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Moment equations and closure schemes in chaotic dynamics

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Abstract. Closure schemes for the infinite hierarchy of moment equations describing the time evolution of averages of observables over a non-equilibrium ensemble of initial conditions for the logistic map model are derived with the aid of the Frobenius–Perron equation in the long-time regime. For the growth parameter $r = 4$ the approximations compare well with exact results derived for specific initial probability densities.

1. Introduction

It is well known that far from phase transition points, and in sufficiently high dimensions, the probability distribution of a macroscopic observable in a system close to equilibrium composed of a large number of particles is strongly peaked around a privileged value, corresponding to both the average and the most probable value of the observable [1]. As a result the fluctuations around the average are small, entailing the existence of a closed form evolution law describing the relaxation of the observable towards its asymptotic value.

In dissipative systems driven out of equilibrium by external constraints, the dynamics of macroscopic observables can be very complex, and relaxation towards a steady-state value may not even occur. A particularly interesting form of such complexity is associated with chaotic dynamics, both purely temporal and spatio-temporal. In a system possessing sufficiently strong ergodic properties a probabilistic description of this behaviour can be carried out, and probability distributions again attain an invariant form as in classical problems of statistical mechanics [2, 3]. However, contrary to this latter case, they are no longer peaked sharply but are, as a rule, delocalized in phase space, implying that fluctuations may now be comparable to the averages [4]. As a corollary, the ensemble average of the observable will not obey a closed equation, but will be coupled to higher moments. As these will in turn be linked to still higher-order averages, one typically arrives at an infinite hierarchy of coupled equations. Several examples of such hierarchies are known, one of the most important being the set of moments associated with fully developed turbulence [5]. Clearly, in all these instances it is desirable to obtain information on the low-order averages, which are the most closely related to experimentally accessible quantities, without having to resort each time to a full-scale evaluation of the entire set of moments. The development of such a *closure scheme* for a simple system exhibiting chaotic dynamics is the principal objective of this work.

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The specific model that we consider is the logistic map. In section 2 the time-dependent moment equations are derived and their invariant (asymptotic in time) values are summarized for a specific parameter value. As straightforward closure schemes fail in this case we resort, in section 3, to a totally different approach. Specifically, we conjecture (and show this to be rigorously the case for the fully developed chaotic regime) that for long times all moments vary on the same timescale, given by the second largest eigenvalue of the corresponding Frobenius–Perron operator. This leads to closed sets of equations giving the correct asymptotic values and linear stability properties of the time-dependent moments. In section 4 the results are compared with numerical simulations. The main conclusions are drawn in section 5.

2. Moment dynamics of the logistic map

The probability density $\rho_n(x)$ associated to the logistic map

$$x_{n+1} = f(x_n, r) = rx_n(1 - x_n) \quad 0 \leq x_n \leq 1 \quad (2.1)$$

evolves according to the Frobenius–Perron equation [2, 3]

$$\rho_{n+1}(x) = \sum_{\alpha} \frac{1}{|f'(f_{\alpha}^{-1}(x))|} \rho_n(f_{\alpha}^{-1}(x)) \quad (2.2)$$

where the pre-images $f_{\alpha}^{-1}(x)$, $\alpha = 1, 2$ are given by

$$f_{\alpha}^{-1}(x) = \frac{1 \pm \sqrt{1 - \frac{4}{r}x}}{2}. \quad (2.3)$$

We define the k th moment of $\rho_n(x)$ by

$$m_k(n) = \int_0^{\frac{r}{4}} dx x^k \rho_n(x). \quad (2.4)$$

Using equations (2) and (3) one obtains

$$m_k(n+1) = \frac{r}{4} \left[\int_0^{\frac{r}{4}} dx \frac{x^k}{4\sqrt{1 - \frac{4}{r}x}} \rho_n \left(\frac{1 + \sqrt{1 - \frac{4}{r}x}}{2} \right) + \frac{x^k}{4\sqrt{1 - \frac{4}{r}x}} \rho_n \left(\frac{1 - \sqrt{1 - \frac{4}{r}x}}{2} \right) \right]. \quad (2.5)$$

Introducing the new variables $y = \frac{1 + \sqrt{1 - \frac{4}{r}x}}{2}$ and $y = \frac{1 - \sqrt{1 - \frac{4}{r}x}}{2}$ in the first and second integral and using the familiar binomial expansion one arrives at an expression linking m_k to higher-order moments up to m_{2k} [6]:

$$m_k(n+1) = r^k \sum_{l=0}^k \binom{k}{l} (-1)^l m_{k+l}(n) \quad k = 1, 2, \dots \quad (2.6)$$

As an example, in the regime of fully developed chaos $r = 4$, the first few moment equations read

$$m_1(n+1) = 4[m_1(n) - m_2(n)] \quad (2.7)$$

$$m_2(n+1) = 16[m_2(n) - 2m_3(n) + m_4(n)]. \quad (2.8)$$

Furthermore, the steady-state values ($n \rightarrow \infty$) of all moments can be determined explicitly from equation (2.4) after inserting the invariant distribution $\rho_s(x) = \frac{1}{\pi\sqrt{x(1-x)}}$ [7]. The result is

$$m_{k,s} = \frac{2}{\pi} \int_0^{\frac{\pi}{4}} dy \sin^{2k} y = \frac{(2k-1)!!}{(2k)!!}. \tag{2.9}$$

We observe a rather slow decay of the $m_{k,s}$ with increasing k . This also holds true for the variances associated with the different moments, and is one of the origins of the failure of closures based on straightforward truncation. For instance, expressing the first two equations in terms of the variances $(x - \bar{x})^k$ ($k = 1, 2, 3, 4$) and dropping all terms beyond $k = 2$ one arrives at a system of two equations possessing only unstable fixed points. The situation gets even worse if truncation is carried out at a higher-order. As for the cumulants, their asymptotic values may not even decay with increasing k .

3. A closure scheme for the long-time regime

In order to cope with the above-mentioned fundamental difficulty we now limit ourselves to the regime of ‘long’ times that is bound to arise after an initial transient period, as long as the Frobenius–Perron operator, equation (2.2), has sufficiently strong ergodic properties. The additional assumption that we shall make is that there exists a *spectral gap* separating the invariant eigenvalue $\lambda_0 = 1$ of this operator and the next largest ones $\lambda_1, \lambda_2, \dots$, ($|\lambda_2| < |\lambda_1| < 1$). A number of instances in which the logistic system for $r \neq 4$ satisfies this condition are known [8]. Possible exceptions include the regime of intermittency, which prevails in the logistic map near the regime of period 3.

3.1. Closure at the level of the first moment

First, consider the effect of the eigenvalue λ_1 dominating the rest of the spectrum apart from $\lambda_0 = 1$. The solution of equation (2.2) for long times will be of the form

$$\rho_n(x) = \rho_s(x) + \lambda_1^n c_1 \phi_1(x) \tag{3.1}$$

where c_1 is determined from the initial condition and $\phi_1(x)$ is the right eigenfunction associated with λ_1 . The dominant contribution to the first few moments in this long-time regime will be given by

$$m_1(n) = m_{1,s} + c_1 \lambda_1^n \int_0^{\frac{\pi}{4}} dx x \phi_1(x) \tag{3.2}$$

$$m_k(n) = m_{k,s} + c_1 \lambda_1^n \int_0^{\frac{\pi}{4}} dx x^k \phi_1(x) \tag{3.3}$$

showing that, eventually, all moments vary on the *same* timescale. This entails, in turn, that in the long-time regime higher-order moments vary in time entirely through the first moment $m_1(n)$. Specifically, from the first equation (3.2) one has

$$c_1 \lambda_1^n = \frac{m_1(n) - m_{1,s}}{\int_0^{\frac{\pi}{4}} dx x \phi_1(x)}. \tag{3.4}$$

Substituting in the second, third, etc equation one then obtains

$$m_k(n) = m_{k,s} + \frac{\int_0^{\frac{\pi}{4}} dx x^k \phi_1(x)}{\int_0^{\frac{\pi}{4}} dx x \phi_1(x)} (m_1(n) - m_{1,s}). \tag{3.5}$$

Combined with equation (2.6) the above result provides us with a closure of the moment hierarchy at the level of m_1 .

As an example, consider the case of fully developed chaos $r = 4$. We adopt the more explicit notation $m_1(n) = \bar{x}_n$. Furthermore, we introduce in the first equation (2.7) the variance

$$\overline{\delta x^2_n} = m_2(n) - m_1^2(n) \quad (3.6)$$

in order to disentangle the role of the averages and fluctuations. We thus obtain

$$\bar{x}_{n+1} = 4[\bar{x}_n(1 - \bar{x}_n) - \overline{\delta x^2_n}]. \quad (3.7)$$

The closure relation (3.5), applied for $k = 2$ and for the variance rather than the second moment reads, also using equation (3.6)

$$\frac{\overline{\delta x^2_n} - \overline{\delta x^2_s}}{\overline{\delta x^2_s}} = 4 \left(\frac{\int_0^{\frac{r}{4}} dx x^2 \phi_1 - \int_0^{\frac{r}{4}} dx x \phi_1}{\int_0^{\frac{r}{4}} dx x \phi_1} \right) \left(\frac{\bar{x}_n - \bar{x}_s}{\bar{x}_s} \right) \quad (3.8)$$

with $\bar{x}_s = \frac{1}{2}$, $\overline{\delta x^2_s} = \frac{1}{8}$. It can be shown [8–10] that the dominant eigenvalue of the Frobenius–Perron operator for $r = 4$ is $\lambda_1 = \frac{1}{4}$ and the corresponding eigenfunction is

$$\phi_1 = \frac{1}{\pi \sqrt{x(1-x)}} B_2 \left(\frac{1}{\pi} \arcsin \sqrt{x} \right) \quad (3.9)$$

where B_2 is the second Bernoulli polynomial. Inserting this into equation (3.8) and integrating one finds

$$\frac{\overline{\delta x^2_n} - \overline{\delta x^2_s}}{\overline{\delta x^2_s}} = -\frac{1}{4} \frac{\bar{x}_n - \bar{x}_s}{\bar{x}_s}. \quad (3.10)$$

Substituting this explicit closure into equation (3.7) one obtains

$$\bar{x}_{n+1} = 4 \left[\bar{x}_n(1 - \bar{x}_n) - \frac{5}{32} + \frac{\bar{x}_n}{16} \right]. \quad (3.11)$$

This is a closed equation for \bar{x}_n . It admits a unique fixed point at $\bar{x}_s = \frac{1}{2}$, the exact asymptotic value of the first moment. To see whether this point is stable we set $\bar{x}_n = \bar{x}_s + \xi_n$ and linearize equation (4.3) with respect to ξ_n . The result is

$$\xi_{n+1} = \frac{1}{4} \xi_n \quad (3.12)$$

showing that \bar{x}_s is indeed stable. Notice that equation (3.12) exhibits the dominant eigenvalue $\lambda_1 = \frac{1}{4}$ of the Frobenius–Perron operator.

3.2. Closure at the level of the variance

We next consider the set of the first two equations of the hierarchy (equation (2.6) for $k = 1, 2$). As in section 3.1 we express the right-hand sides in terms of the variances. In addition to $\overline{\delta x^2_n}$ (equation (3.6)) one now has to also consider third- and fourth-order variances.

$$\overline{\delta x^3_n} = m_3(n) - 3m_2(n)m_1(n) + 2m_1^3(n) \quad (3.13)$$

and

$$\overline{\delta x^4_n} = m_4(n) - 4m_3(n)m_1(n) + 6m_2(n)m_1^2(n) - 3m_1^4(n). \quad (3.14)$$

The first two equations (2.6) then generate the coupled set

$$\bar{x}_{n+1} = r[\bar{x}_n(1 - \bar{x}_n) - \overline{\delta x^2_n}] \tag{3.15}$$

$$\overline{\delta x^2_{n+1}} = r^2[\overline{\delta x^2_n}(1 - 2\bar{x}_n)^2 - (\overline{\delta x^2_n})^2 + \overline{\delta x^4_n} - 2\overline{\delta x^3_n}(1 - 2\bar{x}_n)]. \tag{3.16}$$

Linearizing the terms containing the higher-order variances we find

$$\begin{aligned} \overline{\delta x^4_n} - 2\overline{\delta x^3_n}(1 - 2\bar{x}_n) &= \overline{\delta x^4_s} + [m_4(n) - m_{4,s}] - 2m_3(n) \\ &+ \frac{3}{2}[m_2(n) - m_{2,s}] - \frac{1}{2}[m_1(n) - m_{1,s}] \end{aligned} \tag{3.17}$$

(note that only the term $\overline{\delta x^4_n}$ contributes in the first order). Now, according to (3.5) in the long-time limit all moment deviations are proportional to $m_1(n) - m_{1,s}$. It follows that the fourth-order variance also varies in time entirely though the first or second moment. An appropriate ansatz for the closure in equation (3.16) is, therefore, to express the terms containing higher-order variances as a linear combination of $\bar{x}_n - \bar{x}_s$ and $\overline{\delta x^2_n} - \overline{\delta x^2_s}$

$$\overline{\delta x^4_n} - 2\overline{\delta x^3_n}(1 - 2\bar{x}_n) = \overline{\delta x^4_s} + \alpha(\bar{x}_n - \bar{x}_s) + \beta(\overline{\delta x^2_n} - \overline{\delta x^2_s}). \tag{3.18}$$

To determine the coefficients α and β in this expression we now have to extend equations (3.1)–(3.3) to include the effect of the next largest eigenvalue $\lambda_2 = \frac{1}{16}$ and the corresponding eigenfunction Φ_2 . Specifically, we require that the eigenvalues σ_1, σ_2 of the linearized system of equations (3.15) and (3.16) must be identical to the second- and third-largest eigenvalue of the Frobenius–Perron operator, respectively. For $\sigma_1 + \sigma_2 = \frac{r^2}{2}(-2\overline{\delta x^2_s} + \beta) = \frac{5}{16}$ and $\sigma_1\sigma_2 = r^3\alpha = \frac{1}{64}$ we find

$$\alpha = \frac{1}{4096} \quad \beta = \frac{5}{16}. \tag{3.19}$$

Inserting in equations (3.15) and (3.16) we thus have a set of equations closed at the level of the second moment,

$$\bar{x}_{n+1} = r[\bar{x}_n(1 - \bar{x}_n) - \overline{\delta x^2_n}] \tag{3.20}$$

$$\overline{\delta x^2_{n+1}} = r^2[\overline{\delta x^2_n}(1 - 2\bar{x}_n)^2 - (\overline{\delta x^2_n})^2 + \frac{1}{4096}(\bar{x}_n - \bar{x}_s) + \frac{5}{16}(\overline{\delta x^2_n} - \overline{\delta x^2_s})]. \tag{3.21}$$

The equations admit the fixed point $(\frac{1}{2}, \frac{1}{8})$, the exact asymptotic values for the first moment and the variation. By virtue of our ansatz this fixed point is stable with eigenvalues equal to $\frac{1}{4}$ and $\frac{1}{16}$, respectively.

4. Comparison with exact results for specific initial distributions

An alternative way to proceed for the logistic map at $r = 4$ is to evaluate the successive moments as a function of time starting from the explicit time-dependent solution

$$x_n = \sin^2[2^n \arcsin \sqrt{x_0}] \tag{4.1}$$

and averaging it over an initial distribution $\rho(x)$

$$m_k(n) = \int_0^1 dx \rho(x) [\sin^2 2^n \arcsin \sqrt{x}]^k. \tag{4.2}$$

For a uniform distribution $\rho(x)$ the integrals can be calculated exactly and take the simple form

$$m_k(n) = m_{k,s} \prod_{i=1}^k \frac{1}{1 - \frac{1}{i^2 4^n}} \quad n > 0. \tag{4.3}$$

Note that the denominator in equation (4.3) is defined in terms of k products, each of which is linear in the term $\frac{1}{4^n}$. In particular, for the first moment $m_1(n)$ we have

$$m_1(n) = m_{1,s} \frac{1}{1 - \frac{1}{4^n}}. \quad (4.4)$$

We now eliminate the explicit time dependence in equation (4.3). Since according to equation (4.4)

$$\frac{1}{4^n} = \frac{m_1 - m_{1,s}}{m_1} \quad (4.5)$$

one can express *all* higher moments in terms of the first via

$$m_k = m_{k,s} \prod_{i=1}^k \frac{1}{1 - \frac{1}{i^2} \frac{m_1 - m_{1,s}}{m_1}}. \quad (4.6)$$

Note that in contrast to equation (3.5), equation (4.6) is *exact*, and the whole spectrum of the eigenvalues $\lambda_n = \frac{1}{4^n}$ of the Frobenius–Perron operator contributes.

Linearization of equation (4.6) eventually leads to the counterpart of equation (3.5)

$$m_k = m_{k,s} + \frac{m_{k,s}}{m_{1,s}} (m_1 - m_{1,s}) \sum_{i=1}^k \frac{1}{i^2}. \quad (4.7)$$

Evaluation of the integrals in equation (3.5) for $r = 4$ yields

$$\frac{\int_0^1 dx x^k \phi_1(x)}{\int_0^1 dx x \phi_1(x)} = \frac{m_{k,s}}{m_{1,s}} \sum_{i=1}^k \frac{1}{i^2} \quad (4.8)$$

and we recover equation (4.7).

Note also that for $r = 4$, the term $\frac{1}{4^n}$ specifies both, the n th power of the dominant eigenvalue λ_1 and the n th eigenvalue λ_n of the Frobenius–Perron operator of the logistic map and the tent map as well. In other words, as should be expected, all eigenvalues contribute to the transient (short-time) regime: it is only in the limit of long times that the details of the initial distribution no longer matter and one obtains general closure relationships involving solely the dominant eigenvalue.

In order to study the contribution of higher-order corrections we introduce the deviations from the invariant moment values $\Delta m_k = m_k - m_{k,s}$ and expand the *relative* deviations

$$\frac{\Delta m_k}{m_{k,s}} = \prod_{i=1}^k \frac{1}{1 - \frac{\frac{\Delta m_1}{m_{1,s}}}{1 + \frac{\Delta m_1}{m_{1,s}}}} - 1 \quad (4.9)$$

in powers of $\Delta m_1/m_{1,s}$. We find

$$\frac{\Delta m_k}{m_{k,s}} = a_k^{(1)} \frac{\Delta m_1}{m_{1,s}} + a_k^{(2)} \left(\frac{\Delta m_1}{m_{1,s}} \right)^2 + a_k^{(3)} \left(\frac{\Delta m_1}{m_{1,s}} \right)^3 + \dots \quad (4.10)$$

with

$$a_k^{(1)} = \sum_{i=1}^k \frac{1}{i^2} \quad (4.11)$$

$$a_k^{(2)} = \sum_{1 < i < j}^k \frac{1}{(ij)^2} + \sum_{i=2}^k \frac{1}{i^4} \quad (4.12)$$

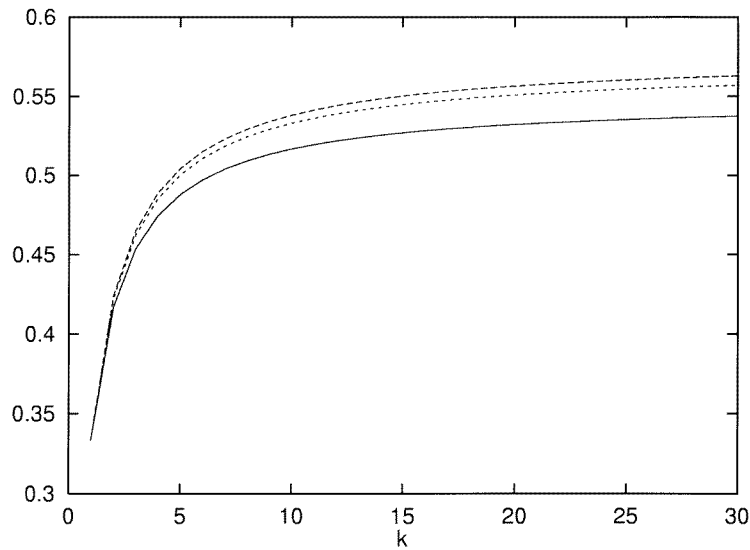


Figure 1. First-, second- and third-order approximations for $\Delta m_k/m_{k,s}$ at time $n = 1$ (lower, upper and middle curve, respectively) as a function of k .

and

$$a_k^{(3)} = \sum_{1 < i}^k \frac{1}{i^2} \sum_{1 < i}^k \frac{1}{i^4} - \sum_{1 < i}^k \frac{1}{i^4} - \sum_{1 < i < j}^k \frac{1}{(ij)^2} + \sum_{1 < i < j < l}^k \frac{1}{(ijl)^2}. \quad (4.13)$$

In the large k -limit the coefficients can be evaluated with the aid of the infinite series

$$s_i = \sum_{n=1}^{\infty} \frac{1}{n^{2i}} = \frac{\pi^{2i} 2^{2i-1}}{(2i)!} B_{2i} \quad (4.14)$$

where B_{2i} are the Bernoulli numbers. We obtain

$$a_{\infty}^{(1)} = s_1 = \frac{\pi^2}{6} \quad a_{\infty}^{(2)} = \frac{7}{4}s_2 - s_1 = \frac{7\pi^4}{360} - \frac{\pi^2}{6} \quad (4.15)$$

and

$$a_{\infty}^{(3)} = \frac{31}{16}s_3 - \frac{7}{2}s_2 + s_1 = \frac{31\pi^6}{15120} - \frac{7\pi^4}{180} + \frac{\pi^2}{6}. \quad (4.16)$$

Figure 1 shows a plot of the relative moment deviations $\Delta m_k/m_{k,s}$ as a function of k in the three approximations equations (4.11)–(4.13) at time $n = 1$, where for a uniform initial distribution $\Delta m_1/m_{1,s}$ takes the value $\frac{1}{3}$.

In contrast to the deviations Δm_k , the *relative* deviations from the invariant values $\Delta m_k/m_{k,s}$ equation (4.9) *increase* with increasing k approaching their asymptotic values for $k \rightarrow \infty$.

The time evolution of the relative moment deviations $\Delta m_k/m_{k,s}$ ($k = 1, 2, 3, 4$) equation (4.13) for the first few timesteps are shown in figure 2. We see that in a logarithmic plot as a function of n they follow straight lines with essentially the same slope, a property that again supports the validity of our main ansatz, equation (3.5).

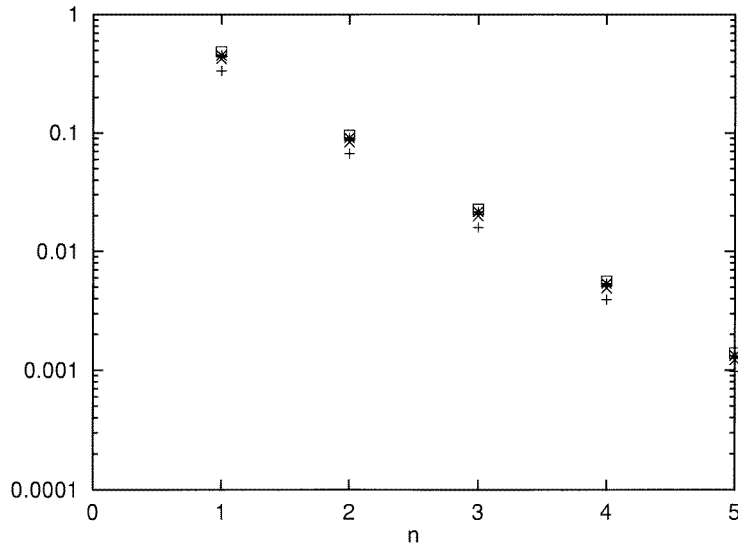


Figure 2. Time evolution of $\Delta m_k/m_{k,s}$ for $k = 1, 2, 3, 4$ (from top to bottom).

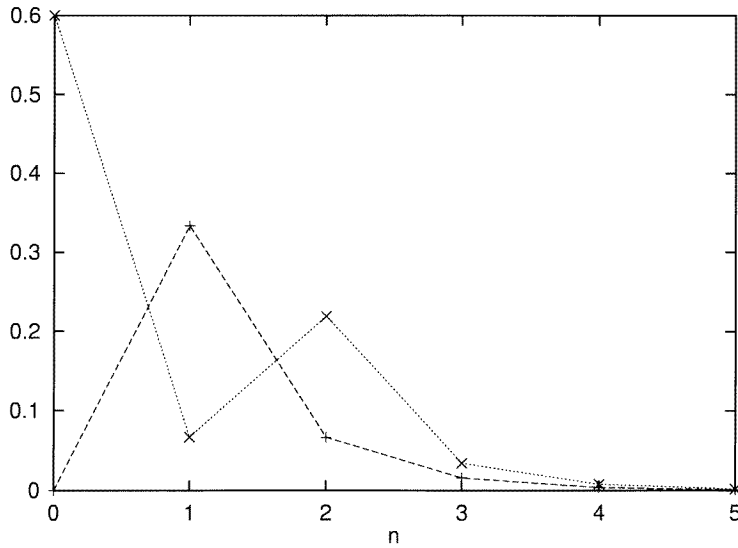


Figure 3. Initial timesteps of $\Delta m_1/m_{1,s}$ for densities $\rho(x) = 1$ (broken line) and $\rho(x) = 4x^3$ (dotted line).

In figures 3 and 4 we compare the time evolution of $\Delta m_1/m_{1,s}$, for an initial uniform probability density $\rho(x) = 1$ (broken lines)

$$\frac{\Delta m_1(n)}{m_{1,s}} = \frac{1}{4^n - 1} \tag{4.17}$$

and for the initial probability density $\rho(x) = 4x^3$ (dotted lines)

$$\frac{\Delta m_1(n)}{m_{1,s}} = \frac{1}{4^n - 1} \frac{2 - \frac{9}{4^n}}{1 - \frac{9}{4^n}} \tag{4.18}$$

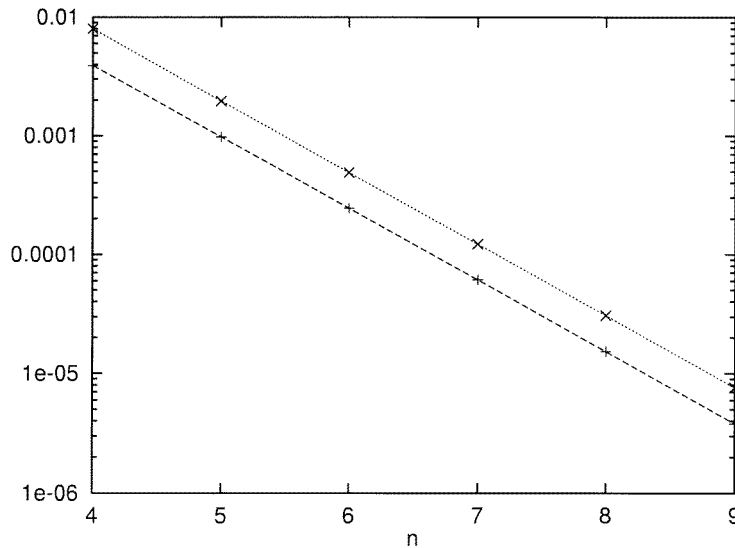


Figure 4. Further time evolution of $\Delta m_1/m_{1,s}$ for densities $\rho(x) = 1$ (broken line) and $\rho(x) = 4x^3$ (dotted line).

evaluated according to the integral, equation (4.2) for $k = 1$. The transient regime and the onset of the long-time behaviour are depicted in figure 3, while the logarithmic plot (figure 4) illustrates that for $n > 3$ the convergence rate $\frac{\Delta m_1(n+1)}{\Delta m_1(n)}$ is already close to $\frac{1}{4}$ for *both* initial densities [11], as predicted by the theory. Note, however, that the initial uniform probability density is always one step ahead (factor of 2 in equation (4.18)).

5. Conclusion and outlook

It has long been recognized that in systems following nonlinear evolution laws, the moments of the underlying probability distribution do not obey closed evolution laws but give rise, instead, to an infinite hierarchy. A problem of central concern in statistical mechanics and nonlinear science is to derive appropriate ‘constitutive’ relations closing such hierarchies at a reasonably low level. Close to thermodynamic equilibrium a solution to this problem is available, providing a basis for transport theory and for the hydrodynamic description of macroscopic systems [12].

The situation is far more involved in the range far-from-equilibrium phenomena and in particular, in the regime where the macroscopic observables undergo deterministic chaos. This paper reports an attempt in this direction. The general idea, reminiscent of the Bogolubov ansatz closing the Bogolubov–Born–Green–Kirkwood–Yvon hierarchy in kinetic theory [13, 14], is that in the long-time regime all moments vary on the same scale and are thus essentially driven by the first one. We have implemented this idea on a toy model—the logistic map—and established full agreement with the exact solution. The sole limitation of the procedure followed in this work is the existence of a set of ‘dominant’ non-degenerate eigenvalues separated from the invariant one by a finite gap. Future work should aim at relaxing this condition to account, for instance, for degeneracies: in turn, a necessary step for tackling spatially extended systems.

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