

Deterministic uncertainty

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Equations of motion with delays naturally emerge in the analysis of complex biological control systems which are organized around biochemically mediated feedback interactions. We study the properties of a Mackey-Glass-type nonlinear map with delay – the deterministic part of the stochastic cerebral blood flow map (CBFM) recently introduced to elucidate the scaling properties of cerebral hemodynamics. We point out the existence of *deterministic* and *nondeterministic subspaces* in the reconstructed phase space of delay-difference equations and discuss the problem of detection of nonlinearities in time series generated by such dynamical systems.

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Attractor reconstruction is certainly one of the more fundamental methods of analysis of nonlinear dynamical systems [1]. Time series prediction, nonlinear filtering, chaos control and targeting of trajectories all exploit the properties of phase space [2]. However, the number of variables accessible to measurement is frequently limited. In many cases even the dimensionality of the system is not known. The fact that phase space may be reconstructed using the time evolution of just a *single* dynamical variable in multidimensional system paves the way for applications of nonlinear methods in natural sciences.

As early as 1985 Babloyantz *et al.* demonstrated that certain nonlinear measures, first introduced in the context of chaotic dynamical systems, changed during slow-wave sleep [3]. The flurry of research work that followed this discovery focused on the application of nonlinear dynamics in quantifying brain electrical activity during different mental states, sleep stages, and under the influence of the epileptic process (for a review see for example [4]). Despite various technical difficulties, the number of applications of nonlinear time series analysis has been growing steadily and now includes prediction of epileptic seizures [5], the characterization of encephalopathies [6], monitoring of anesthesia depth [7], characteristics of seizure activity [8], fetal ECG extraction [9], and control of human atrial fibrillation [10].

We have recently studied middle cerebral artery blood flow velocity in humans using transcranial Doppler ultrasonography (TCD) [11, 12]. We found that scaling properties of time series of the axial flow velocity averaged over a cardiac beat interval may be characterized by two exponents. The short-time scaling exponent determines the statistical properties of fluctuations of blood flow velocity in short-time intervals while the Hurst exponent describes the long-term fractal properties. To elucidate the nature of two scaling regions characteristic

of *healthy* individuals we introduced a stochastic cerebral blood flow map (CBFM). The deterministic part of the CBFM is reminiscent of the Mackey-Glass differential equation originally introduced to describe the production of white blood cells [13, 14] so that we refer to it as the *Mackey-Glass map (MGM)*:

$$x_n = x_{n-1} - bx_{n-1} + a \frac{x_{n-\eta}}{1 + x_{n-\eta}^{10}}. \quad (1)$$

Herein we investigate the detailed properties of the above difference equation from the viewpoint of detection of nonlinearities and determinism. One invariably faces this detection problem when dealing with short, noisy physiological time series.

It is well established that the presence of delays even in such dynamically simple systems as first-order differential equations may lead to intricate and multidimensional evolution. Therefore, we begin our analysis with the attractor reconstruction [15, 16, 17].

Let $\{x_i\}_{i=1}^N$ be the time series generated by (1). In the methods of delays the reconstructed trajectory is made up of the following points:

$$\mathbf{X}_n = [x_{n-(m-1)J}, x_{n-(m-2)J}, \dots, x_{n-J}, x_n], \quad (2)$$

where J is the *delay* or *lag* and m is the *embedding dimension*. Thus, the reconstruction depends upon two parameters which are not known a priori. Considerable effort has been devoted to finding the best approach to selecting judicious values of the lag J see, for example, [18] and references therein. This is because for finite data sets, especially those contaminated by noise, the choice of delay determines the outcome of reconstruction. In Fig. 1 we compare the autocorrelation function and mutual information of the Mackey-Glass map time series ($a = 1.3$, $b = 0.7$, $\eta = 6$). These two methods are routinely used

to estimate the proper reconstruction lag. Typically J is chosen as the delay for which the autocorrelation function drops to a certain fraction of its initial value, e.g. $1/e$ [19] or the first local minimum of the mutual information [20]. Thus, we obtain the lag equal to 1 and 3, respectively. It is apparent that the mutual information has distinct peaks at integer multiples of the delay η and therefore is particularly well suited to detection of dynamical delays. The exponentially decreasing amplitude of the consecutive maxima is a strong indication of sensitive dependence on initial condition characteristic of chaotic dynamics so that we proceed to calculations of the attractor dimension and the largest Lyapunov exponent.

Fig. 2 illustrates the process of calculation of the correlation integral $C_m(r, J)$ for embedding spaces of increasing dimension m with $J = 1$ [21]. The slope of the linear scaling regions in a double logarithmic plot converges to the correlation dimension $D_2 = 4.85$. We obtain the same value for $J = 3$.

In Fig. 3 we graph the average divergence of initially nearby trajectories as a function of the number of iterations of the MGM [18]. In the semilogarithmic graph the slope of the dashed straight line yields the value of the largest Lyapunov exponent $\lambda_1 = 0.069$ which confirms that the underlying dynamics is indeed chaotic. One can see in this plot that the average time after which neighboring trajectories reach the boundaries of the available phase space (as indicated by the constant value of their separation) roughly coincides with the delay time interval where the maxima of the mutual information are clearly pronounced *cf.* Fig. 1.

Difference equations with delays such as the Mackey-Glass map are seldom discussed in standard nonlinear dynamics textbooks. However, let us revisit one of the three most fundamental nonlinear models – the Henon map:

$$\begin{aligned} x_n &= a - x_{n-1}^2 + by_{n-1} \\ y_n &= x_{n-1}. \end{aligned} \quad (3)$$

From the second equation in (3) we have $y_{n-1} = x_{n-2}$ and using this expression we arrive at:

$$x_n = a - x_{n-1}^2 + bx_{n-2}. \quad (4)$$

Hence, the two-dimensional Henon map is equivalent to the single difference equation (4) with delay equal to 2. In the same vein, we can rewrite (1) as a set of η ordinary difference equations:

$$x_n^{(1)} = (1 - b)x_{n-1}^{(1)} + a \frac{x_{n-1}^{(\eta)}}{1 + (x_{n-1}^{(\eta)})^{10}} \quad (5)$$

$$\begin{aligned} x_n^{(2)} &= x_{n-1}^{(1)} \\ x_n^{(3)} &= x_{n-1}^{(2)} \\ &\vdots \\ x_n^{(\eta)} &= x_{n-1}^{(\eta-1)}, \end{aligned}$$

which may be interpreted as a perturbed *periodic shift map*:

$$\begin{aligned} x_n^{(1)} &= x_{n-1}^{(\eta)} \\ x_n^{(2)} &= x_{n-1}^{(1)} \\ &\vdots \\ x_n^{(\eta)} &= x_{n-1}^{(\eta-1)}. \end{aligned} \quad (6)$$

This *linear* map yields periodic orbits of length η regardless of the initial conditions. For brevity's sake, the evolution of a difference equation with delay may be written with the help of the shift operator D_f :

$$\mathbf{x}_{n+1} = D_f \mathbf{x}_n = [f(x_n^{(\eta)}, x_n^{(1)}), x_n^{(1)}, \dots, x_n^{(\eta-1)}]^T. \quad (7)$$

Now we turn the problem around and ask about the prospects of detecting determinism in short, possibly corrupted with environmental noise, time series generated by a difference equation with delay, such as the MGM (1). Distinguishing chaos from environmental noise has been a longstanding challenge to the life sciences where observed time series usually have relatively few data points. Sugihara and May [22] pointed out that for chaotic dynamical systems the accuracy of the nonlinear forecasting exponentially falls off with increasing prediction-time interval at a rate related to the value of the Lyapunov exponent. On the other hand, for uncorrelated noise the forecasting accuracy is roughly independent of prediction interval. Their original idea of using short-term prediction to detect determinism was later extended [2, 23, 24, 25]. In Fig. 4 we display the normalized prediction error as a function of the prediction time. The simplest zeroth order phase-space algorithm [2] was employed to forecast the values of the MGM time series. The forecasting accuracy not only initially *does improve* with the *increasing* prediction-time interval but also exhibits strong oscillations. For some relatively short forecasting steps, the accuracy for the MGM time series is essentially the same as that of the corresponding surrogate data (data which as closely as possible share both the spectral properties and distribution with the original time series, but from which all nonlinear correlations have been excised [26, 27]). To shed some light on this effect, let us assume that we forecast one step ahead ($s = 1$) and embed the MGM time series with $\eta = 6$ in three dimensions ($m = 3$) with delay $J = 2$ (for such delay we simply choose every other element of the original time series to form three dimensional

delay vectors (2)). For clarity of presentation we disregard the influence of the linear term in the shift operator D_f , i.e. $f(x_n^{(\eta)}, x_n^{(1)}) \approx g(x_n^{(\eta)})$. Using the projection operator $P_{ijk}\mathbf{x}_n = [x_n^{(i)}, x_n^{(j)}, x_n^{(k)}]^T$, we may describe the prediction in the reconstructed phase-space as:

$$\begin{aligned} P_{135}\mathbf{x}_{n+1} &= P_{135}(D_g\mathbf{x}_n) \\ &= P_{135}[g(x_n^{(6)}), x_n^{(1)}, x_n^{(2)}, \dots, x_n^{(5)}]^T \quad (8) \\ &= [g(x_n^{(6)}), x_n^{(2)}, x_n^{(4)}]^T = \mathcal{F}_1(P_{624}\mathbf{x}_n). \end{aligned}$$

The propagator \mathcal{F}_1 depends on variables which have been *discarded* in the embedding process so that it should not come as a surprise that accurate forecasting in this case is precluded since we selected a *nondeterministic subspace* with respect to the prediction-time interval. However, if we choose to forecast two steps ahead ($s = 2$) then

$$\begin{aligned} P_{135}\mathbf{x}_{n+2} &= P_{135}D_g\mathbf{x}_{n+1} \\ &= P_{135}[g(x_n^{(5)}), g(x_n^{(6)}), x_n^{(1)}, \dots, x_n^{(4)}]^T \quad (9) \\ &= [g(x_n^{(5)}), x_n^{(1)}, x_n^{(3)}]^T = \mathcal{F}_2(P_{135}\mathbf{x}_n) \end{aligned}$$

and the chosen subspace is closed with respect to the propagator \mathcal{F}_2 . We refer to such subspace as *deterministic*. In Fig. 5 we verify our analysis by plotting the normalized prediction error as a function of the neighborhood size used to construct a locally linear approximation of the MGM dynamics [25, 28]. It is apparent that for $s = 1$ the forecasting accuracy is hardly different from that of the corresponding surrogate data. On the other hand, for $s = 2$ the error curve with a clearly pronounced minimum at small neighborhood sizes is characteristic of nonlinear dynamical systems. The conclusions we have drawn are valid also for small to moderate linear coupling we so far ignored by setting $f(x_n^{(\eta)}, x_n^{(1)}) \approx g(x_n^{(\eta)})$. However, strong couplings may give rise to even more subtle effects which we shall discuss elsewhere.

The forecasting error is one of many statistics applicable to testing for nonlinearities in time series. For example, higher-order autocorrelations such as

$$\langle (x_n - x_{n-d})^3 \rangle / \langle (x_n - x_{n-d})^2 \rangle \quad (10)$$

may be used to measure time asymmetry, a strong signature of nonlinearity [2]. Such autocorrelations are also helpful in pinpointing another interesting property of delay-difference equations. Upon inspection of (6), one immediately realizes that the evolution of the periodic shift map amounts merely to “shuffling” of the components of the state vector. However, *random* shuffle of the data is the crudest way of generation of surrogate data. If the dimensionality of the system determined by the delay η is sufficiently high, it is not surprising that this type of time reversal test may not detect nonlinearities.

We generated the MGM time series ($a = 1.3$, $b = 0.7$, $\eta = 20$) along with 39 surrogate data sets and calculated the corresponding value of (10). For 11 out of 20 delays d taken from the interval $[1, 20]$, we could not reject the hypothesis that at the 95% confidence level the MGM time series results from a Gaussian linear stochastic process.

Delay-difference equations naturally emerge in the analysis of complex biological control systems [11]. The unique properties of such dynamical systems may lead to difficulties in recognizing nonlinearities in their evolution especially when experimental time series are short and delays are long. To draw attention to this issue we gave this paper a somewhat provocative title *Deterministic Uncertainty*.

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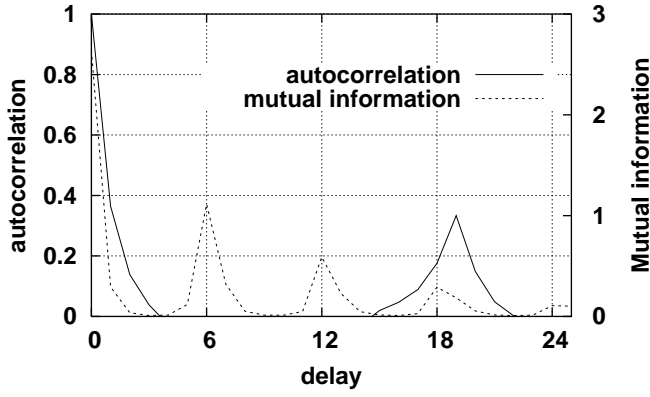


FIG. 1: Autocorrelation function (dashed line) and mutual information (solid line) for the time series generated by the MGM (1) with the following parameters: $a = 1.3$, $b = 0.7$, $\eta = 6$.

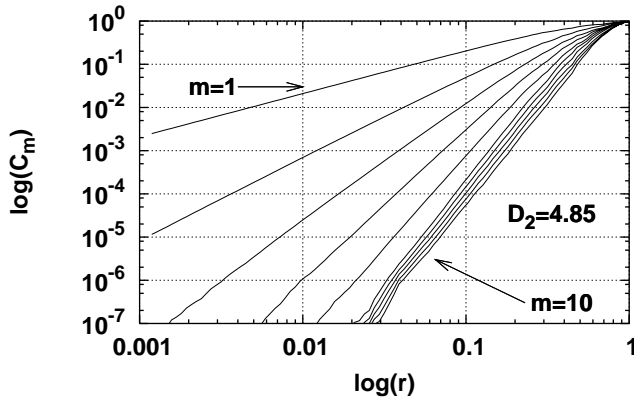


FIG. 2: Correlation integral C_m for embedding spaces of increasing dimension m calculated for the MGM time series used in Fig. 1 .

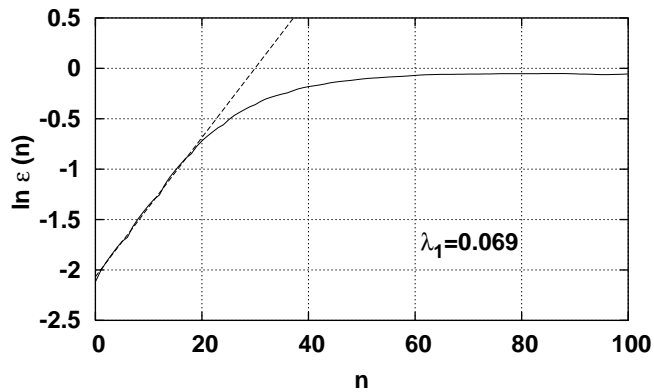


FIG. 3: Average divergence ϵ of initially close trajectories as a function of number of iterations n of the MGM ($a = 1.3$, $b = 0.7$, $\eta = 6$) is plotted in semilogarithmic scale. The slope of the straight dashed line yields the value of the largest Lyapunov exponent λ_1 . The reconstruction was done with $m = 7$ and $J = 1$.

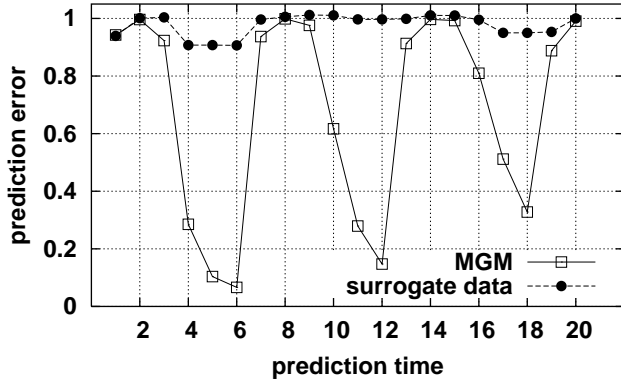


FIG. 4: The normalized forecasting error as a function of prediction time. The simplest zeroth order phase-space algorithm was employed to predict the values of the MGM time series and the corresponding surrogate data. The embedding was done in three dimensions with the lag $J = 1$. The forecasting error was normalized by the standard deviation of the time series.

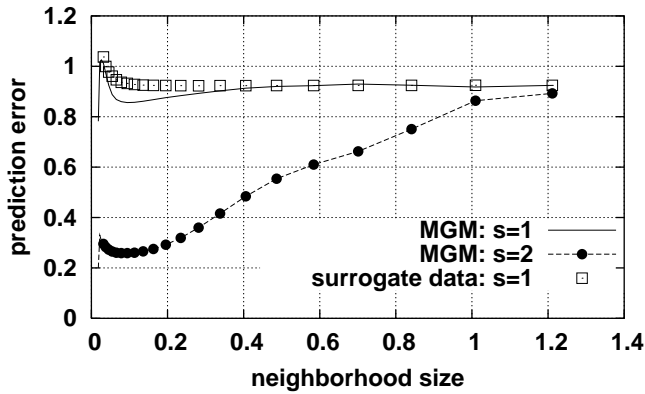


FIG. 5: The normalized prediction error as a function of the neighborhood size used to construct a locally linear approximation of the MGM dynamics ($a = 1.3$, $b = 0.7$, $\eta = 6$) or that of the surrogate data. The embedding was done in three dimensions with the lag $J = 2$. The displayed curves correspond to the length s of the prediction-time interval