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Inverting chaos: Extracting system parameters from experimental data

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Given a set of experimental or numerical chaotic data and a set of model differential equations with several parameters, is it possible to determine the numerical values for these parameters using a least-squares approach, and thereby to test the model against the data? We explore this question (a) with simulated data from model equations for the Rossler, Lorenz, and pendulum attractors, and (b) with experimental data produced by a physical chaotic pendulum. For the systems considered in this paper, the least-squares approach provides values of model parameters that agree well with values obtained in other ways, even in the presence of modest amounts of added noise. For experimental data, the ''fitted'' and experimental attractors are found to have the same correlation dimension and the same positive Lyapunov exponent. © *1996 American Institute of Physics.*
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Model equations are often used to simulate chaotic data. However, a more challenging task is the fitting of model equations to real experimental chaotic data. We describe a simple ''least-squares'' approach to this ''inverse'' problem that is robust against modest amounts of data noise. The technique is successfully applied to data from an experimental chaotic pendulum.

I. INTRODUCTION

The possibility of devising a dynamical model empirically from chaotic data has been explored in a variety of contexts.[1] In the most challenging scenario no specific model is known and one attempts to determine the form of the ordinary differential equations or maps that govern the behavior of a given time series of a single dynamical variable. See, for example, papers by Brown, Rulkov, and Tracy, and references contained therein.[2] Typically the model is expressed as a set of first order ODEs, $d\mathbf{x}/dt = \mathbf{F}(\mathbf{x})$ where $\mathbf{x}$ is a vector in state space. Then $\mathbf{F}(\mathbf{x})$ is constructed from linear combinations of polynomials of the state space variables using simulated or experimental data.[3] Various refinements have been added to this technique, including the use of singular value decomposition to facilitate an efficient choice of polynomials for the ODEs and to help filter noise from the data.[4] Methods have also been developed to reconstruct vector fields from scalar time series when the model equations *are* known.[5] In a recent example, model parameters are obtained by synchronization of a parameter-dependent response system with the original dynamical system.[6]

In this paper we attempt a less difficult but nevertheless practical problem of determining parameters for a dynamical system given a proposed ODE model and an experimental chaotic time series. The invariants of the ''fitted'' attractor can then be compared to those of the ''raw'' attractor in order to assess the adequacy of the model. There are two distinct cases. In the simpler case the model parameters enter *linearly* into the ODEs. Typical examples are the dynamical systems of Lorenz[7] and Rossler.[8] In more complex situations, such as the chaotic pendulum, some model parameters enter linearly, while others enter nonlinearly. We show that a least-squares approach to finding the parameters works well in both cases.

While least-squares methods are of course ubiquitous in data analysis, they appear not to have been previously applied to the problem of determining parameters of dynamical systems in this way. Ultimately we hope to apply the method to test models of spatiotemporal chaos, where the state variables are functions of both position and time and therefore the model equations are partial differential equations.

II. THE FITTING METHOD

We consider a typical third-order dynamical system represented by a set of ODEs

$$\frac{dx_1}{dt} = F_1(x_1, x_2, x_3, a_1, a_2 \cdots a_m),$$

$$\frac{dx_2}{dt} = F_2(x_1, x_2, x_3, a_1, a_2 \cdots a_m), \quad (1)$$

$$\frac{dx_3}{dt} = F_3(x_1, x_2, x_3, a_1, a_2 \cdots a_m),$$

where $\{a_k\}$ is a set of m adjustable parameters for the model. The method is to construct a function of the parameters $S(a_k)$ that has a global minimum[9] with respect to those parameters. A common choice is a ''least-squares'' function and thus our choice for this dynamical system is

$$S = \sum_{j=1}^{N} \left\{ \sum_{i=1}^{3} [x_i'(j) \right.$$

$$\left. - F_i(x_1(j), x_2(j), x_3(j), a_1, a_2 \cdots a_m)]^2 \right\}, \quad (2)$$

where the prime indicates differentiation with respect to time, the first sum is taken over N data points, and the second sum is taken over the three dynamical variables. To obtain a minimum, the derivatives with respect to each parameter a_k are set equal to zero; that is

$$\frac{\partial S}{\partial a_k} = 0. \quad (3)$$

The data set $\{x_i(j)\}$ is assumed given and the derivatives $x_i'(j)$ are calculated using finite-difference derivatives from the data set. The selected algorithm, which approximates a derivative from equally spaced data points, is

$$x_i'(j) = \frac{-x_i(j+2) + 8x_i(j+1) - 8x_i(j-1) + x_i(j-2)}{12\Delta t}. \quad (4)$$

The resulting error is $O(\Delta t^4)$. When the ''true'' parameters are known, the fitted values can be compared with them by defining an error measure E as follows.

$$E = \frac{1}{n} \sum_{k=1}^{n} \frac{[a_k - a_k^0]^2}{a_k^0}, \quad (5)$$

where a_k^0 is a member of the ''true'' parameter set. We also examine the sensitivity of the fit to noise added to the data.

III. APPLICATION TO SIMULATED DATA

To test the method, it is applied first to numerically generated time series from the Rossler and Lorenz systems, and, with modification, from the chaotic pendulum. The Rossler attractor is generated by the following equations with three parameters:

$$x' = -y - z,$$
$$y' = x + ay, \quad (6)$$
$$z' = b + xz - cz.$$

For the Rossler system, Eq. (3) results in the following expressions for the numerical parameters a, b, and c:

$$a = \frac{-\Sigma xy + \Sigma y'y}{\Sigma y^2},$$

$$b = \frac{\Sigma z'\Sigma z^2 - \Sigma xz\Sigma z^2 + \Sigma z\Sigma xz^2 - \Sigma z\Sigma z'z}{n\Sigma z^2 - (\Sigma z)^2}, \quad (7)$$

$$c = \frac{n\Sigma xz^2 - n\Sigma z'z + \Sigma z\Sigma z' - \Sigma z\Sigma xz}{n\Sigma z^2 - (\Sigma z)^2}.$$

(All the summations are carried out over all the data points.) For the numerical simulation we use the parameter set, $a = 0.15$, $b = 0.2$, and $c = 10$, and generate phase space data using a fourth-order Runge–Kutta integrator. The fitted re-

sults obtained from the minimization process as given in Eq. (6) agree within seven decimal places with the original parameter set. For the Rossler system $E \cong 10^{-13}$ when $\Delta t = 0.01$, indicating a remarkably close fit, given the roundoff errors (or equivalent numerical noise) associated with the fact that our numerical derivative is $O(\Delta t^4)$, whereas the numerical integrator is $O(\Delta t^5)$.

We test the *robustness* of the minimization technique by adding extra functional terms and parameters to the fitting model for the Rossler simulation. First we allow the coefficients that are unity for the simulation to *differ* from unity in the fitting model. With this condition application of the minimization technique leads to new equations with these new parameters as well as the usual parameters, a, b, and c that replace Eq. (7). We find that the additional fitted parameters are unity to within about one part in 10^5. In the second test we add several spurious second degree terms to one of the differential equations of the ''fitting'' model, each new term having its own linear parameter. Again, application of the minimization technique results in new equations involving the new parameters and a, b, and c. We find that the new fitted parameters are all zero to within about one part in 10^5, and that a, b, and c are essentially unaffected.

The fitting procedure is also applied to the Lorenz system:

$$x' = -\sigma x + \sigma y,$$
$$y' = -xz + rx - y, \quad (8)$$
$$z' = xy - bz,$$

with minimization resulting in the following equations for the parameters:

$$\sigma = \frac{\Sigma x'y - \Sigma x'x}{\Sigma x^2 - 2\Sigma xy + \Sigma y^2},$$

$$r = \frac{\Sigma xy' + \Sigma x^2 z + \Sigma xy}{\Sigma x^2}, \quad (9)$$

$$b = \frac{-\Sigma zz' + \Sigma xyz}{\Sigma z^2}.$$

Again all summations are carried out over all data points. For the simulation we choose $\sigma = 10$, $r = 28$, and $b = 2.666\,67$. The agreement of the parameters determined by minimization with those used in the simulation is again excellent. The error as defined in Eq. (5) for the Lorenz system is $E \cong 10^{-14}$ when $\Delta t = 0.001$.

Finally we numerically simulate a chaotic pendulum that mimics the physical pendulum of Blackburn *et al.*[10] (In Sec. V we consider *experimental* data from such a pendulum.) This pendulum may be modeled by the equation

$$I \frac{d^2\theta}{dt^2} + b \frac{d\theta}{dt} + \omega_0^2 I \sin\theta = T \sin(\omega_f t + \phi), \quad (10)$$

where I is the moment of inertia, b is a friction parameter, ω_0 is the natural angular frequency, T is the amplitude of the

applied forcing torque, ω_f is the forcing angular frequency, and ϕ is the initial phase of the forcing. Dividing by I eliminates one parameter:

$$\omega' + \alpha\omega + \beta \sin \theta = \gamma \sin(\delta t + \phi), \tag{11}$$

where $\alpha = b/I$, $\beta = \omega_0^2$, $\gamma = T/I$, and $\delta = \omega_f$. Of the five parameters only α, β, and γ enter as linear coefficients of terms in the ODE, as do the parameters in the Rossler and Lorenz systems. The remaining two parameters, δ and ϕ, enter nonlinearly as part of the argument of the trigonometric forcing function. (A dimensionless version of this equation has only three parameters[11] but use of that model implies knowledge of both the natural frequency and the initial phase of the pendulum. Such information would typically be lacking from experimental data, which only consists of sequences of angles θ_i and angular velocities ω_i.) In the simulation we treat the ''nonlinear'' parameters δ and φ as known quantities and therefore only apply the minimization technique to the linear parameters. (In Sec. V, we show how these ''nonlinear'' parameters can be determined from the data.)

As before we form a least-squares function

$$S = \sum_{i=1}^{n} [\omega_i' - (-\alpha\omega_i - \beta \sin \theta_i + \gamma \sin(\delta t + \phi))]^2, \tag{12}$$

where the sum extends over all the points $\{\theta_i, \omega_i\}$ of the data set, and time is incremented by a fixed amount, Δt. The angular acceleration ω_i' is determined for each data point with the finite-difference approximation defined in Eq. (4),

$$\omega_i' = \frac{-\omega_{i+2} + 8\omega_{i+1} - 8\omega_{i-1} + \omega_{i-2}}{12\Delta t}.\neg \tag{13}$$

For the present, we assume knowledge of δ and ϕ, and follow the minimization procedure of setting the partial derivatives of S with respect to α, β, and γ equal to zero. This calculation results in cumbersome but straightforward linear equations for α, β, and γ that may be solved by standard methods

$$\alpha\sum \omega^2 + \beta\sum \omega \sin \theta - \gamma\sum \omega \sin(\delta t + \phi)$$

$$= -\sum \omega'\omega,$$

$$\alpha\sum \omega \sin \theta + \beta\sum \sin^2 \theta - \gamma\sum \sin \theta \sin(\delta t + \phi)$$

$$= -\sum \omega' \sin \theta, \tag{14}$$

$$\alpha\sum \omega \sin(\delta t + \phi) + \beta\sum \sin \theta \sin(\delta t + \phi)$$

$$- \gamma\sum \sin^2(\delta t + \phi) = -\sum \omega' \sin(\delta t + \phi).$$

(As usual, the summations are over all data points.) Figure 1 shows a numerical simulation of the chaotic pendulum with $\Delta t = 0.001$ s. The parameters δ and ϕ are set at $\delta = 5.9628$
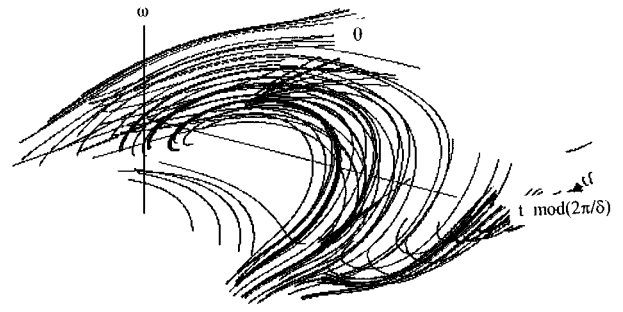

FIG. 1. Attractor for the simulated chaotic pendulum. The values of the parameters used in the simulation are $\alpha = 2.12508$ s^{-1}, $\beta = 76.1236$ s^{-2}, $\gamma = 117.212$ s^{-2}, $\delta = 5.9628$ rad s^{-1}, and $\phi = 1.05$ rad. The fitted parameters from the minimization process agreed with these simulation parameters to within at least eight decimal places.

rad/s and $\phi = 1.05$ rad. The *simulation* values of α, β, and γ (see the caption of Fig. 1) are chosen so as to coincide with those used in acquiring the experimental data of Sec. V. Using the equation set (14), the *fitted* values of the latter three parameters coincide with those used in the simulation to eight significant figures. Consequently, the error measure is $E \cong 10^{-15}$.

For all three dynamical systems we find the error to decrease with smaller Δt. However if Δt is less than about 10^{-4} (for the pendulum) the error increases slightly as numerical error becomes relatively more significant.

IV. THE EFFECT OF ADDITIVE NOISE

In this section we consider the effect of noise on the fit of the ''linear'' parameters for the simulated Rossler, Lorenz, and pendulum systems. In each case Gaussian noise with fractional standard deviation σ is added to the simulated phase space coordinates to represent the effects of measurement uncertainty. Derivatives are calculated from the noisy coordinates. Application of the minimization scheme leads to a power-law dependence of E on σ for modest values of σ. Figure 2 shows a least-squares regression to an equation of the form

$$E = A\sigma^B \tag{15}$$

for numerical pendulum data. While the prefactor A varies from one system to another and depends on the time step Δt, the exponent B is relatively system independent as indicated in Table I. If the integration time step is shortened, E decreases. However, this dependence is primarily due to change in A; B is relatively unchanged as shown in Table I.

If σ is more than about 1% of the attractor size, Eq. (15) still holds but B increases to more than 3 and is somewhat system dependent. Nevertheless, the minimization process itself remains fairly robust until the noise approaches an appreciable fraction of the size of the attractor.
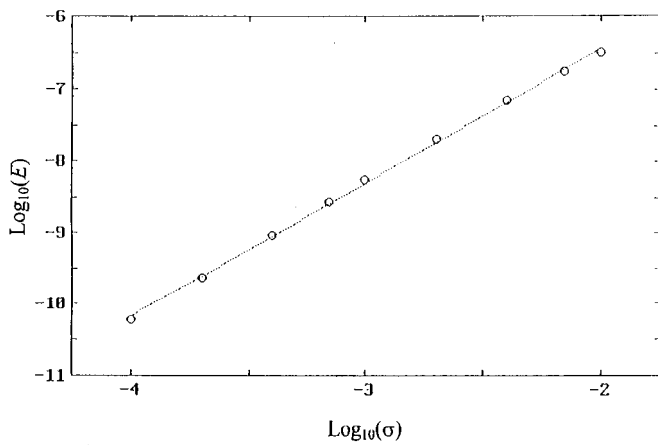
FIG. 2. Effect of Gaussian additive noise of standard deviation σ (expressed as a fraction of the coordinate range) on the error parameter E for numerical pendulum data. A least-squares fit of log E vs log σ suggests a power-law relationship. For small σ, the exponent is about 2.

V. APPLICATION TO EXPERIMENTAL DATA FROM A CHAOTIC PENDULUM

In this section we apply the minimization technique to *experimental* data from the pendulum of Blackburn *et al.*[10] While the numerical values of the parameters for the experimental data were approximately known to us, we treat the data as ''blind'' and only allow ourselves to use our knowledge of the *general* range these parameters might take for this pendulum.

The range of typical values for the physical parameters of the Blackburn pendulum are

$$2 < \alpha < 10,$$

$$60 < \beta < 100 \quad \text{(this is a constant for a given pendulum)},$$

$$80 < \gamma < 200,$$

$$0 < \delta < 12,$$

$$0 < \phi < 2\pi.$$

If δ and ϕ are known then the procedure duplicates that used for the simulated data (Sec. III) where knowledge of these parameters *was* assumed. In practice, these parameters are determined independently by an iterative process. The

TABLE I. Exponents governing the growth of the error parameter with standard deviation of added noise for various integration time steps. (The time step Δt is dimensioness for the Rossler and Lorenz systems and is expressed in units of the drive period for the pendulum.)

System¬	Δt	B
Rossler¬	0.01¬	2.00
	0.005¬	1.98
Lorenz¬	0.002¬	2.03
	0.001¬	1.94
Pendulum¬	0.001¬	1.98
	0.0001¬	2.11
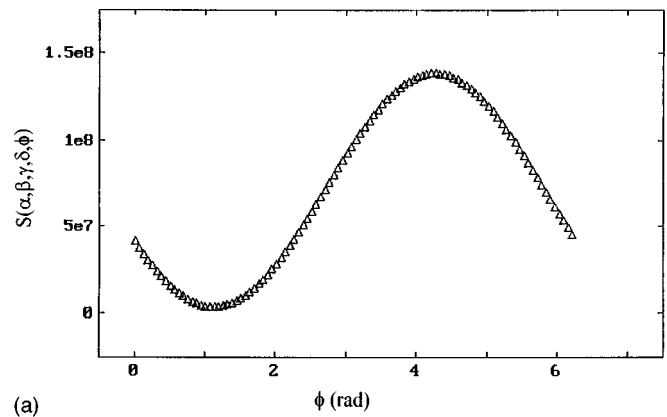
(a)
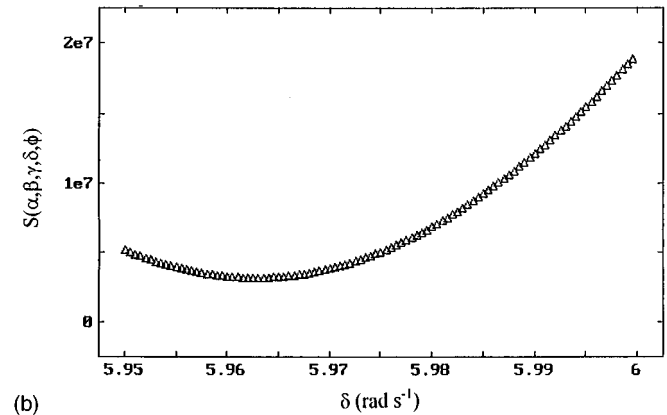
(b)

FIG. 3. (a) Least-squares sum plotted as a function of the initial phase φ for the experimental pendulum data. The minimum is fairly insensitive to initial estimates of α, β, and γ, and represents a first and close estimate to the final result of φ=1.05 rad. (b) The least-squares sum as a function of the angular forcing frequency δ for the experimental pendulum. The minimum has converged to the final result δ=5.9628 rad s^{-1}.

forcing frequency δ is first estimated using a fast Fourier transform. The power spectrum of the angular velocity has a strong maximum at 1.00 ± 0.05 Hz; this leads to an initial estimate of $\delta = 6.28 \pm 0.32$ rad/s that can then be used to determine a rough estimate of ϕ. The fitted value of ϕ is not sensitive to the choice of values for α, β, and γ, and therefore it is possible to look for a minimum in the ''least-squares'' function S [Eq. (12)] as a function of ϕ using somewhat arbitrary values of α, β, and γ, and the estimate of δ. The minimum in S is shown to be at φ=1.13 rad in Fig. 3(a). In the next iteration, these estimates for δ and ϕ and the minimization algorithm are used to determine the α, β, and γ more precisely. With the latter three values in hand the value of the forcing frequency δ can be refined further by looking for the minimum of S, as shown in Fig. 3(b). Then these four parameters can be used to further refine the fitted phase ϕ. This series of steps is iterated a few times (except for the initial spectral estimate for δ) to achieve convergence of the values of the parameters.

Figure 4 shows the attractor for the chaotic pendulum as drawn from 4800 experimental data pair sets $\{\theta_i, \omega_i\}$ with a time interval of Δt=0.007 s. For this data file the values of the parameters of the physical pendulum were determined
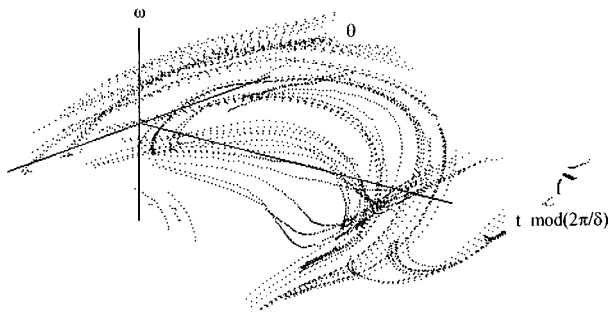
FIG. 4. Attractor of the experimental pendulum data. The fitted and experimental values for the parameters are compared in Table II. A numerically simulated attractor using the fitted values is shown in Fig. 1.

TABLE III. Comparison of invariants for the experimental attractor and a numerically generated attractor using parameters obtained by fitting the experimental data.

	Experimental data	Simulated using fitted parameters
Dimension¬	2.2±0.15¬	2.1±0.1
Lyapunov exponent¬	0.9±0.1¬	0.9±0.1

experimentally and are given in Table II. (The initial phase angle ϕ is not known for this file.)

The fitted values obtained by least-squares fitting are also given in Table II for comparison. The agreement is generally good (though not as good as for the numerical data of Sec. III), with the exception of β. The favorable comparison suggests that the method described in this paper shows promise for testing models to account for chaotic data when parameters are unknown. In general, parameters that appear nonlinearly must be treated by more sophisticated methods. One such method is the Levenberg–Marquardt technique.[12] With this technique one also minimizes a least-squares type of function but through an iteration technique, rather than analytically as in the ''linear'' parameter cases. However, the use of the power spectrum and ''manual'' iteration rendered the Levenberg–Marquardt method unnecessarily complex for the case of the chaotic pendulum.

While initial results for the fitted parameters seem promising and the attractors in Figs. 1 and 4 seem qualitatively similar, it would be useful to have more quantitative measures of the similarity of the simulated and experimental attractor. We compare some of these invariants in the next section.

VI. A COMPARISON OF INVARIANTS

Two attractors can be compared by considering their invariant properties such as the attractor dimension and values of the positive Lyapunov exponent. We compare these invariants for the attractors reconstructed from the experimental data (Fig. 4) and the numerical simulation (Fig. 1). For the experimental data we utilize the time series of the angular velocity. A three-dimensional space is sufficient for the embedding. The attractor dimension is calculated with the Grassberger–Procaccia algorithm.[13] Similarly, the positive Lyapunov exponent is evaluated using the method of Wolf et al.[14] Similar calculations are made for the simulation data with the phase data of the simulation using fitted parameters The results are shown in Table III. For the simulation we were also able to determine the other two Lyapunov exponents, $\lambda_2=0$ and $\lambda_3=-3.7\pm0.1$. Based on these numbers the Kaplan–Yorke dimension is found to be about 2.25 ± 0.1, a figure that is consistent with the results in the Table III.

While other methods for characterizing the attractor using periodic orbits can also be used,[15] the evidence at hand is perhaps sufficient to demonstrate that the model equation with fitted parameters obtained from the experimental data provides a good representation of the dynamics.

VII. DISCUSSION AND CONCLUSION

Other parameters may also affect the fitting process. These include (a) the number of data points and (b) the spacing between points that are sampled for use in the fitting process. For a *noise free* simulation we find that the goodness of fit, as measured by the parameter E, is relatively independent of both the number of points and the spacing between sampled points. A good fit can be achieved with less than ten sampled points from just a single forcing cycle or from up to 15 forcing cycles of the simulation of the chaotic pendulum. In contrast, when *noise* is added to the simulation, the goodness of fit depends strongly on the number of sampled points. Figure 5 shows the goodness of fit for two

TABLE II. Experimental values of the parameters of the pendulum, along with values obtained from the least-squares fitting procedure.

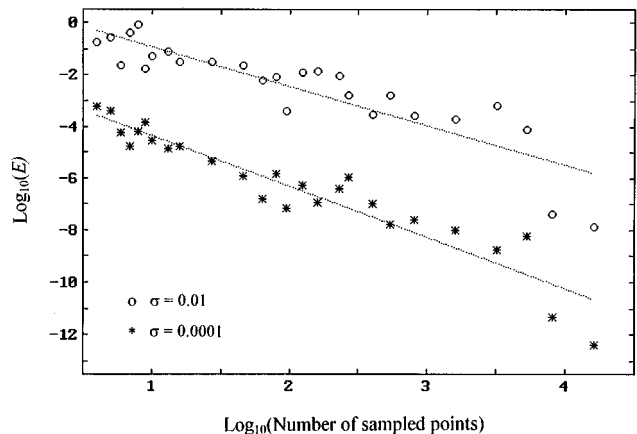| Parameter¬	Experimental value¬	Fitted (from experimental data)
α (rad s^{-1})	2.24±0.1¬	2.12
β (rad s^{-2})	80.6±0.1¬	76.1
γ (rad s^{-2})	121±6¬	117
δ (rad s^{-1})	5.98±0.02¬	5.96
ϕ (rad)	unknown¬	1.05

FIG. 5. Effect on E caused by varying the number of points sampled from two simulations of a noisy chaotic pendulum. Each simulation provided 16 000 points.

different noise levels. In each case the simulation was created with about 16 000 data points and the fit is made with various numbers of points sampled at regular intervals from the simulation. The general trend appears to be an approximate power-law relationship between E and the number of points sampled, but scatter precludes a more definitive statement. Nevertheless, it is clear that a high sampling rate is desirable in the presence of noisy data.

In conclusion, we have presented a method of testing the applicability of model ODEs to chaotic data. A least-squares process is used to determine the model parameters, and then the invariants of the resulting attractor are compared to those of the data. The method was tested on numerical data and on experimental data. It is found to be both accurate and fairly robust with respect to additive noise. The fitting process is especially straightforward when the system parameters enter linearly into the model differential equations, as they do in the case of the Rossler or Lorenz systems.

Whether a similar method will also work for spatiotemporal chaos described by partial differential equations remains to be seen. D. P. Vallette and one of the authors (JPG) have done preliminary work on a model for a Hopf bifurcation of a parity-invariant cellular pattern in one space dimension, which was motivated by experiments on the ''rimming flow'' of a fluid inside a horizontally rotating cylinder.[16] The model, originally proposed in another context by Daviaud et al.,[17] involves two coupled complex fields: the amplitude of oscillation $A(x,t)$ and the spatial phase $\phi(x,t)$ of the underlying cellular pattern. The fitting process is more complicated in this case, since both space and time derivatives must be computed from the data. The coefficients (in this case eight of them) can be quite accurately obtained from the numerical data.[18] On the other hand, the fitting process is much more sensitive to added noise than in the ODE examples discussed in this paper, so the possibility of using the method successfully on experimental spatiotemporal data is not yet clear.

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