\sigma^2(m)$ in Eq. (19) leads again to Eqs. (13) and (14). Using Eq. (17) instead of Eq. (8) as estimator for $\langle c_t\rangle$ in Eq. (14) is a better approximation, when $|\Sigma_{t=1}^{T}(n-t)\tilde{\Delta}_t| < |d\,\Sigma_{t=1}^{T}(n-t)\Delta_t|$, i.e., roughly when $T^2 < \tau n$.

IV. THE "BLOCKING" METHOD

We now describe a way to estimate $\sigma^2(m)$ which is computationally more economical than that of the previous section. It elegantly avoids the computation of c_t and the choice of T. In addition it gives information about the quality of the estimate of $\sigma^2(m)$. The method involves repeated "blocking" of data, and computation of increasing lower bounds for $\sigma^2(m)$ in the following way.

We transform the data set $x_1, \ldots, x_n$ into half as large a data set $x_1', \ldots, x_{n'}'$, where

$$x_i' = \frac{1}{2}(x_{2i-1} + x_{2i}), \tag{20}$$

$$n' = \tfrac{1}{2}n. \tag{21}$$

We define m' as $\bar{x}'$, the average of the n' "new" data, and have

$$m' = m. \tag{22}$$

We also define $\gamma_{i,j}'$ and γ_t' as in Eqs. (6) and (7) but from primed variables x_i'. One easily shows that

$$\gamma_t' = \begin{cases} \tfrac{1}{2}\gamma_0 + \tfrac{1}{2}\gamma_1 & \text{for } t = 0 \\ \tfrac{1}{4}\gamma_{2t-1} + \tfrac{1}{2}\gamma_{2t} + \tfrac{1}{4}\gamma_{2t+1} & \text{for } t > 0 \end{cases} \tag{23}$$

and that

$$\sigma^2(m') = \frac{1}{n'^2}\sum_{i,j=1}^{n'} \gamma_{i,j}' = \sigma^2(m). \tag{24}$$

Equations (22) and (24) show that the two quantities we wish to know, m and $\sigma^2(m)$, are *invariant* under the "blocking" transformation given in Eqs. (20), (21), and (22). Thus, no information we desire is lost in this transformation of the data set to half as large a set. Not only is nothing lost, but something is gained: the value of $\sigma^2(m)$ unravels gradually from γ_r by repeated application of the "blocking" transformation. From Eq. (5) we know

$$\sigma^2(m) \geqslant \frac{\gamma_0}{n} \tag{25}$$

and from Eqs. (21) and (23) it is clear that γ_0/n increases every time the "blocking" transformation is applied, unless $\gamma_1 = 0$. In that case γ_0/n is invariant.

It is not difficult to show that $(\gamma_t/n)_{t=0,1,2,\ldots} \propto (\delta_{t0})_{t=0,1,2,\ldots}$ is a *fixed point* of the linear transformation [Eqs. (21)–(23)], and any vector $(\gamma_t/n)_{t=0,1,2,\ldots}$ for which γ_t decreases faster than $1/t$ is in the basin of attraction of this fixed point. *At* this fixed point $\sigma^2(m) = \gamma_0/n$, since $\gamma_t = 0$ for $t > 0$. $\sigma^2(m)$ is estimated by using Eqs. (9) or (18) to eliminate γ_0 from Eq. (25), using $\Delta_0 = \tilde{\Delta}_0 = 0$, and solving for $\sigma^2(m)$:

$$\sigma^2(m) \geqslant \left\langle \frac{c_0}{n-1} \right\rangle, \tag{26}$$

where c_0 is defined in Eq. (8), and the identity is satisfied at the fixed point. Knowing this, one proceeds as follows.

Starting with a data set $x_1, \ldots, x_n$, $c_0/(n-1)$ is computed, and used as estimate for $\langle c_0/(n-1)\rangle$. Then the "blocking" transformation Eqs. (20)–(21) is applied to the data set, and $c_0'/(n'-1)$ is computed as estimate for $\langle c_0'/(n'-1)\rangle$. This process is repeated until $n' = 2$. The sequence of values obtained for $c_0/(n-1)$ will increase until the fixed point is reached, where upon it remains constant within fluctuations. The constant value is our estimate for $\sigma^2(m)$.

At the fixed point the "blocked" variables $(x_i')_{i=1,\ldots,n'}$ are independent Gaussian variables—Gaussian by the central limit theorem, and independent by virtue of the fixed point value of γ_t'. Consequently, we can easily estimate the standard deviation on our estimate $c_0'/(n'-1)$ for $\sigma^2(m)$. It is $(\sqrt{2/(n-1)})\, c_0'/(n'-1)$:

$$\sigma^2(m) \approx \frac{c_0'}{n'-1} \pm \sqrt{\frac{2}{n'-1}}\frac{c_0'}{n'-1}, \tag{27}$$

$$\sigma(m) \approx \sqrt{\frac{c_0'}{n'-1}}\left(1 \pm \frac{1}{\sqrt{2(n'-1)}}\right). \tag{28}$$

Knowing this error is a great help in determining whether the fixed point has been reached or not in actual calculations, as we shall see in Sec. VII.

If the fixed point is not reached before $n' = 2$, this is signalled by $c_0/(n-1)$ not becoming constant. The largest value obtained for $c_0/(n-1)$ is then a lower bound on $\sigma^2(m)$.

Notice that at no stage in these calculations were $(c_t)_{t=0,1,2,\ldots}$ evaluated, and the estimate for $\sigma^2(m)$ was obtained by $\mathcal{O}(2n)$ operations, while computation of $(c_t)_{t=0,1,\ldots,T}$ requires $\mathcal{O}(Tn)$ operations.

V. ANALYTICAL EXAMPLE WITH FINITE CORRELATION TIME

Assume $x_1, \ldots, x_n$ are correlated with one finite correlation time τ:

$$\gamma_t = \begin{cases} \sigma^2(x) & \text{for } t = 0 \\ Ae^{-t/\tau} & \text{for } t > 0 \end{cases}. \tag{29}$$

The "blocking" transformation maps the four parameters $[n, \tau, \sigma^2(x), A]$ into new values $[n', \tau', \sigma^2(x'), A']$, where

$$\begin{aligned} n' &= \tfrac{1}{2}n, \\ \tau' &= \tfrac{1}{2}\tau, \\ \sigma^2(x') &= \tfrac{1}{2}[\sigma^2(x) = Ae^{-1/\tau}], \\ A' &= \tfrac{1}{2}(1 + \cosh \tau^{-1})A. \end{aligned} \tag{30}$$

From Eq. (5) we get to leading order (we do not *have* to do this approximation, but do it to keep formulas as simple as possible in this example) in $1/n$ that

$$\sigma^2(m) = \frac{1}{n}\left(\sigma^2(x) + \frac{2A}{e^{1/\tau} - 1}\right) \tag{31}$$

which is invariant under the "blocking" transformation (30). Using $(1/n)\sigma^2(x)$ for $1/(n-1)\langle c_0\rangle$ in Eq. (26) and comparing with Eq. (31), we see that Eq. (26) underestimates $\sigma^2(m)$ by an amount δ, which can be inspected in the present example:

$$\delta = \frac{2A}{n(e^{1/\tau} - 1)}. \tag{32}$$

From (30) follows that "blocking" gives

$$\delta' = \tfrac{1}{2}(1 + e^{-1/\tau})\delta \tag{33}$$

from which we see that "blocking" makes $1/(n-1)\langle c_0\rangle$ grow to $\sigma^2(m)$ essentially with geometric progression. This is what one might have expected, knowing $\tau' = \tau/2$. However, this rate of convergence does *not* depend on τ being finite, as the example in the next section shows. It does not express a property of the time series being analyzed, but is due to the efficiency of the "blocking" algorithm.

VI. ANALYTICAL EXAMPLE WITH INFINITE CORRELATION TIME

Assume $x_1, ..., x_n$ are correlated with infinite correlation time, i.e., the correlation function decreases as a power of the difference in time:

$$\gamma_t = \begin{cases} \sigma^2(x) & \text{for } t = 0, \\ A/t^{\alpha} & \text{for } t > 0. \end{cases} \tag{34}$$

Then (5) gives to leading order in $1/n$

$$\sigma^2(m) = \frac{1}{n}[\sigma^2(x) + 2A\zeta(\alpha)], \tag{35}$$

where $\zeta(\alpha)$ is Riemann's zeta function:

$$\zeta(\alpha) = \sum_{t=1}^{\infty} \frac{1}{t^{\alpha}}, \quad \mathrm{Re}\,\alpha > 1. \tag{36}$$

We see that if $\alpha < 1$ the data are too correlated to give a finite value for $\sigma^2(m)$. The "blocking" transformation Eqs. (20)–(23) does not leave the form of the correlation function (34) invariant, since

$$\gamma'_t = \begin{cases} \tfrac{1}{2}[\sigma^2(x) + A] & \text{for } t = 0 \\ A/(2t)^{\alpha}\left(1 + \dfrac{\alpha(1+\alpha)}{16t^2} + \mathcal{O}(t^{-4})\right) & \text{for } t > 0 \end{cases}. \tag{37}$$

So this example is not entirely analytically tractable. However, in the most interesting situation, where α is not much larger than 1, $\sigma^2(m)$ in Eq. (5) receives a dominating contribution from γ_t with t large, as Eqs. (35) and (36) shows. For large t, γ_t is well approximated by the first term on the RHS of Eq. (37). This term *is* form invariant under the "blocking" transformation, giving

$$\begin{aligned} n' &= \tfrac{1}{2}n, \\ \alpha' &= \alpha, \\ \sigma^2(x') &= \tfrac{1}{2}[\sigma^2(x) + A] \quad \text{(not reliable)}, \\ A' &= 2^{-\alpha}A. \end{aligned} \tag{38}$$

As one would expect, Eq. (38) shows that "blocking" leaves the infinite correlation time infinite, and the power law unchanged, while the amplitude A is scaled in accordance with the power law.

Equation (38) is based upon an approximation which improves with distance t, so its relation between $\sigma^2(x')$ and $\sigma^2(x)$—quantities defined at zero distance—is not reliable. The relations for α and A are more reliable, and they are all we need. Comparing Eq. (35) with (25), remembering $\gamma_0 = \sigma^2(x)$, we see that $(1/n - 1)c_0$ underestimates $\sigma^2(m)$ by an amount δ, for which we have the explicit, approximate result

$$\delta = \frac{2A}{n}\zeta(\alpha). \tag{39}$$

From Eq. (38) then follows that the "blocking" transformation gives

$$\delta' = 2^{1-\alpha}\delta, \tag{40}$$

i.e., δ vanishes geometrically, when we block transform it, even in this case of correlations with infinite range.

VII. NUMERICAL EXAMPLE FROM MONTE CARLO SIMULATION

We have simulated the two-dimensional Ising model on a 20×20 lattice at inverse temperature $\beta = 0.30$ using the heat bath algorithm and checker board update. After a hot start and 1000 thermalization sweeps we made 131 072 ($= 2^{17}$) measurements of the instantaneous magnetization with consecutive measurements being separated by one sweep. With x_t denoting the instantaneous magnetization and $n \equiv 131\,072$ Eq. (3) gave $m = -0.0011$ for the magnetization.

We chose to measure the magnetization of this system to have a transparent example well known to most readers. The magnetization is easy to measure and even easier to discuss, since we know its exact value is zero. Consequently our numerical estimate for the magnetization should differ from zero only by an amount that is justified by its error. Furthermore, with $\beta = 0.30$ the correlation time is short, and any method discussed above will work, so different methods can be compared easily.

We computed c_t as defined in Eq. (8). Figure 1 is a semilog plot of $c(t)$ *vs* t. For $t \leqslant 30$ we see a straight line signaling a decrease of c_t with a single correlation time τ that we read off the plot to be $\tau = 5.1$. We also read off $c_0 = 0.022$. It will be self-consistently correct to neglect $\sigma^2(m)$ in Eq. (9), and therefore to use c_t as estimator for γ_t. When Eq. (28) is used with $A = \sigma^2(x) = 0.022$ we find that $\sigma(m) = 0.0013$.

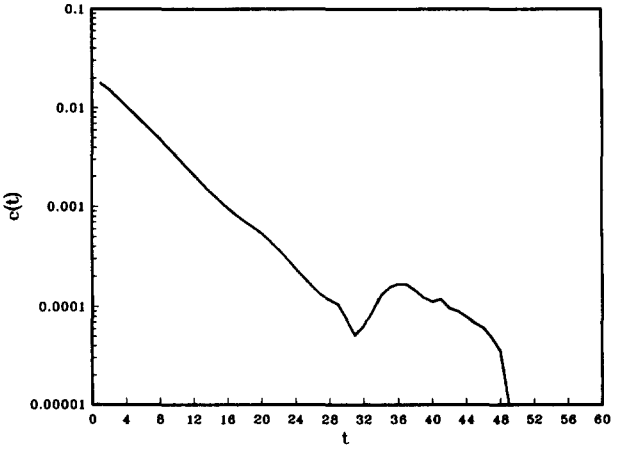

FIG. 1. c_t vs t. c_t was computed from $n = 2^{17}$ measurements of the magnetization $(x_t)_{t=1,...,n}$ using the defining Eq. (8). For $0 \leqslant t \leqslant 16$ $c_t \simeq 0.022 \exp(-t/5.1)$.

Figure 2 shows estimates for $\sigma(m)$ obtained from the same time series using the expression inside the angular bracket in Eq. (14) with increasing cutoff T as abscissa. From $15 \leqslant T \leqslant 300$ we see that $\sigma(m) = 0.0012$ independent of T. This constancy of T is a convincing signal that the value found for $\sigma(m)$ really is its true value. For $T > 300$ the values for $\sigma(m)$ become increasingly noisy. This is because c_t for $t \gg \tau$ is an essentially random number, and when T is increased more such numbers are included in Eq. (14), giving rise to increasing noise.

Figure 3 shows estimates for $\sigma(m)$ obtained from the same time series and its block transformed series defined in Eqs. (20) and (21). Equation (28) has been used. After approximately 6 block transformations $\sigma(m)$ reaches a value of 0.0012, where it remains (within error bars) during further block transformations. The distinct plateau that is seen in this plot of $\sigma(m)$ vs the number of block transformations applied, is a fully convincing signal, that the fixed point for the block transformation has been reached, and $\sigma(m) = 0.0012$ is the true standard deviation on m. This value agrees with the previous estimate for it, and differs little from the estimate based on τ read off Fig. 1. It also makes our estimate $m = -0.0011$ for the magnetization differ less than one standard deviation from zero.

Now let us make a more detailed comparison of the result obtained with the two methods: Fig. 4 shows Figs. 2 and 3 plotted on top of each other. The abscissa of the points from Fig. 3 have been chosen such that $T = \frac{1}{2}(2^{\#} - 1)$ where # is the number of block transformations applied. At this T value the number of pair correlations $\overline{x_{t_1} x_{t_2}}$ taken into account by the estimate for $\sigma(m)$ based on c_t is equal to the number of such pair correlations taken into account by the estimate for $\sigma(m)$ obtained with the blocking method. In Fig. 4 it is very clear that the two methods give the same estimate for $\sigma(m)$. The *length* of the plateau giving this estimate is also the same for both methods. And the noise on the sequence of estimates obtained with one method stays within the error bars on the estimates obtained with the other method. So as far as the quality of results in concerned, both methods are equal, as they should be, since they both extract all relevant information from the time series. There is a great

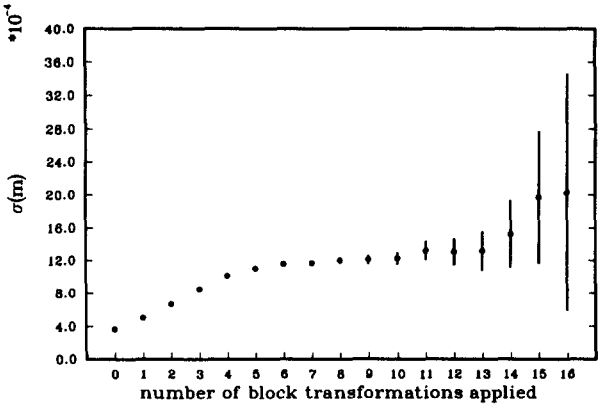

FIG. 3. Estimate for $\sigma(m)$ obtained with the blocking method. After ~ 6 block transformations the estimates remain constant within error bars at 0.0012.

difference in the computational efficiency with which this is done, however. The data plotted in Fig. 2 was obtained with $\mathcal{O}(nT_{\max}) = \mathcal{O}(10^{10})$ arithmetical operations, whereas those in Fig. 3 required only $\mathcal{O}(n) = \mathcal{O}(10^5)$ operations. $T_{\max}$, which is the efficiency ratio between the two methods is 10^5 here only because we wanted to show the reader the noise in Fig. 2. Just the same, we could not have chosen $T_{\max}$ much less than 10^2, if we want to see the plateau in the estimate for $\sigma(m)$. Only if we *know* that $\tau \simeq 5$, can we legitimately choose $T_{\max}$ as low as $\simeq 20$ in Eq. (14). On the other hand, to obtain this knowledge we have to compute c_t at least for $0 \leqslant t \leqslant \max(\tau, 3)$, which requires $\mathcal{O}(n \max(\tau, 3))$ operations. In conclusion, there is no way to obtain $\sigma(m)$ which is more efficient than the blocking method; not even the crude method consisting in reading $c_0 \approx \sigma^2(x)$ and τ off Fig. 1 and using them in Eq. (28) with $A = \sigma^2(x)$.

Another difference between Figs. 2 and 3 is the lack of error bars in Fig. 2. Only if we are willing to assume that $(x_t)_{t=1,\ldots,n}$ are *Gaussian* variables with correlation matrix γ_{t_1,t_2} [compare Eq. (6)] can these error bars be estimated. (Doing this is more than an exercise, we warn the reader.)

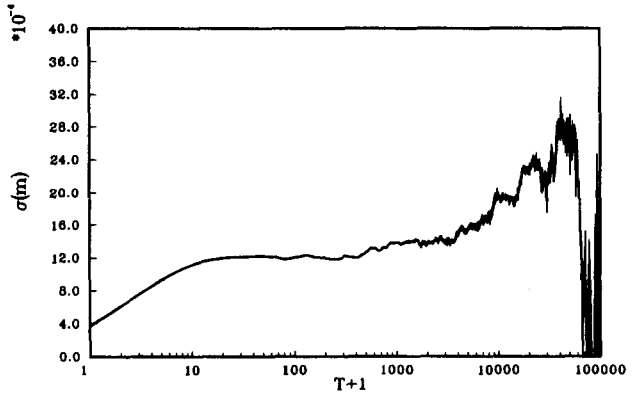

FIG. 2. Estimates for $\sigma(m)$ using Eq. (12) vs cutoff T. For $15 < t < 400$ $\sigma(m) \simeq 0.0012$ independent of T.

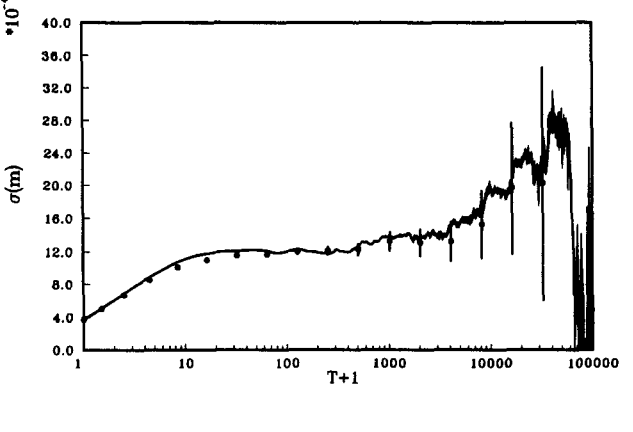

FIG. 4. Figures 2 and 3 plotted on top of each other. For reasons given in the text, the abscissa of the points from Fig. 3 have been chosen such that $T = \frac{1}{2}(2^{\#} - 1)$ where # is the number of block transformations applied.

The error bars in Fig. 3, on the other hand, are rigorous and independent of assumptions.

VIII. NUMERICAL EXAMPLE FROM MOLECULAR DYNAMICS SIMULATION

The blocking method was tested on the results of a molecular dynamics run of 50 000 time steps of the Stockmayer fluid, using $\mu^* = 1.5$, $T^* = 1.35$, $\rho^* = 0.8$, $N = 108$, where the symbols have their usual meaning.[8] This is an example with very long time correlations. The Ewald summation was used to evaluate the dipolar interactions in periodic boundary conditions using a value of $\varepsilon' = \infty$ for the dielectric constant of the surroundings.[8,9] The same state point has been studied by Pollock and Alder,[8] and our result for the Kirkwood factor g agree with theirs. Their result for the g was

$$g = \frac{1}{N\mu^2}\left(\sum_{i=1}^{N} \boldsymbol{\mu}_i\right)^2 = 3.5 \pm 0.2. \tag{41}$$

although they give no details of how their error estimate was arrived at.

The block transformation Eqs. (20)–(22) was used to estimate the error in g. Where n was odd one of the n measures of g was discarded before performing the next block transformation. The result of doing this is shown in Table I. $\sigma[c_0(n-1)]$ is calculated from Eq. (27). A plateau in $c_0/(n-1)$ is observed between 9 and 12 block transformations, and from this we find $\sigma(g) \cong \sqrt{0.024} \cong 0.15$. In the last few rows in the table there are so few blocks, that the error on $c_0/(n-1)$ is close to the value of $c_0(n-1)$ itself. In Ref. 11 the blocking method was used to obtain error estimates for the Kirkwood factor in other simulations.

TABLE I. Results of repeated application of the block transformation to a time series from a molecular dynamics simulation of the Stockmayer fluid.

Number of block transformations	n	$c_0/(n-1)$	$\sigma[c_0/(n-1)]$
0	50 000	1.4×10^{-4}	
1	25 000	2.9×10^{-4}	
2	12 500	5.8×10^{-4}	
3	6 250	1.1×10^{-3}	
4	3 125	2.2×10^{-3}	
5	1 562	4.4×10^{-3}	
6	781	8.1×10^{-3}	
7	390	1.3×10^{-2}	
8	195	1.8×10^{-2}	0.2×10^{-2}
9	97	2.1×10^{-2}	0.3×10^{-2}
10	48	2.4×10^{-2}	0.5×10^{-2}
11	24	2.0×10^{-2}	0.6×10^{-2}
12	12	2.0×10^{-2}	0.9×10^{-2}
13	6	1.6×10^{-2}	1.0×10^{-2}
14	3	1.2×10^{-2}	1.2×10^{-2}

IX. CONCLUSION

We hope the reader to whom the blocking method was new, has learned enough from our presentation to apply it with confidence. The brevity of the literature on the method inspires the vain hope that even workers using the method might have learned a little. Our main message was that no other method is comparable with the blocking method in computational and intellectual economy.

We should add that there are situations in which the method does not apply in the form presented here. Suppose, for example, we compute a correlation length from a correlation function. This involves taking the logarithm of the correlation function. To do that our estimate for the correlation function must be positive. To ensure the positivity, we first average the correlation function over simulation time, and *then* take the logarithm. In contrast, application of the blocking method to the correlation length requires first taking the logarithm to obtain a time series for the correlation length, and *then* do the averaging and blocking. This procedure is clearly not possible, when fluctuations are large enough to give the instantaneous correlation function negative values. In general, this problem may occur whenever one wants to determine a function of a fluctuating quantity, and the function is not defined for the entire range of values that the fluctuations may cover. A rather straightforward procedure based on the jackknife method[11] makes blocking possible also in such situations.[1,3]

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