Numerical Analysis of Dynamical Systems and the Fractal Dimension of Boundaries

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Abstract

A set of MapleV R.4/5 software routines for calculating the numerical evolution of dynamical systems and flexibly plotting the results is presented. The package consists of an initial condition generator (on which the user can impose quite general constraints), a numerical solving manager, plotting commands that allow the user to locate and focus in on regions of possible interest and, finally, a set of routines that calculate the fractal dimension of the boundaries of those regions. A special feature of the software routines presented here is an optional interface in C, permitting fast numerical integration using standard Runge-Kutta methods, or variations, for high precision numerical integration.

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PROGRAM SUMMARY

Title of the software package: Ndynamics.

Catalogue number: (supplied by Elsevier)

Software obtainable from: CPC Program Library, Queen’s University of Belfast, N. Ireland (see application form in this issue)

Licensing provisions: none

Operating systems under which the program has been tested: Linux (RedHat 5.2 and Debian 2.0.34), Windows 95, Windows 98.

Programming languages used: Maple V Release 4 and 5 and ANSI C.

Memory required to execute with typical data: 32 Megabytes.

No. of lines in distributed program, including On-Line Help, etc.: 1370.

Keywords: Dynamical systems, fractal dimension, symbolic computing.

Nature of mathematical problem
Computation and plotting of numerical solutions of dynamical systems and the determination of the fractal dimension of the boundaries.

Methods of solution
The default method of integration is a 5th order Runge-Kutta scheme, but any method of integration present on the MAPLE system is available via an argument when calling the routine. A box counting method is used to calculate the fractal dimension of the boundaries.

Restrictions concerning the complexity of the problem
Besides the inherent restrictions of numerical integration methods, this first version of the package only deals with systems of first order differential equations.

Typical running time
This depends strongly on the dynamical system. With a Pentium II 450 PC with 128 Mb of RAM, the integration of one graph (among the thousands it is necessary to calculate to determine the fractal dimension) takes from a fraction of a second to several seconds. The time for plotting the graphs depends on the number of trajectories plotted. If there are a few thousand, this may take 20 to 30 seconds.

Unusual features of the program
This package provides user-friendly software tools for analyzing the character of a dynamical system, whether it displays chaotic behavior, etc. Options within the package allow the user to specify characteristics that separate the trajectories into families of curves. In conjunction with the facilities for altering the user’s viewpoint, this provides a graphical interface for the speedy and easy identification of regions with interesting dynamics. An unusual characteristic of the package is its interface for performing the numerical integrations in C using a 5th order Runge-Kutta method. This potentially improves the speed of the numerical integration by some orders of magnitude and, in cases where it is necessary to calculate thousands of graphs in regions of difficult integration, this feature is very desirable.
1 Introduction

A large number of problems in physics, chemistry, etc., can be represented in terms of a set of differential equations, which constitute a (very often nonlinear) dynamical system. Among these systems of interest, autonomous dynamical systems are particularly common. A $d$-dimensional autonomous dynamical system can be represented by

$$\frac{d\mathbf{X}(t)}{dt} = \mathbf{F}(\mathbf{X}),$$

where $\mathbf{X} = (X_1(t), X_2(t), \ldots, X_d(t))$ and $\mathbf{F} = (F_1(\mathbf{X}), F_2(\mathbf{X}), \ldots, F_d(\mathbf{X}))$. The $X_i(t)$, with $i = 1, \ldots, d$, represent field variables, usually related to quantities associated with the specific problem under consideration, $t$ is a continuous parameter, which can often be considered as the time, while the functions $F_i(\mathbf{X})$, $i = 1, \ldots, d$, are general functions of their arguments. The $d$-dimensional space constituted by the $X_i(t)$ is called the system’s phase space, with trajectories in this phase space representing the solutions of (1). It is possible to interpret the trajectories generated by all the initial conditions in phase space as analogous to the paths followed by the particles of a flowing fluid with velocity field $\dot{\mathbf{X}}$, where an overdot represents a derivative with respect to $t$. If $F_i = F_i(\mathbf{X}, t)$, the system is said to be a non-autonomous dynamical system. However, introducing a new variable $X_{d+1} = t$, the $d$-dimensional non-autonomous dynamical system can be transformed into a $(d+1)$-dimensional autonomous system. An autonomous system is said to be Hamiltonian if (1) represents the set of Hamilton’s equations and the phase space has a simplectic structure. Otherwise we have a dissipative or non-Hamiltonian system. In this case, volumes in phase space are not conserved, or, equivalently, $\nabla \cdot \dot{\mathbf{X}} = \nabla \cdot \mathbf{F} \neq 0$.

Consider a general nonlinear autonomous dynamical system with dimension $d \geq 3$. Among these systems those exhibiting chaotic behavior have assumed particular interest and constitute a rule than an exception. Roughly speaking, chaos means extreme sensitivity to small changes in the initial conditions. Due to nonlinearity, fluctuations in the initial conditions of chaotic systems evolve such that they can completely alter the asymptotic outcome of the unperturbed trajectories in phase space. There are several ways of analyzing chaos in dynamical systems, such as the Lyapunov exponents or the technique of Poincaré surface of sections for Hamiltonian systems. (For good reviews and books on chaotic dynamical systems see, for instance [1, 2].) We are particularly interested in certain features underlying chaotic dynamical systems, namely sets characterized by a non-integer dimension. Such sets are known as fractals. In the realm of dissipative systems, attractors with fractal properties have been called strange attractors, whereas in Hamiltonian systems there exist the strange repellers [3], identified as repellers with fractal properties. An important numerical task in investigating chaotic behavior in dynamical systems is therefore the determination of the fractal dimension [2].

The presence of fractals is related to chaos, and so these structures are also associated with sensitivity to small changes in initial conditions. To show this relation, we follow closely the procedure of [4]. Let us consider a non-fractal basin boundary $\Sigma$ that separates two attractors $A_-$ and $A_+$, usually fixed points (this will be explained further in section 3).
An uncertainty in our initial condition \( X(t_0) = X_0 \) that has strength \( \epsilon \) means that the initial condition lies somewhere in the region \( |X - X_0| \leq \epsilon \). According to Figure 1, given an uncertainty \( \epsilon \), the initial condition 1 always goes to the attractor \( A_+ \). On the other hand, since the point 2 lies near the boundary \( \Sigma \), due to the uncertainty \( \epsilon \) the actual trajectory may go to either attractor \( A_+ \) or attractor \( A_- \). The initial condition 1 is said to be \( \epsilon \)-certain, and the initial condition 2 is \( \epsilon \)-uncertain. Obviously, \( \epsilon \)-uncertain initial conditions are those which lie within a distance \( \epsilon \) of the basin boundary \( \Sigma \). Let us call \( f(\epsilon) \) the probability of obtaining an \( \epsilon \)-uncertain initial condition, in the sense that it is the fraction of the \( d \)-dimensional volume of the phase space which lies within \( \epsilon \) of the boundary \( \Sigma \). In the case of a simple non-fractal boundary, \( f(\epsilon) \sim \epsilon \). This scaling law tells us that an improvement in the accuracy of the initial condition by, say, a factor 10 (a reduction of \( \epsilon \) by 10), reduces \( f(\epsilon) \), and hence our probability of potential error, by a factor of 10. For the case of a fractal boundary the scaling law (see Appendix)

\[
f(\epsilon) \sim \epsilon^\alpha
\]

is valid, where \( \alpha \) is the uncertainty exponent. The box-counting dimension of the basin boundary, \( D_0 \), is given by

\[
D_0 = d - \alpha ,
\]

with \( d \) denoting the dimension of the phase space. For a fractal boundary, \( D_0 > d - 1 \), implying that \( \alpha < 1 \), whereas for a non-fractal boundary, \( D_0 = d - 1 \), and \( \alpha = 1 \). Suppose that, for instance, \( \alpha = 0.2 \) and \( f(\epsilon) \sim \epsilon^{0.2} \). Then, in order to reduce the probability of error \( f(\epsilon) \) by a factor of 10, a reduction of \( \epsilon \) by an order of \( 10^5 \) is needed. The improvement in prediction by increasing the accuracy of the initial conditions is seen to be less favorable the smaller \( \alpha \) is.

Related to the above discussion, this paper presents a set of software routines, implemented in MapleV R.4/5, together with an optional interface in C for fast numerical integration, which, among other things, calculates the dimension of the fractal basin boundary. The main goal is to determine numerically the scaling law (2) and therefore the fractal dimension. Consider an initial condition \( X_0 \) and perturb one of the coordinates, say \( X_k \), in order to obtain two initial conditions \( X - \epsilon \) and \( X + \epsilon \). By integrating numerically we can determine to which attractor or asymptotic state both of the perturbed initial conditions goes. We call the original initial condition uncertain if the perturbed initial conditions have distinct attractors. If a large number of initial conditions are chosen randomly in a given region of the phase space, it is possible to determine the fraction \( \overline{f}(\epsilon) \) of these that are uncertain, where \( \overline{f}(\epsilon) \) is the ratio between the number of uncertain conditions and the total number of initial conditions. This process can be repeated for several values of \( \epsilon \). According to Bleher et. al. in [4], the quantities \( f(\epsilon) \) and \( \overline{f}(\epsilon) \) are proportional, so that the parameter \( \alpha \) can be determined by the scaling of \( \overline{f}(\epsilon) \) with \( \epsilon \).

The package has the following features:

- user-friendly software tools for fast numerical integration of both Hamiltonian and non-Hamiltonian dynamical systems, as well as a set of commands for the flexible presentation of the results;
- an optional C interface for fast high-precision numerical integration;
• tools for determining sets of initial conditions that satisfy given constraints, expressed, e.g., as $g(X_1, X_2, \ldots, X_d) \geq 0$, where $g(X_1, X_2, \ldots, X_d)$ is a given function of $X_i$, $i = 1, \ldots, d$;

• the ability to perform combined symbolic and numerical studies by implementing these software tools in a symbolic computing environment.

The paper is organized as follows: in section 2 we give a summary of the package’s commands, followed by a detailed description of its most relevant commands, mainly Nsolve, for the generation of initial conditions and numerical integration of the system allowing 2D or 3D plots, View, for changing the ranges of all variables (including the time) and Fdimension, to determine the dimension of the fractal basin boundary; section 3 illustrates the application of various commands of the package to two examples with known results already presented in the literature; section 4 analyzes the performance of the various integration schemes, and section 5 contains some concluding remarks.

2 The Ndynamics package

Basically the Ndynamics package consists of a set of routines for calculating the numerical evolution of dynamical systems and plotting the results. The package generates initial conditions in a user-defined region, subject to constraints provided by the user. After calculating the evolution of each trajectory, the user may use its plotting commands to locate possible regions of interest — regions where the system presents chaotic behavior, and so on. Finally, a set of routines is available to calculate the fractal dimension of the boundaries using box-counting algorithms.

Summary

A brief review of the commands of the package is as follows:

• Nsolve takes as arguments a dynamical system, the ranges of the initial conditions (from which it generates the initial conditions), the range for the time (independent variable), and the time step to be used when plotting the associated trajectories. The variables to be included in the final plot (which can be 2D or 3D) must also be defined;

• View generates a plot from points already calculated, allows the user to modify the ranges for all the variables (including the time), and to swap between 2D and 3D plots;

• Boxcount applies the box counting algorithm to determine the number of hypercubes of side $\epsilon$ (see the introduction) covering the boundary;

• Fdimension uses Boxcount for many values of $\epsilon$ to calculate the fractal dimension of the boundary.

Aside from this, the package itself contains on-line help in standard Maple format which can be viewed as the user’s manual for all the routines.

This subsection and the next one may contain some information already presented in the previous sections; this is necessary to produce a self-contained description of the package.
Description

A complete description of the *Ndynamics* package's commands is found in the on-line help. Here we present the most relevant part of that description.

2.1 Command name: Nsolve

*Feature:* plot 2D/3D graphs calculated for a set of initial conditions, generated by the program, within ranges defined by the user.

*Calling sequence:*

\[
> \text{Nsolve}(\text{sys}, \left[\text{dep_ranges}, \left[\text{indep_range}, \text{plotstep}\right]\right], \text{Frame}, \text{optional\_parameters});
\]

*Parameters:*

- **sys** - a set of first order ordinary differential equations.
- **dep_ranges** - a list with the ranges for the dependent variables in the format: 
  \([x=a..b, y=c..d, ...]\), where \(x, y\) are the dependent variables and 
  \(a..b, c..d\), are the ranges in which the initial conditions will be 
  generated.
- **indep_range** - the range for the independent variable: \(t=t1..t2\), where \(t\) represents 
  the independent variable.
- **plotstep** - a numerical value defining the interval (in the independent variable) 
  for the plot.
- **Frame** - a list with the variables to be plotted.

*Optional Parameters:*

- **initial** - Forces the command to stop after generating the initial 
  conditions.
- **random** - Tells the program to generate the initial conditions 
  randomly.
- **diagonal** - Makes the program look for the initial conditions 
  along the main diagonal of the hypercuboid defined by 
  the ranges of the dependent variables.
- **method=option** - Indicates which numerical method of integration will 
  be used, where **option** can be any one of the options 
  available to *dsolve* in MAPLE (see the associated help).
- **method=[rk5C,number]** - Tells the program to generate the C code and manage the 
  interface to the C routines, which use a 5th order Runge- 
  Kutta method to integrate the equations more rapidly. The 
  parameter **number** defines the integration step (constant).

*Synopsis:*

The *Nsolve* command is a part of the *Ndynamics* package, which, to brutally sum- 
marize things, is designed to calculate the fractal dimension of boundaries. The command 
that actually does this is *Fdimension*. In order to calculate this dimension, the process

\[4\text{In what follows, the *input* can be recognized by the Maple prompt } >.\]
involves the demarcation of dynamically interesting regions of the system being studied. This demarcation is achieved by running \texttt{Nsolve} and looking for such regions by analyzing the resulting graphs. To facilitate this, \texttt{Nsolve} is designed to calculate and plot the trajectories associated with a given system of differential equations, subject to constraints and adjustments which can be tailored to the specific search at hand. In order to control and customize the output of \texttt{Nsolve}, we have introduced the global and environment variables described below.

\begin{itemize}
  \item Global Variables
    \begin{enumerate}
      \item \texttt{Coloring}
      \item \texttt{constraint}
      \item \texttt{initial\_conditions}
      \item \texttt{number\_ic}
      \item \texttt{initial\_time}
    \end{enumerate}
\end{itemize}

The first item above controls in which color a trajectory will be displayed. \texttt{Coloring} is a boolean condition that is applied to the last calculated point of each trajectory so that different trajectories are displayed in one of two colors, corresponding to the cases where \texttt{Coloring} is true or false. \texttt{Coloring} defines the boundary, since it is defined to discriminate trajectories on either side of it. If \texttt{Coloring} is not assigned, then the command uses a default setting, which produces a plot with a certain color pattern. This is useful when the criteria to define the boundary have not yet been decided, but it is desirable, perhaps for the purposes of defining these criteria, to see the general flow of the trajectories.

The second item, \texttt{constraint}, is a variable that defines the constraints imposed upon the initial conditions. All initial conditions generated will satisfy these constraints. This variable can be any valid boolean Maple condition. For instance, it may be two (or more) simultaneous conditions, such as $100 > x^2 - y^2 + z^4 > 20$, where $x, y, z$ are dependent variables of the differential system. This variable does not have a default value and can be left unassigned, in which case the command freely generates the initial conditions inside the hypervolume defined by the dependent variable ranges.

Item number 3 is a facility that allows the user to supply the program with specific initial conditions. If this global variable is assigned, the program skips the part that generates the initial conditions and uses those supplied by the user. Its syntax is the same as that produced by the program with \texttt{initial\_conditions} unassigned. We refer the reader to the on-line help that comes with the package for this syntax.

In the case that \texttt{initial\_conditions} is not assigned by the user, the global variable \texttt{number\_ic} has to be defined, otherwise the program issues an error message. As the name suggests, it defines the number of initial conditions to be generated.

Finally, the global variable \texttt{initial\_time} allows the user to define the initial value for the independent variable to be anywhere in the interval stipulated for its range.\footnote{In the present version, when using the C interface, this facility is not available.}
The integration of the trajectory is then performed in both directions, up to the limits of the time range.

- Environment Variables

To customize the interface between the program and the user, the following environment variables were introduced:

1. \texttt{Env\_print},
2. \texttt{Env\_store}.

\texttt{Env\_print} controls the level of printing during the execution of the command. When set to zero, no printing takes place; if \texttt{Env\_print} =1, (the default value) basic messages are printed; when set to 2, time-counting messages will be printed and, finally, for the value 3 all possible messages are printed.

The variable \texttt{Env\_store}, controls in which file the results will be stored. The initial conditions, the range for the variables, the differential equation system, etc., are, by default, stored in a file called usedata1 and the calculated points (trajectories) are stored (by default) in a file called usedata2. This arrangement is fine if only one process is running at a time. It will, however, result in file conflicts if the user wishes to perform simultaneous runs of the program from the same directory. The assignment of \texttt{Env\_store} by the user to the desired filenames avoids such problems.

\textit{The arguments}

The first argument of \texttt{Nsolve} is a set containing the system of differential equations. In the present implementation, the program only deals with first order ordinary differential equations (ODEs). This is not a major drawback, since all systems of ODEs can be put into this form. The second argument is a list in which the first element is itself a list giving the ranges of the dependent variables. The second element is a list containing the range of the independent variable and the step (for that variable) for printing the graphs. The third argument gives the variables to be plotted (this can be two or three variables). Finally there are the optional arguments.

\textit{The optional arguments}

The optional arguments can be given alone or in conjunction and in any order. By default, \texttt{Nsolve} takes care of everything for the user — it generates the initial conditions and fully integrates the system. If the optional argument initial is given then it stops after calculating (and saving in the appropriate file) the initial conditions.

The optional arguments random and diagonal act similarly. There are thus three ways in which the command may generate the initial conditions in the hypercuboid defined by the dependent variable ranges. The default is to produce initial conditions homogeneously throughout the hypercuboid. However, if the argument random is used then the initial conditions will be randomly distributed inside hypercuboid. If, instead, diagonal is used, all conditions will be generated along the main diagonal\footnote{By “main diagonal” we mean the straight line inside the hypercuboid which joins the point defined by the minimum value of the ranges of the independent variables to the point defined by the maximum values of those ranges.} of the region.
Many different algorithms can be used to numerically integrate the system. Maple provides a great variety of these and all of them can be used with our command, via the option method. For example, if method=classical[rk2], the second order Runge-Kutta method will be used.

Apart from the numerical methods available in the MAPLE system, our program has a further possibility: a C-based numerical integrator. The only additional requirement for this is that the machine where the program is being run has a C compiler. In this case, the integrator is a fixed-step fifth order Runge-Kutta scheme based on the procedure RKQC in [3]. The idea behind this option is to gain speed over Maple’s interpreted procedures, thereby combining the flexibility of the symbolic environment with the efficiency of the compiled C routine (see section 1 for comparisons). It is our intention to introduce more compilable algorithms in later releases.

2.2 Command name: View

Feature: This command allows easy and efficient viewing of different parts of the trajectories calculated by Nsolve, allowing the user to zoom in and out, and to change the variables being viewed (if necessary the user can even swap between 2D and 3D plots).

Calling sequence:

> View(list_range);

Parameters:

list_range - a list with the new ranges of those (two or three) variables
the user wants to view in detail. The format is: [x=a..b, y=c..d, ...],
where x, y are (dependent or independent) variables and a..b, c..d,
their ranges.

Synopsis:

The importance of this command lies in the search for the relevant regions for studying the system’s behavior. The user generally starts by running Nsolve in a broad region of the variable space and then studying more closely the regions, for example, where chaos is suspected. The graphs that View produces (2D or 3D) do not need to display the same variables that Nsolve uses in its argument Frame.

2.3 Command name: Boxcount

Feature: this command analyzes the effect of a small perturbation on the initial conditions on the fate of a bundle of trajectories.

Calling sequence:

> Boxcount(epsilon, final_time, optional_parameters);
Parameters:
epsilon - defines the size of the perturbation around each initial condition.
final_time - indicates the final value of the independent variable.

Optional Parameters:
method=option - Indicates which numerical method of integration will be used, where option can be any one of the options available to dsolve in MAPLE (see the associated help).
method=[rk5C,number] - Tells the program to generate the C code and manage the interface to the C routines, which use a 5th order Runge-Kutta method to integrate the equations more rapidly. The parameter number defines the integration step (constant).

Synopsis:
Suppose we have generated a set of initial conditions (see 2.1). Boxcount perturbs each of these initial conditions within a neighborhood of radius = \( \epsilon \). For points sufficiently close to the boundary (that separates the different end-point behaviors) the two perturbed trajectories will have different fates. Boxcount then counts the number of initial conditions for which the pairs of perturbed trajectories evolve to different attractors.

2.4 Command name: Fdimension

Feature: Fundamentally applies Boxcount a user-defined number of times, with a different value of \( \epsilon \) each time.

Calling sequence:
> Fdimension(epsilon_range, TF, Nepsilon, optional_parameters);

Parameters:
epsilon_range - defines the range of variation of \( \epsilon \).
TF - indicates the final value of the independent variable.
Nepsilon - indicates how many values of \( \epsilon \) will be considered in epsilon_range.

Optional Parameters:
savefile=filename - Indicates in which file the results will be stored. The default value of filename is XY-file. Since Fdimension makes many calls to Boxcount, only the pairs of data \( \epsilon \), and the logarithm of the ratio of the number of initial conditions on the boundary to the total number of initial conditions (see appendix A) are saved to the file.

method=option - Indicates which numerical method of integration will be used, where option can be any one of the options available to dsolve in MAPLE (see the associated help).
method=[rk5C,number] - Tells the program to generate the C code and manage the interface to the C routines, which use a 5th order Runge-Kutta method to integrate the equations more rapidly. The parameter number defines the integration step (constant).
Synopsis:

Fdimension essentially implements the box-counting process in our program. It uses Boxcount to evaluate the number of points on the boundary for many values of $\epsilon$ thus calculating the fractal dimension of the boundary (using the method described in appendix A).

3 Examples

To illustrate the routines presented in the previous section we consider the well-known Lorenz system:\[6\]:

\[
\begin{align*}
\dot{x} &= \sigma(y - x), \\
\dot{y} &= -y - xz + Rx, \\
\dot{z} &= xy - bz,
\end{align*}
\]

(4)

where $\sigma$, $R$ and $b$ are constant parameters of the problem. $R$ plays a crucial role as far as the dynamics of phase space is concerned. A simple analysis shows the presence of three critical points (the points satisfying the conditions $\dot{x} = \dot{y} = \dot{z} = 0$): the origin $P_0(0, 0, 0)$ and, provided $R > 1$, two further points are symmetrical with respect to the $z$-axis, $P_{\pm} = (\pm \sqrt{b(R - 1)}, \pm \sqrt{b(R - 1)}, R - 1)$. The stability properties of these critical points depend only on $R$, so that we set $\sigma = 10$ and $b = 8/3$. We summarize the behavior of the solutions of the Lorenz system for distinct values of $R > 1$ that will be important in the applications of the routines and commands we have described. For $1 < R < 24.74$ the origin $P_0$ is unstable and $P_{\pm}$ are attracting stationary solutions, therefore representing two possible asymptotic configurations (except for the set of trajectories of measure zero that stay in the neighborhood of $P_0$). However, around the critical value, $R_c \approx 13.926$, $P_0$ develops into a homoclinic point such that, above this value, the basins of attraction around $P_-$ and $P_+$ are no longer distinct. This means that trajectories can cross backwards and forwards between the two before settling down. Another transition occurs when $R \approx 24.74$, for which $P_-$ and $P_+$ become unstable. Lorenz considered $R = 28$ and obtained a remarkable behavior displaying for the first time a strange attractor. As we shall show, the dynamics are highly erratic: a given trajectory can spiral around one of the critical points, $P_+$ or $P_-$, for some arbitrary period then jump to the neighborhood of the other critical point, spiral around that for a while and then jump back to the first one, and so on.

In Figure 1 we show the form of the trajectories for the Lorenz system, with coefficients $\sigma = 10$, $b = 8/3$ and $R = 20.06$. We are therefore inside the parameter range for erratic behavior discussed above. We see that, given enough time (in our case $\geq 50$ units of time), the trajectories settle down around one of the two possible asymptotic points, $P_{\pm}$. Figure 1 was obtained with 10 initial conditions, $(x_0, y_0, z_0)$, that were randomly chosen in the volume of phase space defined by $0.9 < x_0 < 1.1$, $0.9 < y_0 < 1.1$ and $21.9 < z_0 < 22.1$. This is our first illustration of the application of Nsolve. Figure 1 was obtained using the set of commands below. First, we set the accuracy, read the program and define the system:
Digits := 16;
with(Ndynamics);

Boxcount, Fdimension, Nsolve, View

sigma:=10.0: b:=8.0/3: R:=20.06:

Lorenz:={diff(x(t),t)=sigma*(y(t)-x(t)),
  diff(y(t),t)=-x(t)*z(t)+ R*x(t)-y(t),
  diff(z(t),t)=x(t)*y(t)-b*z(t)};

Note that the integers in (4) have been swapped for floating-point numbers. This is important in the case of the parameter \( b \) to avoid truncated integer division occurring in the C subroutines generated.

We then define the input:

x_range := 0.9..1.1: y_range := 0.9..1.1: z_range := 21.9..22.1:
t_range := 0..50:
plot_spacing := 0.03:
Frame := [x(t),y(t),z(t)]:

Now we can call Nsolve:

graph := Nsolve(Lorenz,[[x=x_range,y=y_range,z=z_range],
  [t=t_range,plot_spacing]],Frame,method=[rk5C,time_step]):

The use of Nsolve above illustrates the application of the global variable Coloring. Here we have based the choice of color by specifying the approximate location (x coordinate) of one of the asymptotic points \( P_\pm \). Trajectories ending around this point are colored green, while trajectories ending around the other critical point are colored black. Using Display(graph) gives the result shown in Figure 1.

In this paper we take as a measure of the degree of chaos of a dynamical system, such as the Lorenz system above, the fractal dimension associated with the possible different exit modes under small changes of initial conditions, as discussed in section 1. A note here is in order about our criterion for choosing the intervals between the values of \( \epsilon \) (the variations for the initial conditions as explained in section 2.4). Given ranges for the initial conditions which define a hypervolume \( V_{ic} \) in \( d \) dimensions, and distributing \( N_{ic} \) initial conditions throughout this volume, the largest \( \epsilon \) cannot exceed the average distance \( \bar{l} \) between the initial conditions, since otherwise the “perturbation” \( \epsilon \) for different initial conditions will overlap leading to loss of predictability of the fractal dimension. We take for \( \bar{l} \) the minimum distance between two initial conditions for a uniform distribution, which is easily deduced to be
\[
\bar{l} = \frac{V_{ic}^{1/d}}{N_{ic}^{1/d} - 1}.
\]

In all the numerical tests performed the largest value for \( \epsilon \) is of the order of \( \bar{l} \). The lowest value for \( \epsilon \) used is determined by the statistical error associated with the number of initial conditions \( \bar{N} \) falling inside the fractal boundary. We then have that \( \bar{N}^{1/2} \) will give the statistical uncertainty associated with the probability \( f = \bar{N}/N_{ic} \) of a given initial condition falling within the boundary \([4]\). The numerical tests performed have values of \( \epsilon \) and \( N_{ic} \) such that \( \bar{N} \geq 400 \), thus assuring an estimated error (\( \sqrt{N}/N \)) of at most 5\% in the determination of \( f \).

The fractal dimension can be readily obtained by using the command \texttt{Fdimension}. We begin by generating the initial conditions as explained in section 2.1:

\[
> \text{number_ic} := 10000:
> \text{Nsolve}(\text{Lorenz},[x=x\_range,y=y\_range,z=z\_range],
> \quad \text{[t=t\_range,plotting\_spacing]],[\text{Frame,initial}]):
\]

Note that 10000 initial conditions are used. By omitting the optional parameter \texttt{random} (see section 2.1), these \texttt{number_ic} initial conditions are uniformly distributed throughout the interval volume \( V_{ic} = (0.2)^3 \) defined by the dependent variable ranges. The use of random initial conditions leads to no appreciable change in the results, which always remain within the statistical error defined above. Values of \( \epsilon \) ranging from \( 10^{-5} \) to \( 10^{-4} \) were used in \texttt{Fdimension} when computing the fractal dimension. An easy way to check the number of initial conditions, \( \bar{N} \), which are generated inside the basin boundary is by using \texttt{Boxcount}. For example, having generated 10000 initial conditions, we can use:

\[
> \text{Boxcount}(0.00001, 60, \text{method=[rk5C,0.01]});
\]

From the 10000 points (that were testable), 2202, were close to the boundary.

\[
[2202,10000]
\]

tells us that, for the \( N_{ic} = 10000 \) initial conditions and for \( \epsilon = 10^{-5} \), \( \bar{N} = 2202 \) initial conditions are around the boundary, with a resulting statistical error of around 2\%. If we decrease \( \epsilon \), say to \( 10^{-10} \), we get instead \( \bar{N} = 551 \), and the statistical error is of the order of \( N^{-1/2} \approx 4\% \), close to the 5\% limit of acceptability which we have imposed. Accordingly, for smaller values of \( \epsilon \) we must increase the number of initial conditions in order to assure that we have at least the minimum number of initial conditions on the boundary necessary for statistical acceptability. With this done, the fractal dimension is then obtained by issuing the command:

\[
> \text{Fdimension}(0.00001..0.0001, 60, 10, \text{method=[rk5C,0.01]});
\]

where we are evolving the trajectories through 60 units of time and we are taking 10 equally spaced points in the range \( \ln(10^{-5}) \) to \( \ln(10^{-4}) \). The results obtained are shown in Figure 2 in terms of the logarithm of the number of uncertain initial conditions, (those that change their fate, or “color” on the graph), against \( \ln(\epsilon) \). The slope of the best-fit
straight line through the points gives the number $\alpha$ (see Appendix). The fractal dimension is then defined from (3) as $D_0 = d - \alpha$. We obtain for the fractal dimension the result $D_0 \simeq 2.87 \pm 0.01$, in complete agreement [7] with the known result for the Lorenz system for the choice of parameters $\sigma = 10$, $b = 8/3$ and $R = 20.06$.

In Figure 3 we once again compute the fractal dimension with $\text{Fdimension}$, but with $10^{-8} \leq \epsilon \leq 10^{-7}$. The result is the same up to statistical error.

As a further check of our set of routines, we evaluate the fractal dimension for the set of parameters $\sigma = 10$, $b = 8/3$ and $R = 10$, in the parameter region prior to the onset of transient chaos [2]. Using $\text{Fdimension}$, with $5 \times 10^{-3} \leq \epsilon \leq 9 \times 10^{-3}$ (an interval that ensures the minimum statistical error), we obtain the result shown in Figure 4, from which we conclude that $D_0 \simeq 1.98 \pm 0.05$. Further refinements of this result for a larger number of initial conditions leads us to conclude that $D_0 = 2$ and $\alpha = 1$ and that, as expected, there is no chaos for this choice of parameters.

As a demonstration of the use of $\text{View}$, we illustrate the basin-boundary in the two cases analyzed above. Figure 5 shows the case $R = 10.00$ while Figure 6 illustrates the results for $R = 20.06$. In both cases $\text{numberic}$ is taken to be 100.

The arguments to $\text{View}$ are $[x = -0.1..0.1, y = -0.1..0.1, z = 0.9..1.1]$ (for Figure 5) and $[x = 0.9..1.1, y = 0.9..1.1, z = 21.9..22.1]$ (for Figure 6). From Figure 5 we easily identify a well-defined (non-fractal) boundary separating the sets of initial conditions whose associated trajectories approach $P_+$ and $P_-$. In contrast we see in Figure 6 that neighboring initial conditions may lead to very different end-states. This is the fractal basin boundary discussed in the introduction.

4 Performance

To point out the advantages of our hybrid symbolic/numeric approach, which uses Maple to manage the source code generation and compilation for the number crunching, while maintaining Maple’s flexibility, table [4] presents a comparison of the elapsed time taken to perform the same calculation using the C interface and performing the entire calculation in Maple, using some of its numerical integration routines. To obtain a fair comparison particular care was taken to use methods of the same order and adjusting parameters to produce solutions with the same precision. The following procedure was used: for a given set of initial conditions, namely $x_0 = 0.679149319354506$, $y_0 = -0.5692394267519960$, $z_0 = 22.00017552807044$), Maple’s inbuilt high-precision Taylor Series integrator was used to integrate system (4) from $t = 0$ to $t = 11$ until convergence was obtained to an accuracy of 13 decimal places; subsequently Maple’s global variable $\text{Digits}$ was set equal to 13 (higher values of $\text{Digits}$ seemed to cause problems with Maple’s integrator), and Maple’s inbuilt 5th order Runge-Kutta-Fehlberg integrator, $\text{rkf45}$, was used up to $t = 11$. This integration was found to be accurate to 4 decimal places. The step size in the C routine was then adjusted to give the same precision, resulting in a step size of 0.002. An average was then taken for 200 integrations.

The results below were obtained with Maple V.4 running in Windows 98 on an AMD-K6 266 with 64Mb of SDRAM. The C compiler used was Delorie’s implementation of GNU’s gcc, available form www.delorie.com, with level 3 optimization.

\[\text{in fact, the C routine was slightly more precise}\]
| Integration Method | C-interface | Maple |
|-------------------|-------------|-------|
| rk5               | 0.1         | 7.0   |
| rkf45             |             | 70    |

Table 1: Comparative performances of Maple’s inbuilt numerical integrators and our C interface for the Lorenz system.

5 Conclusions

We have presented a set of software tools which allow great flexibility for the analysis of dynamical systems composed of first-order ordinary differential equations. Even though the construction of these programs was mainly motivated by the computation of fractal dimensions of basin boundaries of chaotic systems, this is not their only use, as was highlighted in the previous section. Large regions of phase space can be readily studied with a fairly large number of initial conditions, allowing the user to quickly find regions of interesting behavior.

The optional numerical interface allows for faster numerical integration than with Maple’s internal routines. The ease of use of the Maple software is thus combined with a faster numerical interface (here implemented in C, though this can be easily modified to use routines written in other languages such as Fortran), thereby allowing intensive numerical study of dynamical systems.

A Fractals

A.1 Fractal Dimension

The idea of a fractal is hard to define precisely. But, when we refer to a set $F$ as a fractal, we typically have the following in mind:

1. $F$ has a “fine structure”, i.e., detail on arbitrarily small scales;
2. $F$ is too irregular to be described in traditional geometrical language, both locally and globally;
3. often $F$ has some form of self-similarity, perhaps approximate or statistical;
4. usually the “fractal dimension” of $F$ (defined in some way) is greater than its “topological dimension”;
5. in most cases of interest, $F$ is defined in a very simple way, perhaps recursively.

There are many ways to define the dimension of a fractal. An important one is the Hausdorff dimension — one possible generalization of the “primitive” notion of dimension.

Suppose that we have a hypercube of side $a$. Its hypervolume is
\[ H_v = a^d, \]  

where \( d \) is the dimension of the hyperspace.

If we divide the hypervolume into \( N \) hypercubic cells of side \( \epsilon \), we have that

\[ H_v = N \epsilon^d. \]  

Dividing (7) by (6) we obtain

\[ 1 = N \left( \frac{\epsilon}{a} \right)^d. \]  

Defining \( \delta \equiv \epsilon/a \) and noticing that the number of cells is a function of \( \delta \) (\( N = n(\delta) \))

\[ 1 = n(\delta) \delta^d. \]

Taking logarithms of both sides of (9) and solving for \( d \), we obtain the standard definition of dimension:

\[ d = -\frac{\ln(n(\delta))}{\ln(\delta)}. \]  

Suppose now that we want to measure the dimension of a Cantor set, constructed as follows (see figure):

We take each segment (figure 7A), divide it into three equal parts, remove the middle segment and replace it with two other segments of the same length (figure 7B), repeating this procedure \textit{ad infinitum} (figure 7C, ..), one gets (figure 7D).

To cover the Cantor set (figure tal n) with segments it would be necessary to use an infinitesimal \( \epsilon \), implying that \( \delta \to 0 \). Hence the analogue of equation (10) would be

\[ d = -\lim_{\delta \to 0} \frac{\ln(n(\delta))}{\ln(\delta)}, \]  

which is the Hausdorff dimension.

In the Cantor set above we can easily determine the value for the limit on (11):

\[ d = -\frac{\ln(4)}{\ln\left(\frac{1}{3}\right)} \sim 1.26. \]

A.2 Fractal Dimension of Boundaries

Consider a \( d \)-dimensional finite region \( R \), and a subset \( S \subset R \). How can we determine the fractal dimension of \( S \), given some criteria as to whether a point of \( R \) belongs to \( S \) or not?

One possible way to determine the fractal dimension of \( S \) is as follows. Without loss of generality, let us suppose that \( R \) is a hypercube of side \( a \). Dividing \( R \) into \( N \) hypercubic “cells” of side \( \epsilon \), and evaluating the number of cells \( N_s \) that contain points belonging to the subset \( S \) we expect that for \( \delta \ll 1 \) we have a good approximation to the exact result given in (11).

However the number of cells

\[ N = \delta^{-d} \]  

(13)
rapidly increases as $\delta \to 0$, and this approach becomes impractical. An alternative approach is that of selecting $N^*$ random cells in $R$ and counting the number of cells $N_s^*$ that have points belonging to $S$. We expect that

$$\frac{N_s^*}{N^*} \to \frac{N_s}{N}$$

as $N^*$ becomes statistically sound. Supposing that, indeed,

$$\frac{N_s^*}{N^*} = \frac{N_s}{N}$$

we have

$$-\frac{\ln(N_s)}{\ln\delta} = -\frac{\ln(N_s^*/N^*)}{\ln\delta} - \frac{\ln(N)}{\ln\delta}.$$  \hspace{1cm} (16)

Defining

$$\alpha \equiv d - d_f = \frac{\ln(N_s^*/N^*)}{\ln\delta},$$

we have

$$\ln \left( \frac{N_s^*}{N^*} \right) = \alpha \ln\delta.$$  \hspace{1cm} (18)

Both $\delta$ and $N_s^*/N^*$ can be measured, allowing us to determine $\alpha$ and the fractal dimension $d_f$ of $S$.

In the previous discussion, little has been said about how to determine whether or not a point belongs to the subset $S$. In our specific case of differential equations, the following criterion is used. For a given cell, a number of points within the cell is chosen, and the trajectories passing through those points are followed. If these trajectories have different attractors, the cell is said to belong to $S$.

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Figure Captions

**Figure 1:** A plot of the Lorenz system using Nsolve.

**Figure 2:** ln($\bar{N}/N_{ic}$) as a function of ln $\epsilon$. $N_{ic} = 10^4$ and $10^{-5} \leq \epsilon \leq 10^{-4}$. The slope of the curve, $0.13 \pm 0.01$, is the exponent $\alpha$ in (3) defining the fractal dimension: $D = 2.87 \pm 0.01$.

**Figure 3:** As for Figure 2, but with $10^{-8} \leq \epsilon \leq 10^{-7}$. The slope of the best-fit straight line is $\alpha = 0.12 \pm 0.01$.

**Figure 4:** The output from Fdimension applied to the non-chaotic (non-fractal) Lorenz system ($\sigma = 10$, $b = 8/3$ and $R = 10$), with $5 \times 10^{-3} \leq \epsilon \leq 9 \times 10^{-3}$. The slope of the best-fit straight line is $\alpha = 1.02 \pm 0.05$.

**Figure 5:** An example of the use of View for a non-fractal system. 100 (random) initial conditions have been taken in the phase space interval $[x = -0.1..0.1, y = -0.1..0.1, z = 0.9..1.1]$.

**Figure 6:** The result of 100 (random) initial conditions taken in the phase space interval $[x = 0.9..1.1, y = 0.9..1.1, z = 21.9..22.1]$, for a chaotic regime.

**Figure 7:** The construction process for the Cantor Set
Figure 1
Figure 3
