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Discretizations of nonlinear differential equations using explicit finite order methods

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Abstract

In this work we study the appearance of spurious solutions when first-order differential equations with unimodal right-hand sides are discretized using Runge–Kutta schemes. These spurious solutions are explained in terms of the iteration functions. Schemes that produce good approximating solutions for much longer times are given.

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1. Introduction

The study of the asymptotic behavior of nonlinear autonomous differential equations depending on one or more parameters has led to different numerical schemes that try to reflect accurately these asymptotic states. If the method of approximation has fixed step size then the asymptotic states of the approximation and the continuous system may differ dramatically as parameters are varied. It has been shown (see [12]) that multi-step methods with bounded trajectories have correct asymptotic behavior, but unfortunately some popular one-step schemes such as explicit Runge–Kutta methods can have asymptotic solutions that satisfy the difference equations but are not approximations to the solutions of the differential equations. These solutions are known as spurious asymptotic solutions.

As a way to avoid these problems one can try to obtain discretizations that are chosen properly in the sense that they really reflect the dynamics of the differential equation. One idea in this direction is to obtain "the best discretization", that is, a scheme with zero local truncation error (see [7, 8]). The problem is that in general it is not clear how to obtain such optimal discretizations. Thus,

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it is necessary to discuss in detail simple examples to attempt to build some intuition concerning the new types of behavior that can arise as a result of approximations. Several attempts have been already done, in particular for the logistic equation, for which spurious asymptotic solutions for explicit Runge–Kutta schemes have been studied together with some local bifurcation analysis [3]. Our interest here is to study some unimodal differential equations, particularly those that provide some discrete models that have been widely used in ecology.

An unimodal differential equation is of the form $\mathrm{d}x(t)/\mathrm{d}t = f(x,\lambda)$ where f satisfies the following properties:

1. f depends continuously on x and λ.
2. There is an interval $(0,b)$ in the domain of f such that $f(x,\lambda) \geqslant 0$ with $f(0,\lambda) = 0 = f(b,\lambda)$.
3. There is $x_M \in (0,b)$ such that $f(x,\lambda)$ is monotone increasing for $x \in (0,x_M)$ and monotone decreasing for $x \in (x_M, b)$.
4. There is a unique fixed point, x_f, of $f(x,\lambda) \in (0,b)$.
5. $f(x,\lambda) > x$ for $(0,x_f)$.

Properties 1–5 are satisfied for every value of λ, where λ is known as the natural parameter.

The cases that we will consider here are $f(x,\lambda)=\lambda x(1-x)$ logistic equation, $f(x,\lambda)=\lambda \sin \pi(x)$ sine equation, $f(x,\lambda)=(\lambda x(1-x)/(1+x))-x$ Monod's equation, and $f(x,\lambda)=\lambda x \cdot \chi_{(-\infty,0.5]}+\lambda(1-x)\cdot \chi_{[0.5,\infty)}$, tent map, here $\chi_{(a,b]}$ is the characteristic function of the interval $(a,b]$.

The importance of unimodal differential equations is based on the facts that in their discrete versions (using Euler's method) chaotic phenomena occurs for some parameter regime, also because they model the behavior expected of a single population with the property of having isolated generations. Of special biological interest is the study of the implications of the discrete maps obtained when dependence on two parameters is allowed, one being the natural parameter and other the step size parameter. It is worth noting that even though we are dealing with unimodal differential equations, the discrete versions that we will obtain are not unimodal maps. One can find a nice treatment of unimodal maps in [2].

Two goals of this work are, first, to study the asymptotic behavior of discrete versions of unimodal differential equations of the form

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x,\lambda) \tag{1}$$

using explicit Runge–Kutta methods (R–K), and second, to provide some alternative methods that can extend the validity of the approximated solutions for larger values of the parameter. We point out that the method of discretization of a equation plays an important role in the dynamics: for example, for the logistic equation, $\dot{x} = \lambda x(1-x)$, the following two models, based on Euler's method, have been considered as its difference equation analogue:

$$x_{n+1} = (1+\lambda)x_n(1-x_n) \quad \text{and} \quad x_{n+1} = x_n \exp\left(\lambda(1-x_n)\right). \tag{2}$$

Even though these two models came from the same equation using the same technique of discretization they behave totally different under small perturbations in some parameter regime, see [11, 9].

The basic idea is to discretize this type of differential equations with explicit Runge–Kutta schemes with fixed step size. In our case the step size is equal to one, but analogous behavior will appear for any finite step size. In general, it is an advantage to use methods with a higher order than one since a decrease in the value of the step size results in a greater gain in accuracy. But we will show it later that this is not always true.

2. Discrete models

The point of departure is the equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = f(x, \lambda), \tag{3}$$

where f is a unimodal function. Explicit Runge–Kutta methods yield corresponding difference equations of the form (see, for example, [1])

$$x_{n+1} = x_n + \phi(x_n, \lambda), \tag{4}$$

where the right-hand side functions are known as the iteration functions. The iteration function for an m stage Runge–Kutta method of order p is of the form $\sum_{j=1}^{m} c_j f(k_i, \lambda)$ where $k_i = x_n + \sum_{j=1}^{m} b_{jl} f(k_l, \lambda)$ with $j = 1, 2, \ldots, m$. The coefficients c_j's and b_{jl}'s are chosen to obtain the desired order.

Assuming that $f(x, \lambda)$ is a polynomial of degree m in x, the iteration function is a polynomial with degree equal to m^s where s is the number of stages of the method. In this case we are approximating the exact solution by a polynomial of order m^s. The fixed points of the differential equations are fixed points of the iteration function, but there are many more fixed points of the iteration function that lead to spurious solutions. When the value of p is large, this problem is related to the problem of global interpolation that it is known for having potential ill-conditioning and numerical instability.

For the logistic equation, $f(x, \lambda)$ is a quadratic polynomial in x and the best iteration function is given by the map $(x_{n+1} - x_n)/(e^h - 1) = x_n(1 - x_{n+1})$, where h is the step size. This is an "exact" scheme as given by [7]. The Runge–Kutta schemes of order one, two, three and four define some iterations functions that we labeled as rk1, rk2, rk3 and rk4. (Runge–Kutta's method of order one is Euler's method, of order two is improved Euler's method. The particular schemes that we considered are given in the appendix.) Their graphs are shown in Fig. 1 with a fixed value of the natural parameter $\lambda = 2$, also we show the graph of the optimal iteration function, labeled as "exact".

As we can notice, the iterated functions approximate the exact function very well in a neighborhood of the origin but as the x-variable increases the iterated functions tend to minus infinity where as the exact function becomes constant. This fact is one of the reasons of the incorrect behavior of the approximations.

If $f(x, \lambda)$ is a periodic function on x, then the iteration function is also a periodic function. Thus, this problem is related to the problem of approximation of a function (exact solution) with a finite collection of periodic functions obtained by Taylor approximations of the exact solution. So, the method can only succeed (obtain a good approximation), if the exact solution is a periodic function; otherwise, one will have to consider a higher-order Runge–Kutta scheme, to increase the period of the approximating function, to be able to approximate the true solution for longer time, but the difficulty will eventually appear. In Fig. 2, we show the optimal iterated function, labeled as exact, for the equation $\dot{x} = \lambda \sin(\pi x)$ and also its iterated functions for the Euler's method (rk1) and improved Euler's method (rk2). Here we can notice that both schemes do not approximate very well

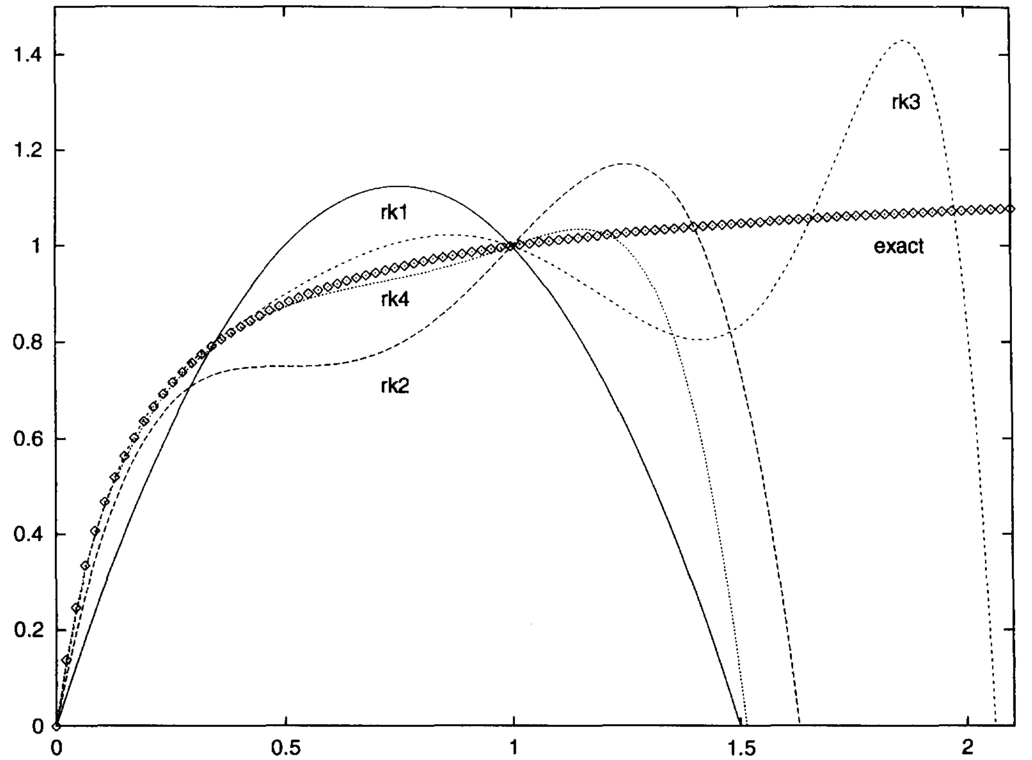

Fig. 1. Iteration functions for the logistic equation for some R–K methods.

the exact iterating function even in a small neighborhood of the origin. This fact will be reflected in its bifurcation diagram were spurious solutions will appear for smaller parameter values than for the logistic equation.

When the iterated function is a linear function in the natural parameter, the step size can be combined with the natural parameter to get a unique bifurcation parameter. The step size can be seen as a scaling of the natural parameter and it can be used to reduce the bifurcation parameter.

In some examples, like the logistic equation, with this scaling one can make the step size parameter as small as possible but it will be eventually overcompensated by the natural parameter. The example above (sine function) is another example where the bifurcation parameter does depend linearly on the step size. Note that the fixed points of the differential equation in both examples do not depend on the bifurcation parameter, so their bifurcation diagrams will consist in a straight line. In their discrete versions (using R–K schemes) we will obtain a straight line followed for some bifurcating spurious solutions.

In Fig. 3, we show a bifurcation diagram for the equation $\dot{x} = \lambda \sin(\pi x)$, here we used a sixth order R–K scheme (see the appendix). As we stated before, the bifurcation diagram consists of a constant line followed by some period doubling branches and then by a complicated chaotic pattern. Notice that even though the order of the scheme is sixth, the bifurcation point appears for values of the parameter less than one, similar behavior is obtained for lower-order methods.

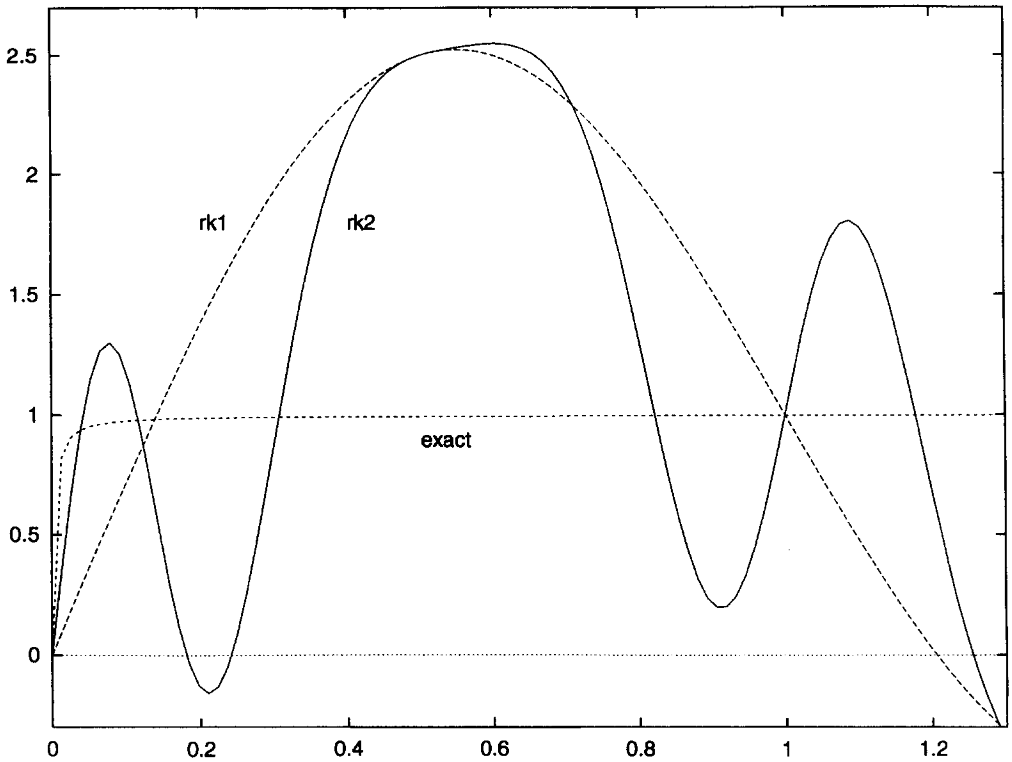

Fig. 2. Some iteration functions for $\dot{x} = \lambda \sin(\pi x)$.

One interesting example is given by the two-dimensional Monod's equation, which has been used to model the bacterial growth, where the rate of growth is proportional to the substrate concentration when the substrate is scarce, but tends toward a constant saturation level as the substrate becomes more plentiful. In a pollution control application, there is a continual flow of substrate into the pool that is matched by a flow of bacterial culture out of the pool. A slightly simplified form of Monod's equation is given by the one-dimensional equation of the form (although no generality is lost in this context)

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\lambda x(1-x)}{k+x} - bx,$$

where k and b are constants. In this case, the natural parameter is not a scaling of the step size parameter; moreover, the fixed points of the differential equation depend on the natural parameter, so a different bifurcation diagram will appear. In Fig. 4, we show a bifurcation diagram of a discrete version of the Monod's equation using a second-order scheme using the values $b = k = 1$. The "bifurcation" diagram for the optimal discretization is also shown in this figure, with small diamonds. As we can see, the approximation is exact until $\lambda = 4$ where there is a branch of two period points. The behavior shown in this picture is the typical of period doubling route to chaos present in most of the discrete versions of unimodal differential equations.

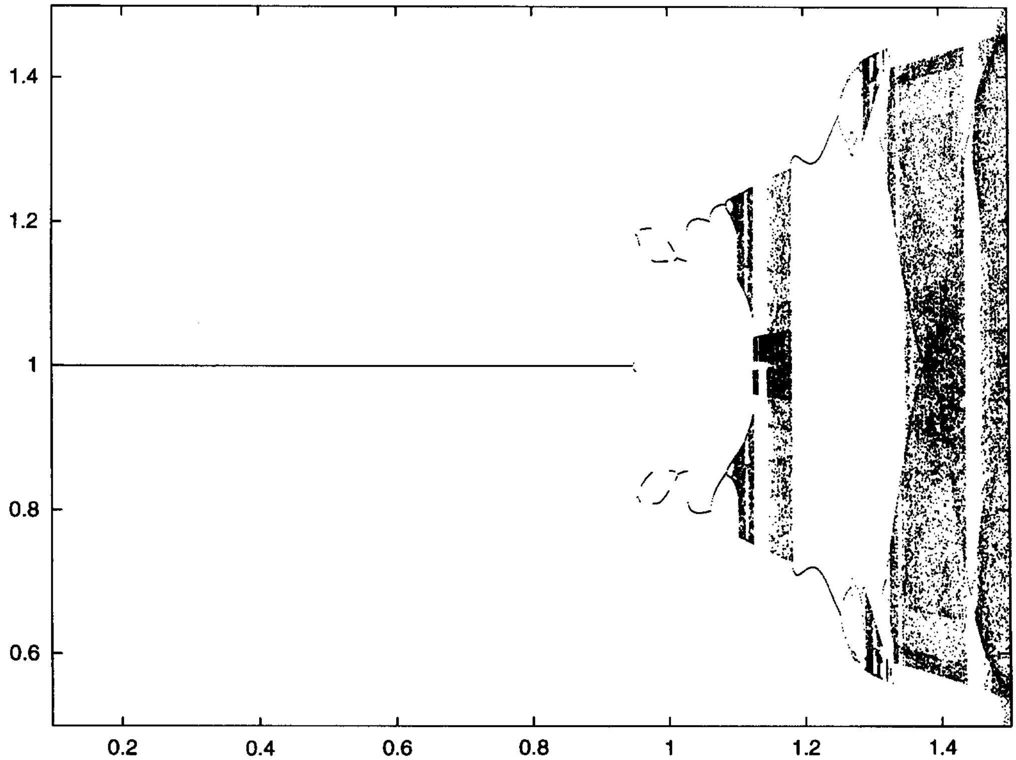

Fig. 3. Bifurcation diagram for the sine equation using a sixth-order R–K scheme.

In the next section we will compare how Runge–Kutta schemes behave for all these examples and others of theoretical interest.

3. Numerical Results

Our next step is to study numerically the system 1 for the particular functions that we mention before. Our interest is to analyze the behavior of the approximates and how the approximations reflect the true asymptotic behavior of the differential equation.

The bifurcation diagrams of the logistic equation are well known, see [5, 3], so we will not get into details of them. Applying the Runge–Kutta schemes to this equation we get that Euler's method (R–K of first order) gives a correct solution up to the value of the parameter $\lambda = 2.0$, which we will define as the critical value. The same critical value is obtained for a R–K second-order method, known as the improved Euler's method. For a R–K method of third order we get $\lambda_c = 2.5127$; for the classical Runge–Kutta method of order 4, we get $\lambda_c = 2.785293$, for a method of sixth-order we get $\lambda_c = 2.8561$; for a fifth-order method the critical value is $\lambda_c = 3.5854336$ and finally for an eighth-order method we get that $\lambda_c = 2.99$. In Fig. 5 we show how these methods interlock between each other. The particular Runge–Kutta methods that we used are given in the appendix.

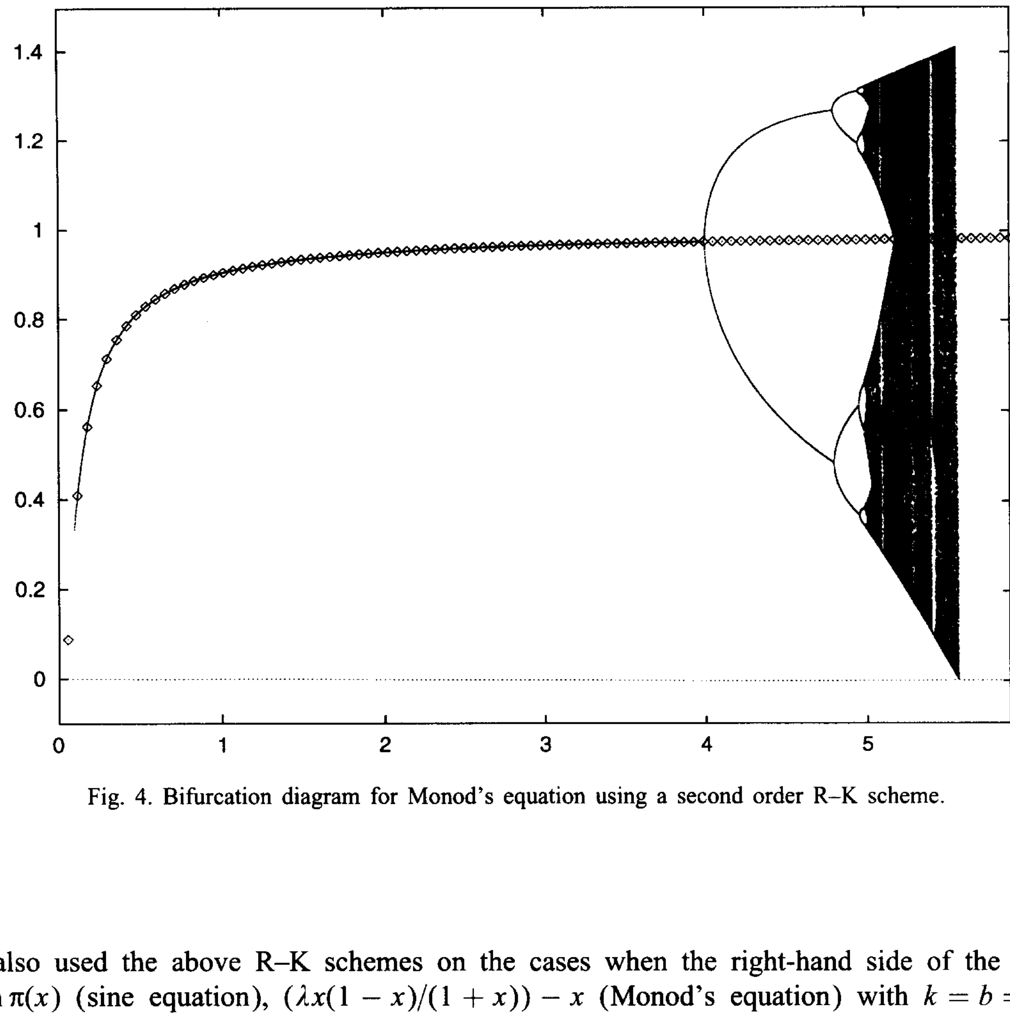

Fig. 4. Bifurcation diagram for Monod's equation using a second order R–K scheme.

We also used the above R–K schemes on the cases when the right-hand side of the system 1 is $\lambda \sin \pi(x)$ (sine equation), $(\lambda x(1-x)/(1+x)) - x$ (Monod's equation) with $k = b = 1$), and the tent function. The tent equation has a special interest on its own, since the function f is only continuous in the variable x, and the bifurcation diagram shows some different qualitative behavior, moreover for some values of the natural parameter, as a map, it is topologically conjugated to the logistic map; see [13]. Another equation of particular interest (not a unimodal equation) is when the function is $\lambda x(1-x)(x-0.5)$. This equation has been studied numerically in [12]. For all of these cases, chaotic behavior is present and spurious solutions are found. The values of the parameter up to which the approximated asymptotic solutions are exact (critical values) are given in Table 1.

One may think that higher order methods will be give better approximations than lower ones, but in our studies this is not always true. A good bound for the bifurcation value is easy to determine since it is the parameter value at which the map has a fixed point with an eigenvalue of the Jacobian matrix on the unit circle. Although this is a necessary condition for the exact bifurcation point, in most cases it is also sufficient. In the case of a single equation, this condition reduces to the derivative of the iteration function with respect to x being plus or minus one at the fixed point. So a priori one can know which R–K method will produce a better scheme.

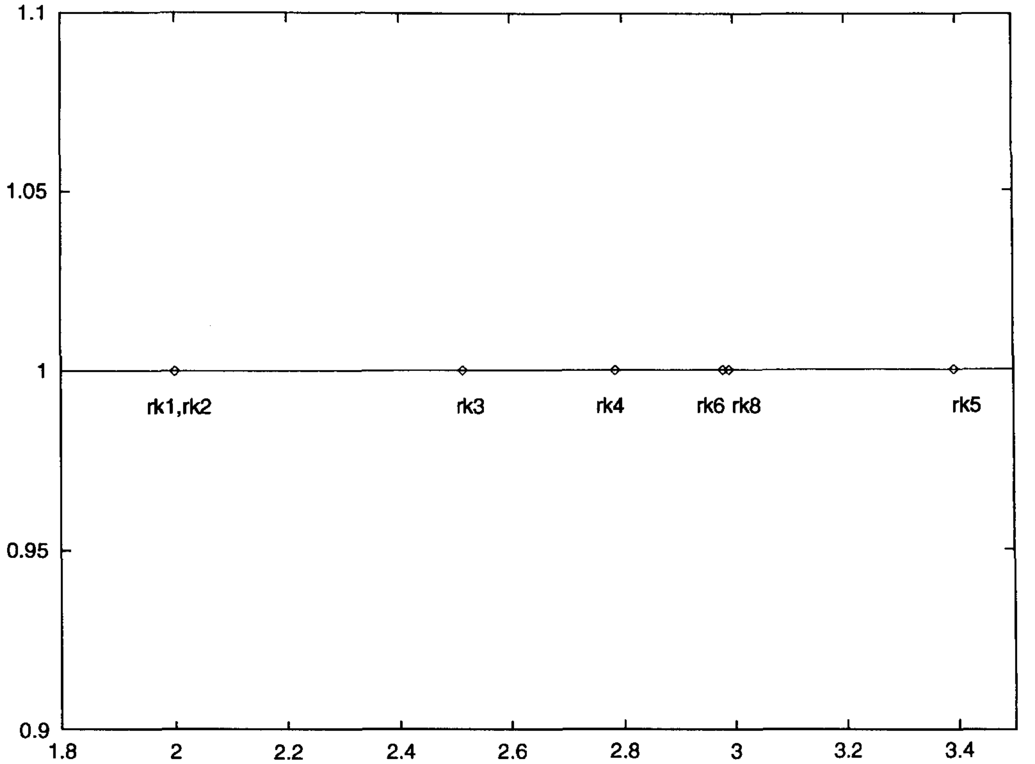

Fig. 5. Critical values for the logistic equation.

Table 1
Critical Values of the natural parameter

Method equation	Logistic	Sine	Monod	Tent	Cubic
RK-1	2.0	0.636	4.0	2.0	4.0
RK-2	2.0	0.636	4.0	2.0	4.0
RK-3	2.5127	0.7998	5.22	2.5	5.025
RK-4	2.7853	0.8866	5.686	2.75	5.57
RK-5	3.394	1.141	7.2	3.21	7.171
RK-6	2.98	0.948	5.648	2.43	5.9584
RK-8	2.99	0.987	5.27	3.11	5.75

4. Combination methods

From the above numerical calculations we observe that there are some basic facts that we can take into account to remove numerical instabilities. When the order of the difference scheme is greater than the order of the differential equation — in our case, one — new fixed points will appear, leading to the existence of asymptotic spurious solutions. Moreover, making the step size smaller, may not improve the method. The first bifurcation point is a crucial factor to test the accuracy of the method

Table 2
Critical values for the logistic equation

Method	Critical value λ_c
RK-12, $\beta = 0.5$	3.464
RK-12, $\beta = 0.28$	5.23
RK-12, $\beta = 0.255$	7.83
RK-34, $\beta = 0.5$	2.9454
RK-34, $\beta = 0.6$	2.9889

used. Another factor is that slopes of the iteration functions plays an important role on the behavior of the difference scheme.

With aid of these facts we suggest the following combination method: Given a collection of explicit Runge–Kutta methods with their iterated functions given by the family $f_{m_1}, f_{m_2}, \dots f_{m_j}, \dots$ with corresponding orders $O_{m_1} < O_{m_2} < \cdots < O_{m_j} < \cdots$, consider the method given by

$$x_{n+1} = \sum_j c_j f_{m_j}(x_n, \lambda)$$

with $\sum_{j=1} c_j = 1$. Note that in general this method is of order O_{m1} but since the coefficients of the linear combination are to be chosen, one will try to find a combination that extends the validity of the solution of the discrete solution to the largest value of the natural parameter possible.

This combination method will improve the given schemes when the derivatives of two of the iteration functions evaluated at the fixed point x_f and critical value λ_c are different. Moreover, if the following condition holds, the improvement is significant:

$$\frac{\mathrm{d}f_{m_j}(x_f, \lambda_c)}{\mathrm{d}x} \frac{\mathrm{d}f_{m_k}(x_f, \lambda_c)}{\mathrm{d}x} < 0 \tag{5}$$

for some j and some k. This condition just guarantees that those two iteration functions have slopes of different sign at the fixed point.

The combined scheme gives us a better approximation in the sense that the limiting solution is correct for larger values of the parameter. This agrees with Mickens' idea (see [7]) that the best discrete version has to be of the same order as the differential equation. This new method will postpone the appearance of spurious solutions when one changes the values of the coefficients c_j's. In fact, we will show how good this method is even when only two basic methods are used.

For example, if we choose a mixed method involving only Euler's method and improved Euler's method, we obtain the following mixed scheme parameterized by β with $0 \leqslant \beta \leqslant 1$:

$$x_{n+1} = x_n + (1 - \tfrac{1}{2}\beta) f(x_n, \lambda) + \tfrac{1}{2}\beta f(x_n + f(x_n, \lambda), \lambda).$$

The method is of order one if $\beta \neq 1$. Condition 5 simplifies to $(\mathrm{d}f/\mathrm{d}x)(x_0, \lambda_0) < -1$. This method gives better results than the fourth-order classical Runge–Kutta method for $\beta = 0.5$, but also it is even better than the methods of sixth and eighth order for other choices of β, e.g. $\beta = 0.255$. In fact, this method gives better approximations for values of $\beta \to 0.25^+$. A combination of a R–K scheme of third and fourth order will be equivalent to a method of eighth-order, but not as good

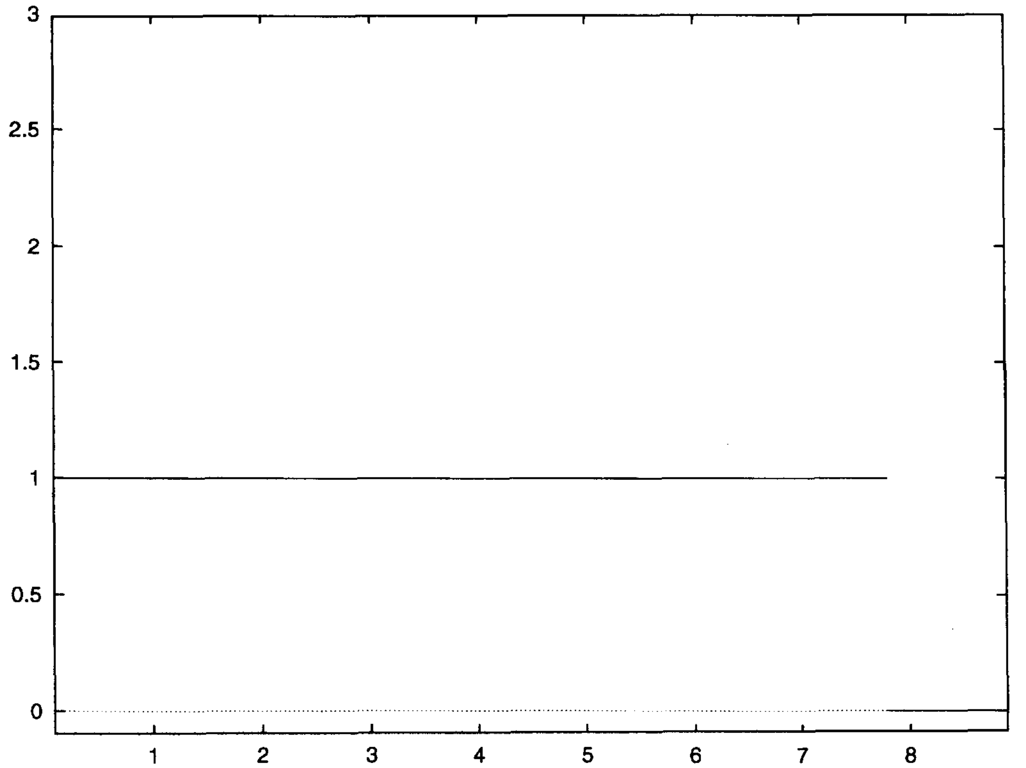

Fig. 6. Bifurcacion diagram for the logistic equation using a combined scheme R–K12.

as a combination of R–K schemes up to fourth-order. In Table 2 we show some combinations of R–K methods applied to the logistic equation to illustrate how the exact solution can be extended by using combined methods. The methods are labeled as R–Kab where a and b stands for the order of each method in the combined method. The values of β is the value of the weight associated to the lower order method, the other coefficient is of course $1-\beta$.

In Fig. 6 we show a bifurcation diagram for the logistic equation using a combination scheme of Euler's and improved Euler's schemes, the value of the weight is $\beta=2.555$; notice the disappearance of spurious solutions.

5. Conclusions

As observed in our study, the asymptotic dynamics of simple nonlinear equations described by the different discrete versions that we presented are similar within an interval of confidence, but special care has to be taken for larger values of the parameter. Hence, an important conclusion of our study is that a single discretization is not enough to make assertions about the exact asymptotic solution of the equation. Thus, we suggest that to check the reliability of a numerical solution is convenient to check several versions of discretizations of the equation and base the statements about the exact solution in the common interval of confidence. An exact scheme maybe hard to find but by considering combined schemes one should have solutions that are close–qualitatively and quantitatively—to that of the continuous equation.

6. Appendix. Runge–Kutta Schemes

We know that the iteration function for an m stage Runge–Kutta method of order p is of the form $f_1(x_n,\lambda)=\sum_{j=1}^{m} c_j f(k_i,\lambda)$ where $k_i=x_n+\sum_{j=1}^{m} b_{jl} f(k_l,\lambda)$ with $j=1,2,\ldots,m$. The coefficients c_j's and b_{jl}'s are the elements of a vector c and a matrix B, respectively.

Here we show which particular schemes we used in our work, and we only give the matrices B and the vectors c for each case; in [1] one can find many more cases.

1. Runge–Kutta method of first order (Euler's method):

$$c=(1),$$
$$B=(0).$$

2. Runge–Kutta method of second order (Improved Euler's method):

$$c=\left(\tfrac{1}{2},\tfrac{1}{2}\right),$$
$$B=\begin{pmatrix}0&0\\1&0\end{pmatrix}.$$

3. Runge–Kutta method of third order:

$$c=\left(\tfrac{1}{6},\tfrac{2}{3},\tfrac{1}{6}\right)$$
$$B=\begin{pmatrix}0&0&0\\\tfrac{1}{2}&0&0\\-1&2&0\end{pmatrix}.$$

4. Runge–Kutta method of fourth order (Runge–Kutta classical method):

$$c=\left(\tfrac{1}{6},\tfrac{1}{3},\tfrac{1}{3},\tfrac{1}{6}\right),$$
$$B=\begin{pmatrix}0&0&0&0\\\tfrac{1}{2}&0&0&0\\0&\tfrac{1}{2}&0&0\\0&0&1&0\end{pmatrix}.$$

5. Runge–Kutta method of fifth order:

$$c=\left(\tfrac{13}{200},0,\tfrac{11}{120},\tfrac{11}{60},\tfrac{2}{75},\tfrac{2}{15}\right),$$
$$B=\begin{pmatrix}0&0&0&0&0&0\\\tfrac{1}{3}&0&0&0&0&0\\0&\tfrac{2}{3}&0&0&0&0\\\tfrac{1}{12}&\tfrac{1}{3}&\tfrac{-1}{12}&0&0&0\\\tfrac{25}{48}&\tfrac{-55}{24}&\tfrac{35}{48}&\tfrac{15}{8}&0&0\\\tfrac{3}{20}&\tfrac{-11}{24}&\tfrac{-1}{8}&\tfrac{1}{2}&\tfrac{1}{10}&0\end{pmatrix}.$$

6. Runge–Kutta method of sixth order:

$$c = \left(\tfrac{13}{200}, 0, \tfrac{11}{40}, \tfrac{11}{40}, \tfrac{4}{25}, \tfrac{4}{25}, \tfrac{13}{200}\right),$$

$$B = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{2}{3} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{12} & \frac{1}{3} & \frac{-1}{12} & 0 & 0 & 0 & 0 \\ \frac{25}{48} & \frac{-55}{24} & \frac{35}{48} & \frac{15}{8} & 0 & 0 & 0 \\ \frac{3}{20} & \frac{-11}{24} & \frac{-1}{8} & \frac{1}{2} & \frac{1}{10} & 0 & 0 \\ \frac{-261}{260} & \frac{33}{13} & \frac{43}{156} & \frac{-118}{39} & \frac{32}{195} & \frac{80}{39} & 0 \end{pmatrix}.$$

7. Runge–Kutta method of eighth order:

$$c = \left(\tfrac{1}{20}, 0, 0, 0, 0, 0, 0, \tfrac{49}{180}, \tfrac{16}{45}, \tfrac{49}{180}, \tfrac{1}{20}\right),$$

$$B = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{4} & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{7} & \frac{-7,-3}{98} & \frac{21,5}{49} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{11,1}{84} & 0 & \frac{18,4}{63} & \frac{21,-1}{252} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{5,1}{48} & 0 & \frac{9,1}{36} & \frac{-231,14}{360} & \frac{63,-7}{80} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{10,-1}{42} & 0 & \frac{-432,92}{315} & \frac{633,-145}{90} & \frac{-504,115}{70} & \frac{63,-13}{35} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{14} & 0 & 0 & 0 & \frac{14,-3}{126} & \frac{13,-3}{63} & \frac{1}{9} & 0 & 0 & 0 & 0 \\ \frac{1}{32} & 0 & 0 & 0 & \frac{91,-21}{576} & \frac{11}{72} & \frac{-385,-75}{1152} & \frac{63,13}{128} & 0 & 0 & 0 \\ \frac{1}{14} & 0 & 0 & 0 & \frac{1}{9} & \frac{-733,-147}{2205} & \frac{515,111}{504} & \frac{-51,11}{56} & \frac{132,28}{245} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{-42,7}{18} & \frac{-18,28}{45} & \frac{-273,-53}{72} & \frac{301,53}{72} & \frac{28,-28}{45} & \frac{49,-7}{18} & 0 \end{pmatrix}.$$

Here $a,b/c$ stands for $(a+b\sqrt{21})/c$.

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