Proc. Indian Acad. Sci. (Chem. Sci.), Vol. 106, No. 2, April 1994, pp. 479–492.

Dynamics from time series: Iteration maps in correlation space

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Abstract. The attractor for the dynamics of a complex system can be constructed from the time series measurement of a single variable. A recently proposed procedure is to construct a covariance matrix using an embedding window on the time series. An analysis of the meaning of the eigenvalues of the covariance matrix of the time series is undertaken here. It is argued that each principal eigenvalue can be decomposed into components which describe the time evolution of the correlations of the system along the given principal direction. A one-dimensional iterative map of these components can be constructed in correlation space. Such a map displays the regular or chaotic nature of the dynamics for each principal direction of the attractor. Illustrative examples of such maps are constructed for regular and random time series and for the Lorenz attractor.

Keywords. Dynamics; time series; correlation maps; singular spectrum.

1. Introduction

Chemical and biological systems have generally phase spaces of large dimensions. Commonly in such systems, self-organisation gives rise to system evolution on low-dimensional manifolds, called attractors. A major aim of the current dynamical studies is to determine the dimension of the attractor and the rate of convergence or divergence of the trajectories of the attractor (Holden 1986). For a real experimental system, we normally do not know the dynamical equations of motion solving which we could in principle construct the attractor. A break-through in this regard was achieved by Takens (1981) and Packard *et al* (1980) who showed that a m-dimensional attractor could be embedded in any R^n space with dimension $n \geqslant 2m+1$. The space R^n is spanned by n successive measurements of a time sequence of a *single* observable, called a time series. The Taken's theorem provides a theoretical foundation for procedures to construct the attractor from experimental time series data. Based on this theorem, Broomhead and King (1986) have proposed a procedure to construct the attractor, which essentially involves construction of the covariance matrix and determining its significant eigenvalues. The number of such eigenvalues provide an upper bound to the dimension of the attractor. The procedure is known as singular system analysis in information theory or as principal component analysis in statistics. Broomhead and King (1986) have applied the procedure to the Lorenz attractor and demonstrated its effectiveness in determining the dimension and in recreating the flows on the attractor.

In this paper we undertake an analysis of the meaning of the singular eigenvalue by decomposing it into correlation components that evolve in time. We construct one-dimensional maps (iterates) of such an evolution and show that the converging or diverging nature of the trajectory along the singular direction can be determined from these maps.

In § 2, the procedure of singular value analysis of the time series is outlined and then our analysis of the singular eigenvalue is presented. In § 3, we illustrate the analysis and construction of iterative correlation maps with idealised examples of systems with constant, periodic and random observables and finally for the strange attractor of the Lorenz system.

2. The singular spectrum and correlation maps

We begin by outlining the construction of the covariance matrix by the method of delays. See Broomhead and King (1986) for details. The observable v of the system is measured at uniform time intervals and the resulting time series consists of the set $\{v_i | i = 1, 2, \ldots, M\}$ of M consecutive observations. An 'n-window' is now applied to the time series, which makes the n consecutive elements of the series visible in the window. The jth window is given as the column matrix:

$$x_j = (v_j, v_{j+1}, \ldots, v_{j+n-1})^T, \tag{1}$$

where T denotes the transpose. Here $j = 1, 2, \ldots, N$ with $N = M - (n-1)$. Hence N is the total number of n-windows possible for M observations. x_j is an $(n \times 1)$ matrix.

The *trajectory matrix* X is now constructed from these windows as:

$$X = \frac{1}{\sqrt{N}} \begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_N^T \end{bmatrix}. \tag{2}$$

X is an $(N \times n)$ matrix and $(1/N^{1/2})$ is introduced as a normalisation factor. From the trajectory matrix X, one constructs the *covariance matrix*, Ξ, by:

$$\Xi = X^T X, \tag{3}$$

which is an $(n \times n)$ matrix.

To make further analysis transparent we may look closely at the nature of the elements of Ξ. As an example, we consider a 4-window ($n = 4$) so that Ξ is (4×4). Let us assume to have made 10 observations ($M = 10$). Therefore, $N = M - (n-1) = 7$, and we have 7 such windows. We denote the time lag between observations as τ.

From the definition of Ξ, (3), it follows that the elements of Ξ have the form:

$$\Xi_{mn} = \sum_{i=0}^{N-1} v_{(m+i)} v_{(m+i)+(n-m)} / N, \tag{4}$$

for $m \leqslant n$. Matrix Ξ is symmetric: $\Xi_{mn} = \Xi_{nm}$.

It is helpful to look at some elements explicitly.

Diagonal elements:

$$\Xi_{11} = (1/7)(v_1^2 + v_2^2 + \cdots + v_7^2),$$

$$\Xi_{22} = (1/7)(v_2^2 + v_3^2 + \cdots + v_8^2),$$

$$\vdots$$

$$\Xi_{44} = (1/7)(v_4^2 + v_5^2 + \cdots + v_{10}^2). \tag{5}$$

Off-diagonal elements:

$$\Xi_{12} = (1/7)(v_1 v_2 + v_2 v_3 + \cdots + v_6 v_7),$$

$$\vdots$$

$$\Xi_{24} = (1/7)(v_2 v_4 + v_3 v_6 + \cdots + v_8 v_{10}), \tag{6}$$

and so on.

The diagonal element Ξ_{mm} of the covariance matrix is thus the average of the self-correlations, $(v_i v_i)$, over the N windows starting with the ith observation and going on to $i + (N-1)$. By self-correlation, we mean the dyadic product $(v_i v_i)$ of the same observation, i.e. between observations of time lag $\tau = 0$. $\Xi_{(m+1)(m+1)}$ obviously represents a similar average of self-correlations, but now over windows displaced forward by time τ from the set of windows corresponding to Ξ_{mm}.

Therefore, the ordered set Ξ_{11}, Ξ_{22}, Ξ_{33}, Ξ_{44} can be thought of as representing the progression of average self-correlations over the trajectory as the dynamics evolves from time 0, τ, 2τ, to 3τ.

For the off-diagonal elements of Ξ, a similar interpretation holds. That is, Ξ_{mn} represents the average over the trajectory, of N dyadic correlations between observations v_i and v_j with a delay time of $(n-m)\tau$ between the observations starting with $v_{i=m}$. For instance, Ξ_{24} represents the average of 7 correlations of observations with delay of $(4-2) = 2\tau$, starting with the product $v_2 v_4$, as is clear from (6). This structure of the matrix Ξ may be schematically written as:

$$\Xi \equiv \begin{bmatrix} (11) & (12) & (13) & (14) & & & \\ \xrightarrow{\tau} & (21) & (22) & (23) & (24) & & \\ \longrightarrow & \xrightarrow{2\tau} & (31) & (32) & (33) & (34) & \\ \longrightarrow & \longrightarrow & \xrightarrow{3\tau} & (41) & (42) & (43) & (44) \end{bmatrix}, \tag{7}$$

where (mn) denotes Ξ_{mn}. Each row of Ξ is displaced forward in time by τ. The elements on the dotted diagonal line are those of a column or equivalently of a row because of the symmetry of Ξ. *The average of the elements of a row (or column) of the covariance matrix is therefore displaced forward in time by* τ.

We can imagine the elements of Ξ as being viewed through a 4-window, *opened upon the dyadic correlations*, in contrast to the window used for observing the elements of the time series. This correlation window monitors the average binary correlations at times 0, τ, 2τ, 3τ in our example.

The next step is the singular value decomposition or equivalently the diagonalisation of Ξ to obtain the eigenvalues (singular values) and eigenvectors (singular vectors). Since Ξ is symmetric and non-negative definite, its eigenvalues σ are real and can be taken as non-negative. We write the eigenvalue equation as:

$$\Xi C = C\Sigma \tag{8}$$

Here Σ is the diagonal matrix of elements $\{\sigma_i\}$ and C is the $(n \times n)$ eigenvector matrix with each column consisting of an eigenvector:

$$C = (C_1, C_2, \ldots, C_n), \tag{9}$$

with

$$C_i = (C_{i1}, C_{i2}, \ldots, C_{in})^T, \tag{10}$$

and $C^T C = 1$.

Clearly, we have from (8),

$$\Sigma = C^T \Xi C. \tag{11}$$

By expanding the r.h.s. of this equation, we have for the ith diagonal element of Σ,

$$\sigma_i = \sum_{j=1}^{n} \sum_{k=1}^{n} C_{ij} C_{ik} \Xi_{jk}. \tag{12}$$

We rewrite this equation as

$$\sum_{j=1}^{n} \left(\sum_{k=1}^{n} C_{ij} C_{ik} \Xi_{jk} / \sigma_i \right) = 1. \tag{13}$$

Or further as

$$\sum_{j=1}^{i} q_j^i = 1, \tag{14}$$

where we have defined,

$$q_j^i = \sum_{k=1}^{n} C_{ij} C_{ik} \Xi_{jk} / \sigma_i. \tag{15}$$

This definition of q_j^i shows that it is the *weighted* average of the elements of the jth row of the covariance matrix Ξ. The weighting factor involves the product of the coefficients, $C_{ij}C_{ik}$, i.e. the j,k components of the ith singular vector. As j goes from 1 to n, we are descending down the rows of Ξ, and according to our earlier interpretation of the elements of these rows, the n q_j^i values should correspond to time delays 0, τ, $2\tau, \ldots, (n-1)\tau$. To remind us of this property, we write (14) in the slightly modified form:

$$q_0^i + q_1^i + q_2^i + \cdots + q_{n-1}^i = 1. \tag{16}$$

We note that these q^i-values represent a certain decomposition of the singular value σ_i. Thus q_j^i is the average over the trajectory projected on to the ith principal (singular) direction, of all binary correlations after a time lag of $j\tau$ units. That their sum over the window length is unity is just a convenient normalisation. It is easy to show that q_j^i as defined by (15) is simply C_{ij}^2, the square of the jth component of the singular vector i, but the form of (15) lends itself more easily to our interpretation in terms of evolving binary correlations.

Thus we may think of the ordered set $\{q^i_j | j = 0, 1, \ldots, (n-1)\}$ as representing the time evolution of the average binary correlations along the singular direction i.

Hence this set of q^i may be used to produce a one-dimensional mapping of the correlations along the singular direction i as

$$q^i_{j+1} = f(q^i_j), \tag{17}$$

by simply plotting q^i_{j+1} against q^i_j.

We expect that the iterates of such a map in the correlation space should reveal the qualitative character of the dynamics along each singular direction. That is, the map could reveal a fixed point, or periodic, or chaotic nature of the attractor along the principal directions in correlation space. These should not however be confused with similar entities in phase space. We test out this expectation by explicit calculations for a few selected dynamical systems in the following section.

3. Illustrative examples

In this section we illustrate the construction of the map of correlation iterates for some typical cases.

Case 1: *Time-invariant trajectory*

If the observations do not change with time, we have a constant trajectory and an $(n \times n)$ covariance matrix with every element equal to, say, a/n. It has only a single non-zero eigenvalue equal to a. The singular eigenvector has all the n components each equal to $1/n^{1/2}$. Consequently the iterates defined by (17) gives a single fixed point, showing the time-invariant nature of the correlations.

Case 2: *Sinusoidal trajectory*

As our next example, we take the observations of the time series to be given by

$$y(t) = \sin \omega t, \tag{18}$$

with $\omega = 5$, say. The spectrum of the singular eigenvalues, in percentage, is given in figure 1. This figure corresponds to 200 equally spaced y values and an embedding window of length 20. The figure shows that there are only 2 significant singular values, out of a possible total of 20. The correlation iterative map for the dominant singular value ($\sigma_1 = 92\%$) is shown in figure 2. The points lie close to the diagonal, the envelope of these points being cigar shaped. This indicates the essential retention of correlations along the direction given by this eigenvector in correlation space. The second singular value ($\sigma_2 = 8\%$) also gives a similar iteration map of retained correlations (not shown in the figure).

Case 3: *Random trajectory*

We now take the extreme case of the observable $y(t)$ to be 200 random numbers generated by a computer, with mean $= 0$ and variance $= 1$. We impose an embedding

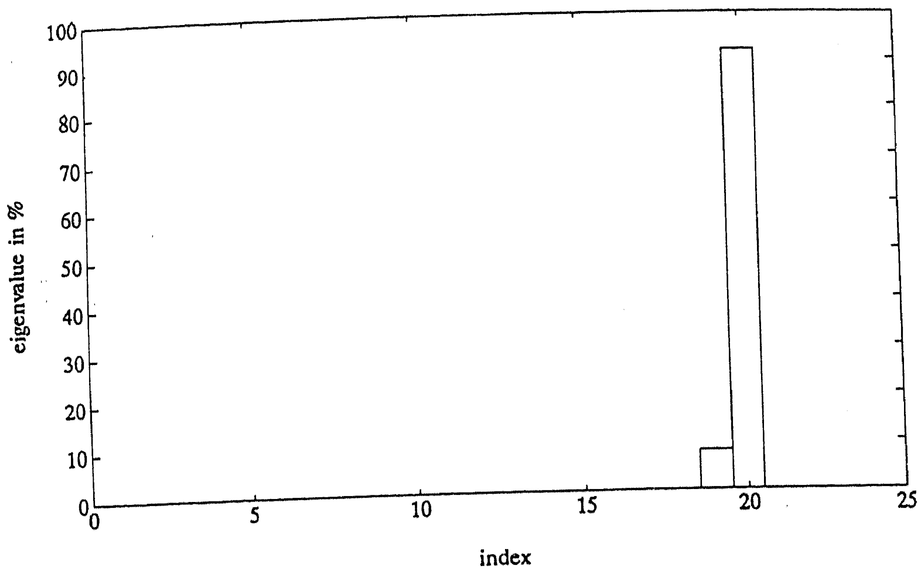


Figure 1. Eigenvalue spectrum for the sinusoidal trajectory of (18) for 200 points with a window length of 20.

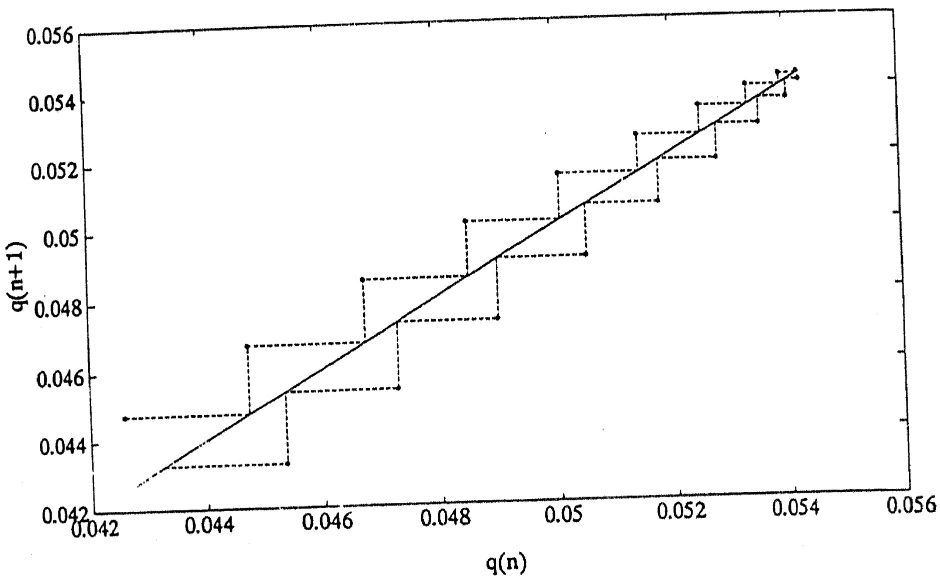


Figure 2. Iterative map of the components of the singular value $\sigma_1 = 92\%$ for the sinusoidal trajectory of (18).

window length of 30. A typical trajectory is given in figure 3 and the corresponding eigenvalue spectrum is shown in figure 4a. The eigenvalues have been taken in increasing order. The values have all comparable magnitudes, showing that the dimension of the attractor is, according to the Broomhead and King (1986) prescription, the same as that of the embedding space, namely 30 in this case. The iteration map of q for the highest ($\sigma = 6{\cdot}5\%$) is given in figure 5a. The random distribution of points away from the diagonal is obvious. In other words, the correlations change randomly along this principal direction as the dynamics evolves. This is the case for all other

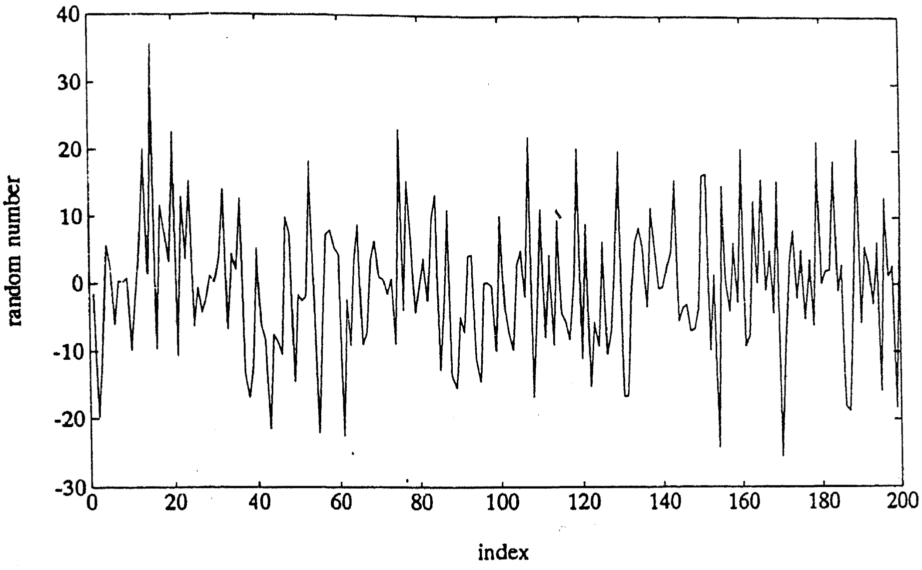


Figure 3. Random trajectory of 200 points generated by a computer.

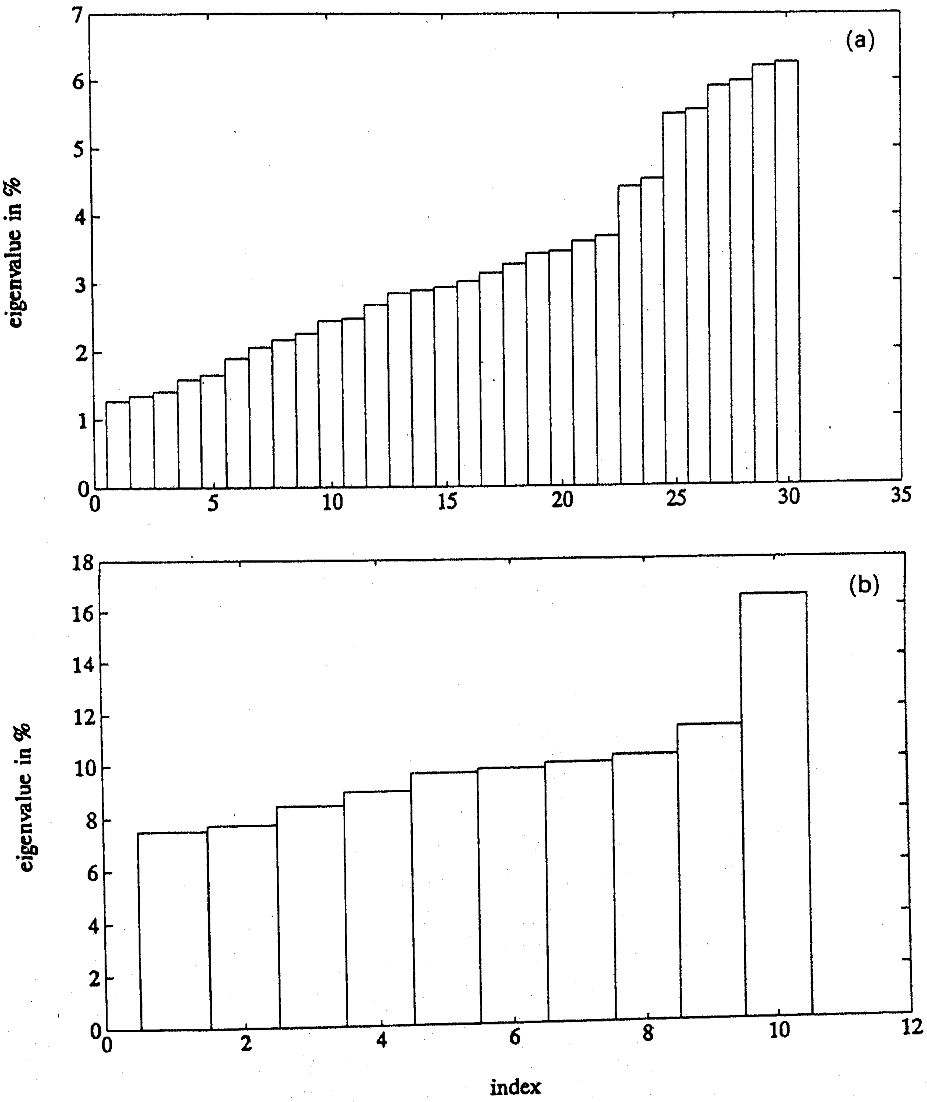


Figure 4. Eigenvalue spectrum for the random trajectory of figure 3, with a window length of 30 (**a**) and 10 (**b**).

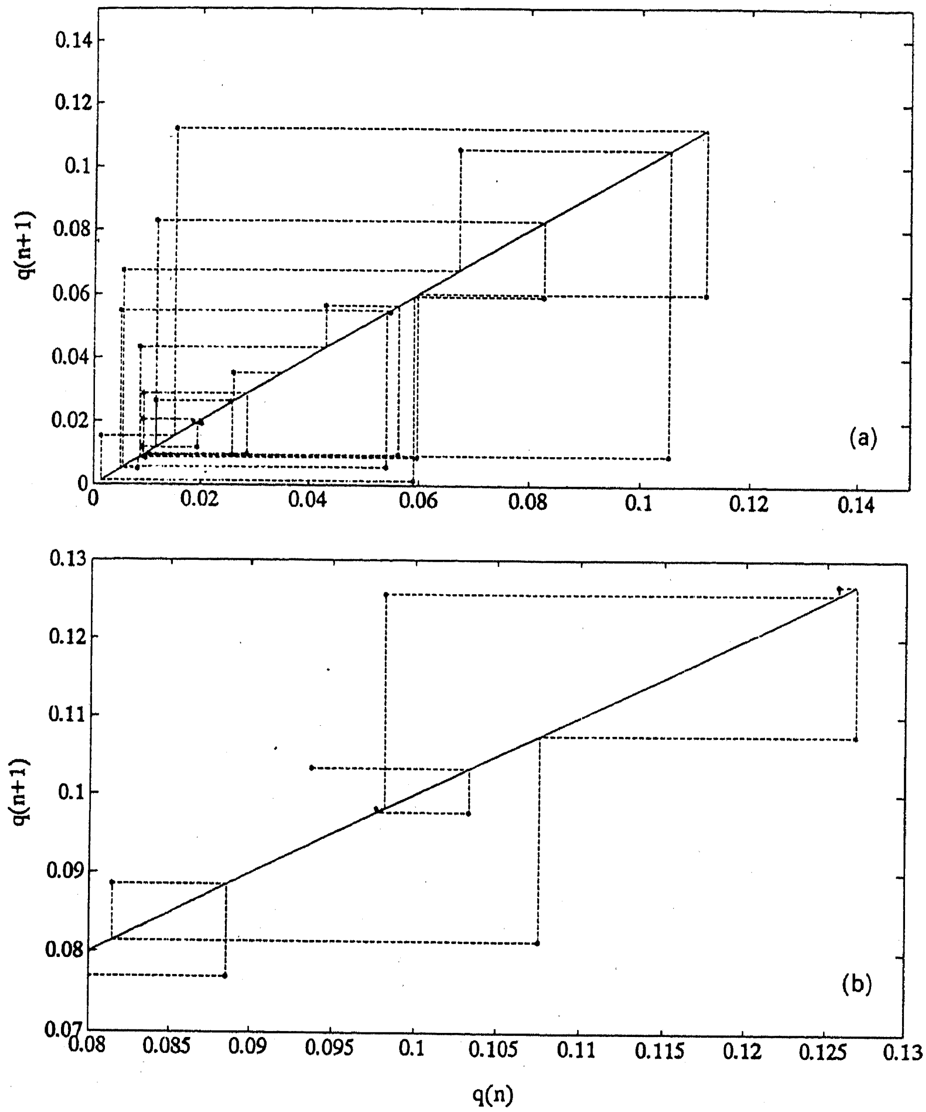


Figure 5. Iterative map of the components of the largest singular value for the random trajectory corresponding to figure 3, with a window length of 30 (**a**) and 10 (**b**).

eigenvalues and principal directions also, which shows that there is no direction in which correlations are retained. This is indeed what one would expect for random observables.

At this point it is necessary to comment on the dependence of the results on the choice of the embedding dimension. Relatively large dimensions are chosen in this example and in the following cases, since the number of points on the iterative map is determined by this dimension and one would like to have sufficient points on the map to decipher its nature. However, it is important to see whether this choice affects the qualitative features of the eigenvalue spectrum or of the iterative maps. We display in figure 4b the eigenvalue spectrum obtained for the same random trajectory, but now with a drastically reduced dimension of only 10. Clearly the same qualitative distribution of the eigenspectrum is obtained. (Compare with figure 4a. Note that the percentages depend on the actual number of eigenvalues.) The iterative map for the highest eigenvalue for this case is shown in figure 5b. It shows the same aperiodic feature as in the case of the larger dimension figure 5a. Studies with various other values for the embedding dimension lead to the same conclusions, showing that the present results are indeed generic.

Case 4: The Lorenz attractor

The well-known Lorenz attractor (see Sparrow 1986) is defined by

$$(\dot{x}, \dot{y}, \dot{z}) = (\sigma(y - x), \quad rx - y - xz, \quad -bz + xy), \tag{19}$$

where we take the parameters to be: $\sigma = 10$, $b = 8/3$ and $r = 28$ for which the system is a strange attractor.

The time series $x(t)$ obtained by numerical solution of (19) by a fourth-order Runge–Kutta routine is shown in figure 6. The singular spectrum for $x(t)$ as the time series with an embedding window of 35 time units is shown in figure 7. The number of *significant* eigenvalues and therefore the dimension of the attractor are not clear from this figure. This depends on the numerical noise level of the computations of the spectrum, and this problem has been discussed in detail by Broomhead and King (1986). The dimension is also sensitive to the parameters of the embedding window, namely the sampling time and the lag time (see Albano *et al* 1991 for a discussion of these problems). In the present case, the first five largest singular values are: 57, 14, 6, 3 and 2·5%. If we set the noise level as 5%, the attractor has a dimension of 3, as is the case for the Euclidian space dimension of the Lorenz attractor. Our present concern, however, is not so much the dimension of the attractor, as the nature of correlations along the principal directions. The iterate maps of q for the above five singular values are given in figures 8a–e. The first two, figures 8a and b, corresponding to $\sigma = 57$ and 14%, show clearly the regular behaviour of correlations in these two directions. These figures are very similar to the map for the sinusoidal function of case 2 (figure 2), where the iterates lie close to the diagonal.

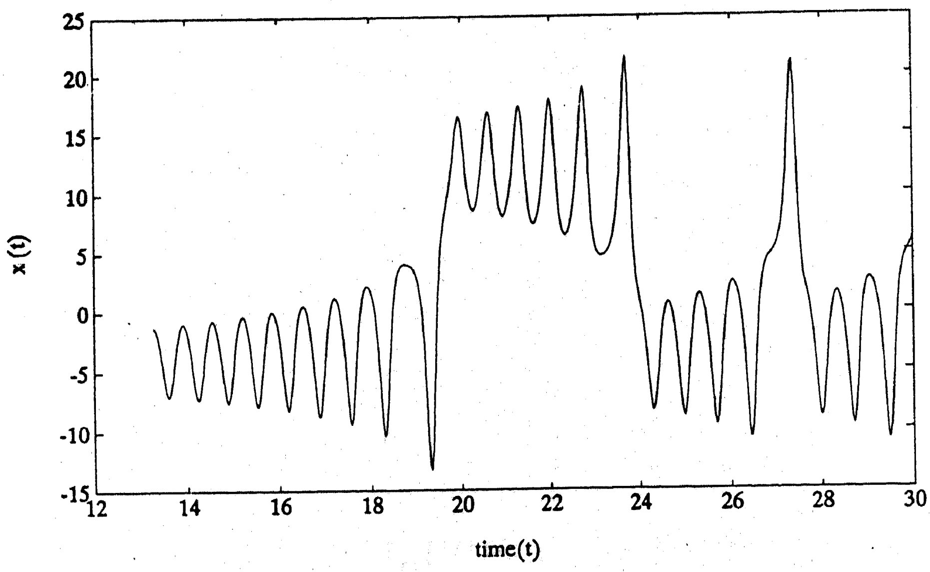


Figure 6. Time series $x(t)$ for the Lorenz attractor obtained by the solution of (19).

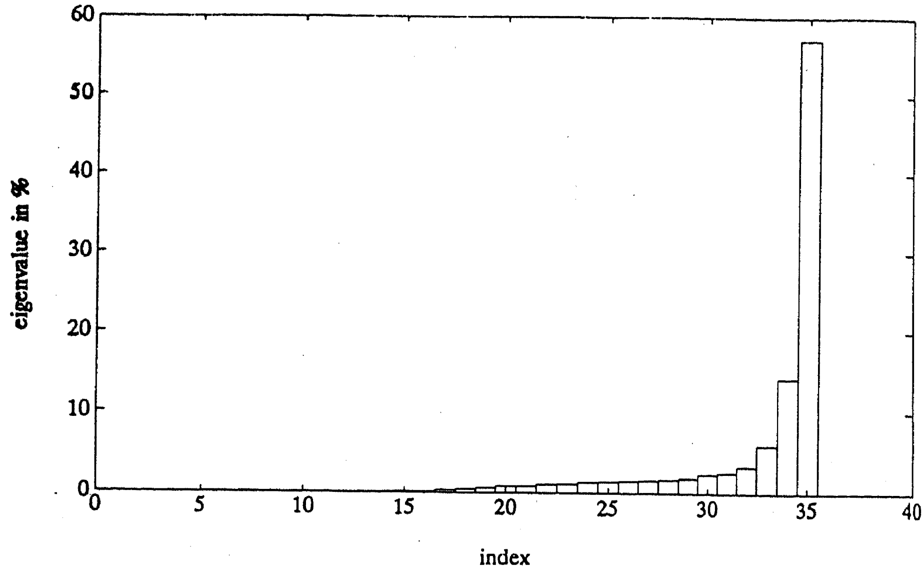
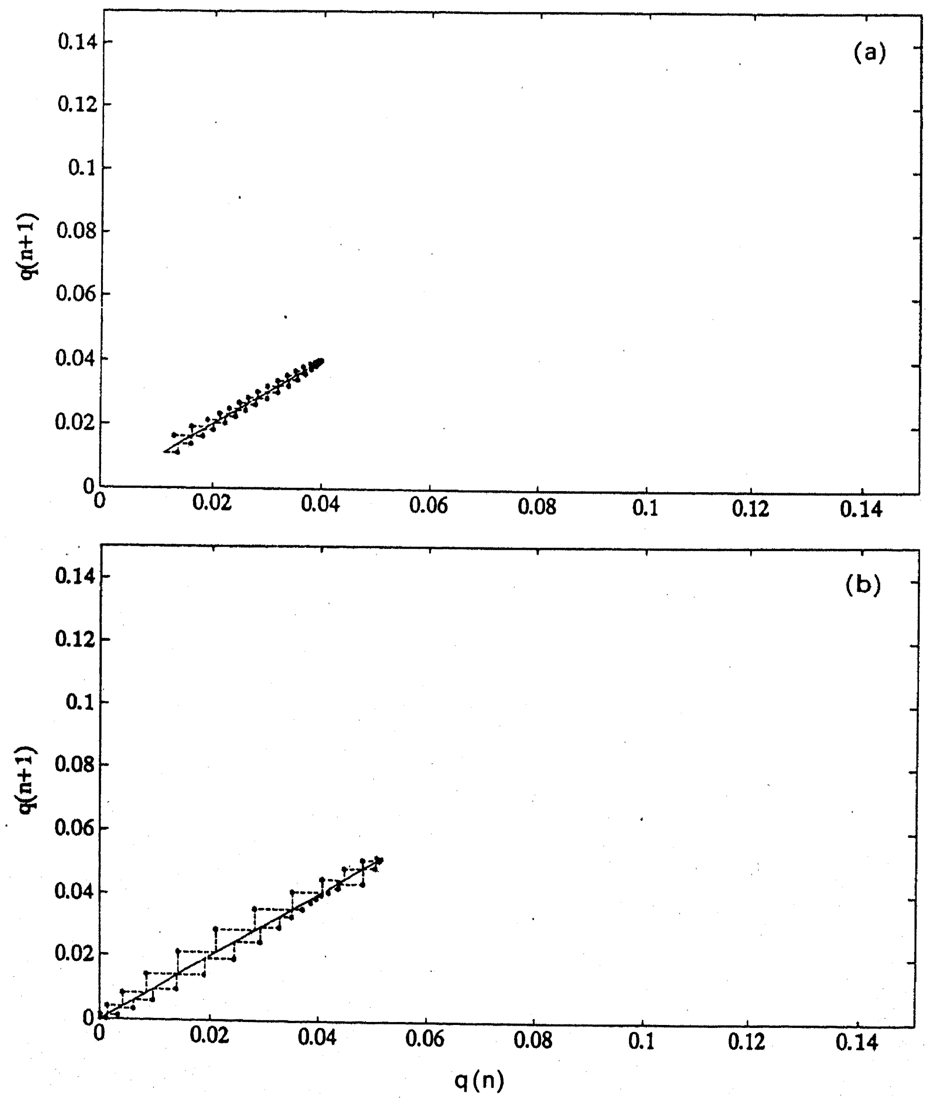


Figure 7. Eigenvalue spectrum for the time series $x(t)$ of figure 6, with 1000 points and a window length of 35.



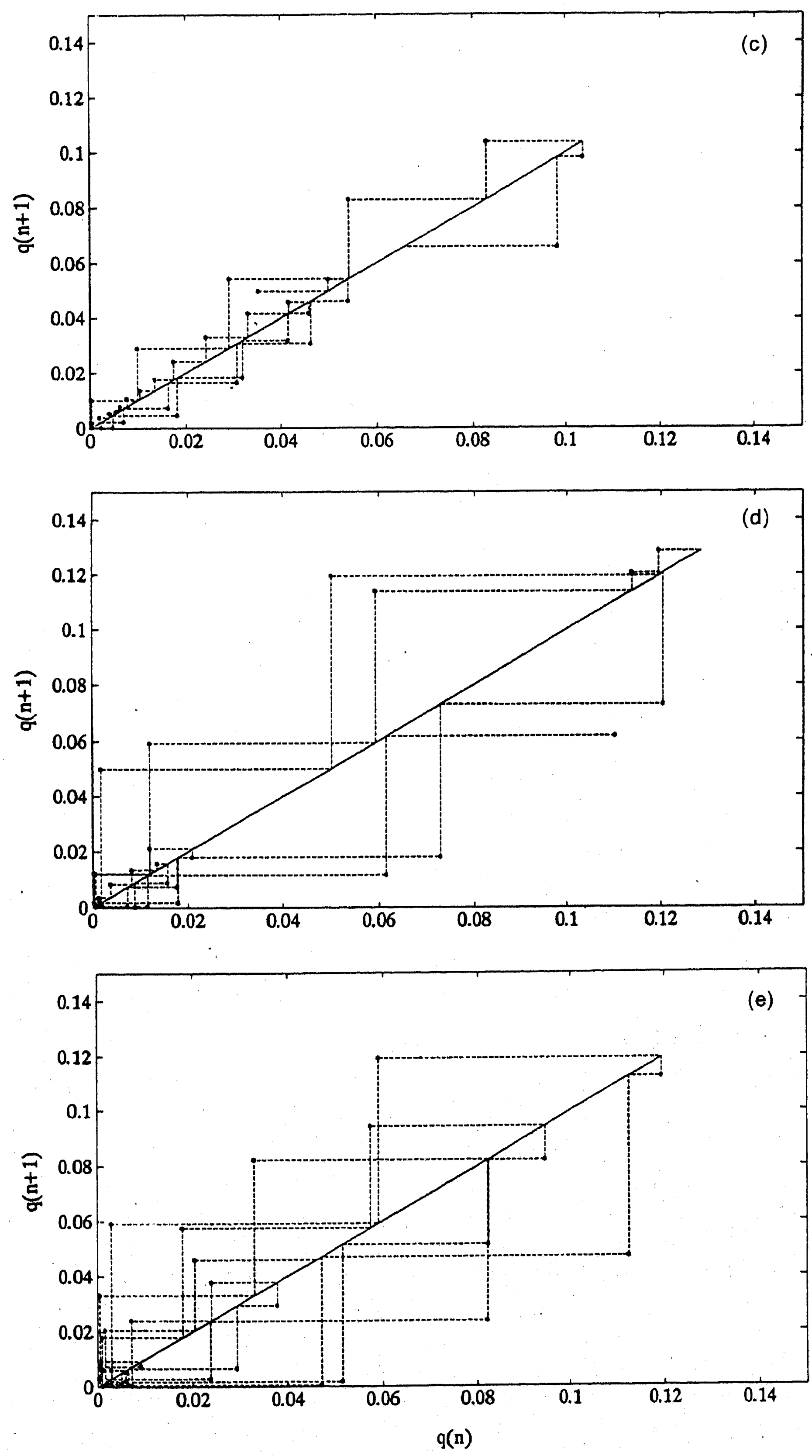


Figure 8. Iterative map of the components of the singular values for $x(t)$ of the Lorenz attractor corresponding to figure 7 (window length = 35). The singular values for the different figures are 57 (**a**), 14 (**b**), 6 (**c**), 3 (**d**) and 2.5 (**e**).

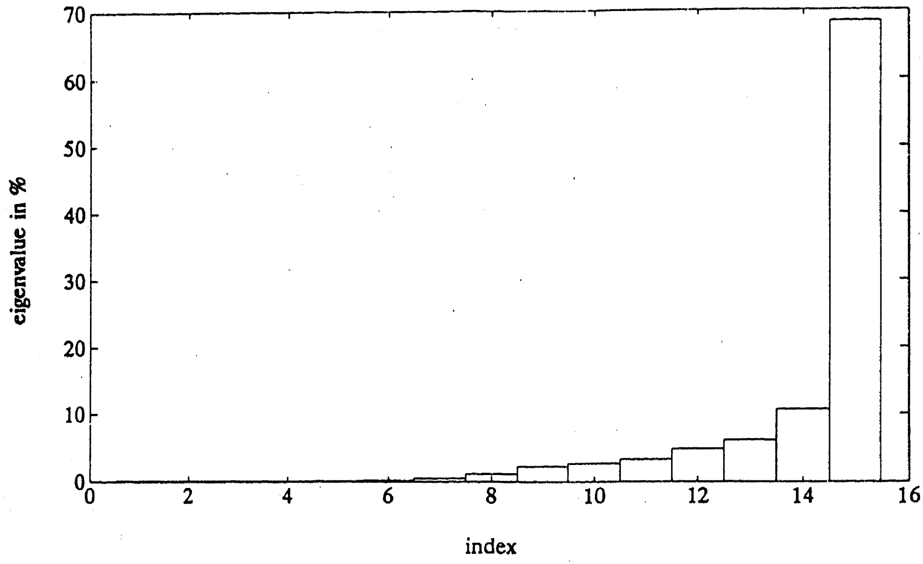


Figure 9. Same as figure 7, but with window length of 15.

The third principal direction with $\sigma = 6\%$, the flow of correlations is again somewhat regular, but shows signs of decorrelation and a greater spread in the values of q (see figure 8c). These findings are reminiscent of the Lyapunov exponents of the Lorenz attractor, which have the signs $(-, 0, +)$ indicating that trajectories in phase space contract exponentially, slower than exponentially and diverge exponentially in the three dimensions (Wolf 1986).

Going on to the fourth ($\sigma = 3\%$) and the fifth ($\sigma = 2{\cdot}5\%$) singular directions (figures 8d and e), we see unmistakable signs of aperiodic or chaotic behaviour of correlations which are now more widely scattered from the diagonal. These diagrams resemble figure 5 for the case of the random observable, indicating the chaotic nature of evolution of correlations along these directions.

As in the case of the random trajectory discussed above, it is important to deterimine whether these results are generic. For this purpose we have carried out studies of the eigenspectrum and the correlation maps for varying embedding dimensions. Typical results, for dimensions 15 instead of 35 used above, are reported. The eigenvalue spectrum (figure 9) has evidently the same features (compare with figure 7), the largest five now being 68, 10·6, 6, 4·7 and 3%, respectively. The correlation map for the principal direction for the largest eigenvalue (figure 10a) shows the same regular behaviour as for the larger dimension case (figure 8a) and the aperiodic nature of the map for the fourth direction (figure 10b), is similar to that for the larger dimension (figure 8d). Note that numerical values of the eigenvector components will differ in the two cases due to the different dimensions and normalization. We thus conclude that the qualitative aspects of the eigenspectrum and the correlation maps of the eigenvectors are independent of the choice of the embedding dimension.

These observations prompt us to conclude that there are at most three orthogonal directions in which the correlations are more or less retained and that the flow is appreciably decorrelated in all other directions of the embedding space. It may be possible to quantify this picture by evaluating the rates of decorrelation along the singular directions and to compute the corresponding exponents. Such efforts which would involve devising a proper definition of the decorrelation exponent in the present

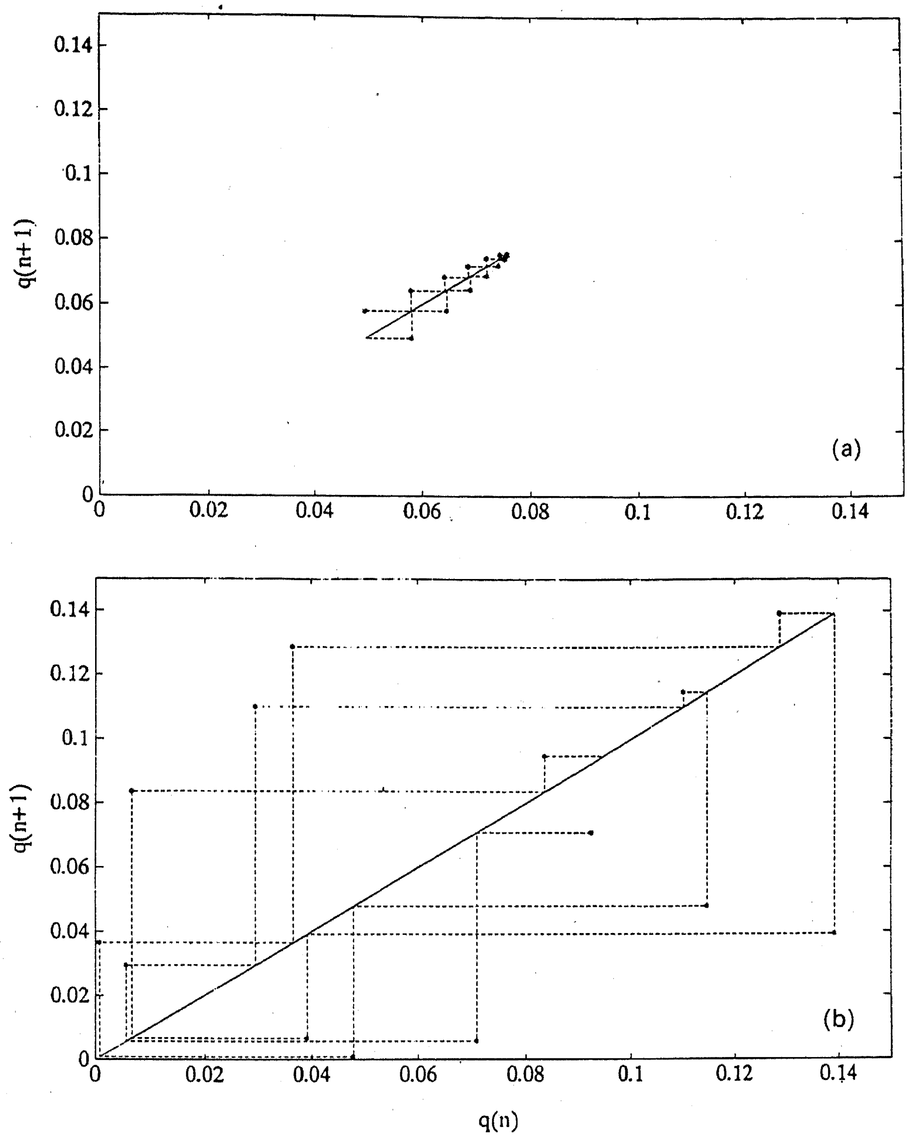


Figure 10. Iterative map of the components of the singular values for $x(t)$ of the Lorenz attractor corresponding to figure 9 (window length $= 15$). The singular values are for 68 (**a**) and 4.7% (**b**).

context and devising a suitable algorithm for its numerical evaluation from the maps, are under way.

4. Summary

We have addressed the problem of determining the nature of the attractor from the time series of a single variable of a multidimensional dynamical system. We have shown that the singular values of the covariance matrix constructed from the trajectory, can be decomposed into components that evolve with time. An iterative one-dimensional map of these correlation components reveal the nature of retention or loss of correlation along a given principal direction of the attractor. Along insignificant directions, i.e. those with small singular values, the flow is fast decorrelated and resembles chaotic behaviour. Along significant directions, i.e. those with large singular values, correlations are retained to a considerable extent. The results are largely independent of the choice of the embedding dimension.

These observations made on the model systems of the present study point the way to the possible use of such correlation maps to determine not only the dimension of the attractor but also the nature of the flow along the singular directions of the attractor from the experimental time series.

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