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A general method for obtaining unconventional and nonstandard difference schemes

R. Meyer-Spasche and D. Düchs

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Abstract

In recent years it has been shown that some unconventional or nonstandard finite difference schemes have very good properties. Some are exact schemes, others give dynamically correct approximations for wide parameter ranges and arbitrary initial values even in the case of blow-up, or they are symplectic on a non-canonical Hamiltonian system. Thus it is highly desirable to know a general method for generating such schemes for any given differential equation, without a priori knowledge of the solution. We show that the 'linearized trapezoidal rule' is such a method: some nonstandard schemes found in the literature are generated by it, others are approximated in a surprizing way. Moreover, the method is nearly a standard method: practitioners in computational plasma physics and fluid dynamics have been using it for years, and it belongs to the family of Rosenbrock methods.

1 Introduction

As pointed out in several recent publications, it is sometimes advantageous to use non-standard difference schemes for the numerical solution of differential equations. Some nonstandard schemes are exact [11, 1], others give dynamically correct approximations for wide parameter ranges and arbitrary initial values even in the case of blow-up [7], or they are symplectic on a non-canonical Hamiltonian system [16, 6]. Until now, no general method seems to be known for constructing nonstandard schemes. According to R.P. Argawal's recent review[1] of Mickens' book [11], the present situation is the following: 'Difference equation approximations are obtained either by using the known forms of the solutions of the differential equations or by ad hoc experimentation. A more effective method is still lacking'.

We present here a simple general method for derivation of nonstandard schemes for any given initial value problem, without a priori knowledge of the solution. We demonstrate its power for a number of often used equations. Moreover we extend the range of pertinent examples for nonstandard schemes by discussing their role in the approximation of blow-up solutions. With this general method, nonstandard schemes could become standard.

We begin by explaining the case of blow-up solutions. The general method is introduced at the end of this section, and applied to the blow-up solution case in some detail in section 2. Sections 3 and 4 provide several more cases of easy derivations of successful 'nonstandard' schemes from our general method (13).

When we approximate the solutions of an initial value problem

$$\dot{u} = f(u), \qquad u(0) = u_o \tag{1}$$

by explicit finite differences, say a Runge-Kutta scheme, we get some difference equations

$$\begin{aligned} t_{n+1} &= g(t_n, y_n), \\ y_{n+1} &= F(t_n, y_n), \qquad y_o = u(0). \end{aligned} \tag{2}$$

If eq. (1) has blow-up solutions, it can happen that $u(t)$ exists only in a bounded time interval $(0, T)$, while the iterates $\{y_n\}$ exist for $t_n \to \infty$.

[1]SIAM Review **37**, Sept. 95, p. 459

Example:

$$\dot{u} = \lambda u^2, \qquad u(0) = u_o \tag{3}$$

has the solutions

$$u(t; u_o) = \frac{u_o}{1 - \lambda u_o t}. \tag{4}$$

If $\lambda u_o < 0$ then $u(t; u_o)$ exists for $t \to \infty$ and $\lim_{t\to\infty} u(t; u_o) = 0$. If, however, $\lambda u_o > 0$ then $u(t; u_o)$ exists only in the bounded time interval $(0, T = \frac{1}{\lambda u_o})$. Such solutions are called **blow-up solutions** [12] or **of explosive type** [13]. If we approximate eq. (3) by Euler's method with constant step size k, we obtain the iterative scheme

$$t_{n+1} = t_n + k, \tag{5}$$

$$y_{n+1} = y_n + \lambda k {y_n}^2, \qquad y_o = u_o, \tag{6}$$

and the iterates exist for all $t_n = nk$, no matter if λy_o is positive or negative. For sufficiently negative values λy_o , the trajectories $\{y_n\}$ do not tend to zero as the trajectories of the differential equation do. Instead, they change sign and tend to $+\infty$ for $t_n \to \infty$. This can be shown in the same way as it was shown for forward Euler on the logistic differential equation in [7]. In addition, there is the well-known problem of stability of the scheme. ◇

All this is no contradiction to the well-known fact that Euler's method is convergent. The convergence theorems assume a compact time interval, and $k \to 0$. Here, however, we consider the behavior of (6) for $t_n \to \infty$, k fixed. Open time intervals without a-priori bounds are the usual case when dealing with dynamical systems. Fixed k is not so realistic for high quality numerical approximations. But it makes it easier to understand basic effects. It seems reasonable to assume that if one method is superior to another for fixed step size, it will be superior as well when used with step size control. The question of how well continuous dynamical systems are approximated by discrete dynamical systems has been formulated by Dahlquist in 1959 [3]. It is at present intensively investigated (see the proceedings 'Numerics of Dynamics - Dynamics of Numerics' [14], especially the article by Sanz-Serna [15]).

If we consider the nonstandard scheme

$$y_{n+1} = y_n + \lambda\ k\ y_n\ y_{n+1}, \qquad y_o = u_o, \tag{7}$$

for equation (3) instead of (6), we find that it solves eq. (3) exactly. And this also is valid for arbitrary variable step size k_n.

Theorem 1 *Scheme (7), and its explicit version*

$$y_{n+1} = \frac{y_n}{1 - k_{n+1}\lambda y_n}, \qquad y_o = u_o, \tag{8}$$

renders the exact solution (4) of (3) for all non-zero $u_o \in \mathbb{R}$ *and all sequences* $\{k_n\}_{n \leq N}$ *satisfying* $k_n > 0$ *and*

$$\lambda y_o t_N = \lambda y_o \sum_{n=1}^{N} k_n < 1. \tag{9}$$

Here we put $t_N := \sum_{n=1}^{N} k_n$. Note that condition (9) bounds the step sizes k_n only if $\lambda y_o > 0$, i.e. in the blow-up case.

Proof: We prove this theorem by induction. For $N = 1$ we get

$$y_1 = \frac{y_o}{1 - \lambda k_1 y_o} = u(t_1), \qquad \text{if } \lambda k_1 y_o < 1.$$

Let it be valid for N. Then

$$\begin{aligned} y_{N+1} &= \frac{y_N}{1 - k_{N+1}\lambda y_N} \\ &= \frac{y_o}{1 - t_N \lambda y_o} \cdot \frac{1}{1 - k_{N+1}\lambda \frac{y_o}{1 - t_N \lambda y_o}} \\ &= \frac{y_o}{1 - (t_N + k_{N+1})\lambda y_o} \\ &= \frac{y_o}{1 - t_{N+1}\lambda y_o} \\ &= u(t_{N+1}), \end{aligned}$$

if the blow-up time has not passed, i.e. if (9) is satisfied. This proves the theorem. $\diamond$

Scheme (7) is called an **exact scheme** because it solves eq. (3) exactly, i.e. because $y_{N+1} = u(t_{N+1})$, as just proved. Exact schemes were introduced by Mickens, see [11, p. 70ff]. He proved that every ordinary differential equation

$$\dot{u} = g(u, t, \lambda), \qquad u(t_o) = u_o \tag{10}$$

has an exact scheme. Using exact solutions of differential equations and methods of mathematical physics, he found several examples of exact schemes. We shall study them in section 3. Scheme (7) is one of Mickens' examples, [11, (3.3.32)].

Scheme (7) is called a **nonstandard scheme** because it cannot be written in one of the standard forms usually considered in Theoretical Numerical Analysis, neither as

$$\frac{y_{n+1}-y_n}{k} = (1-\theta)\lambda y_n^2 + \theta\lambda y_{n+1}^2, \quad 0 \le \theta \le 1, \tag{11}$$

nor as

$$\frac{y_{n+1}-y_n}{k} = \lambda\left((1-\theta)y_n + \theta y_{n+1}\right)^2, \quad 0 \le \theta \le 1. \tag{12}$$

Since standard difference schemes for (10) are always formulated as expressions in g, they cannot lead to a scheme like (7). But the fact that (7) is exact and that many other exact schemes contain terms involving more than one grid point (time level) shows that it is important to consider nonstandard schemes. The best sources for today's knowledge on nonstandard schemes for single ordinary differential equations and parabolic differential equations are probably the books by Mickens [11] and by Agarwal [1, Chap. 3]. Nonstandard modelling rules are offered in [11, p. 81ff]. These rules tell what nonstandard schemes should look like, but do not tell how to produce them.

For this paper we start from the observation that the special difference scheme (7) can be obtained by Taylor-expanding either of the formulas (11) or (12) at y_n for $\theta = \frac{1}{2}$ and neglecting terms of higher order in $\frac{y_{n+1}-y_n}{2}$.

Generalizing this derivation procedure for difference schemes to solve any eq. (1) leads to

$$\frac{y_{n+1}-y_n}{k} = f(y_n) + f'(y_n)\frac{y_{n+1}-y_n}{2} \tag{13}$$

which can be viewed as using a time-centered scheme together with the first step of a Newton iteration.

The time-centered scheme is either taken as the standard trapezoidal rule

$$\frac{y_{n+1}-y_n}{k} = \frac{f(y_n)+f(y_{n+1})}{2} \tag{14}$$

or the standard midpoint rule

$$\frac{y_{n+1}-y_n}{k} = f\left(\frac{y_n+y_{n+1}}{2}\right). \tag{15}$$

Schemes of type (13) have been used for practical applications in computational fluid dynamics [2], [20, p. 1610] and in computational plasma physics [4, 5].

In the following sections we shall compare, for a number of cases, the schemes obtained from (13) with 'nonstandard' schemes found in recent literature. We shall show that (13) provides a unifying approach to these schemes and therefore should be ranked among the standard methods. This is even more so since scheme (13) can also be viewed as the simplest scheme in the family of Rosenbrock methods which are decribed in [9, p. 561].

Scheme (13) is therefore open to improvements in accuracy: either by using higher order Rosenbrock schemes or by performing more Newton iterations. Investigations of the dynamical properties of (13) and of generalizations of it are in progress [10].

In section 2 the modelling of blow-up by nonstandard schemes is discussed for the logistic equation, and the relation between several nonstandard schemes and the scheme obtained from (13). Sections 3 and 4 provide several more cases of easy derivations of successful 'nonstandard' schemes from (13).

2 Nonstandard schemes for the logistic equation

The logistic differential equation

$$\dot{u} = \lambda u(1-u), \quad u(0) = u_o \tag{16}$$

has the two stationary states $\bar{u}(t) \equiv 0$ and $\tilde{u}(t) \equiv 1$ for all λ. The solutions of (16) are given by

$$\begin{aligned} u(t) &= \frac{u_o e^{\lambda t}}{1 + u_o(e^{\lambda t} - 1)} & (17) \\ &= \frac{u_o}{(1-u_o)e^{-\lambda t} + u_o}. & (18) \end{aligned}$$

To describe the behavior of the solutions, we have to consider several different cases.
1) Let $\lambda > 0, \quad u_o > 1$. As long as $u(t) > 1$, we get $\dot{u} = \lambda u(1-u) < 0$, and $\lim_{u\to 1^+} \dot{u} = 0$, $\lim_{t\to\infty} u(t) = 1$. Thus $u(t)$ decays monotonically to $\tilde{u} = 1$. The decay rate depends on λ.

2) Let $\lambda > 0$, $0 < u_o < 1$. As long as $0 < u(t) < 1$, $\dot{u} = \lambda u(1-u) > 0$, and $\lim_{u\to 1^-} \dot{u} = 0$, $\lim_{t\to\infty} u(t) = 1$.

From 1) and 2) follows that $\tilde{u}(t) \equiv 1$ is a stable stationary state of (16), and that all trajectories with $u_o > 0$ approach $\tilde{u}$ monotonically.

3) Let $\lambda > 0$, $u_o < 0$. As long as $u(t) < 0$, $\dot{u} = \lambda u(1-u) < 0$. Thus these solutions tend to $-\infty$.

The denominator in (17) is $d(t) = 1 + u_o(e^{\lambda t} - 1)$. We have $d(0) = 1$ and $d(T) = 0$ with blow-up time

$$T = \frac{1}{\lambda}\ln\frac{u_o - 1}{u_o} = \ln\left(\frac{u_o - 1}{u_o}\right)^{1/\lambda} > 0. \tag{19}$$

From 2) and 3) follows that $\bar{u}(t) \equiv 0$ is unstable from above and from below.

4) In the case $\lambda < 0$, everything is very similar. Stability of the two stationary states is different: $\bar{u}(t) \equiv 0$ is stable, $\tilde{u}(t) \equiv 1$ is unstable.

When we discretize (16) using (13), we get

$$\frac{y_{n+1} - y_n}{k} = \frac{\lambda}{2}(y_n(1 - y_{n+1}) + y_{n+1}(1 - y_n)). \tag{20}$$

This scheme was considered by Wang et al. [19]. Their analysis left several open questions, for instance they could not explain why the scheme is not defined for certain initial values y_o.

To understand the properties of scheme (20), it is illustrative to consider the two schemes of which it is the arithmetic mean:

$$y_{n+1} = y_n + k\lambda y_{n+1}(1 - y_n), \qquad y_o = u_o, \tag{21}$$

which leads to the rational scheme

$$y_{n+1} = \frac{y_n}{1 - k\lambda(1 - y_n)}, \qquad y_o = u_o, \tag{22}$$

and

$$y_{n+1} = y_n + k\lambda y_n(1 - y_{n+1}), \qquad y_o = u_o, \tag{23}$$

which leads to the rational scheme

$$y_{n+1} = \frac{(1 + k\lambda)y_n}{1 + k\lambda y_n}, \qquad y_o = u_o. \tag{24}$$

Schemes (21) and (23) are **adjoint schemes** in the sense of Definition 8.2 of [8, Chap. II]: the map $k \mapsto -k$; $y_{n+1} \mapsto y_n$; $y_n \mapsto y_{n+1}$ replaces scheme (21) by scheme (23), and scheme (23) by scheme (21).

Theorem 2 *The difference equation (22)*

$$y_{n+1} = \frac{y_n}{1 - k\lambda(1 - y_n)}, \qquad y_o \text{ given },$$

has the solution

$$y_n = \frac{y_o}{(1 - k\lambda)^n(1 - y_o) + y_o}. \tag{25}$$

The iteration is defined as long as

$$(1 - k\lambda)^n \neq \frac{y_o}{y_o - 1}. \tag{26}$$

Proof: A proof by induction shows that scheme (22) leads to

$$\begin{aligned} y_n &= \frac{y_o}{(1 - k\lambda)^n + k\lambda y_o \sum_{i=0}^{n-1}(1 - k\lambda)^i}; \\ &= \frac{y_o}{(1 - k\lambda)^n(1 - y_o) + y_o}, \end{aligned} \tag{27}$$

because

$$\sum_{i=0}^{n-1}(1 - k\lambda)^i = \frac{1 - (1 - k\lambda)^n}{k\lambda}.$$

The iteration is defined as long as the denominator of eq. (22) is non-zero, i.e. as long as condition (26) is satisfied.

Theorem 3 *The difference equation (24)*

$$y_{n+1} = \frac{(1 + k\lambda)y_n}{1 + k\lambda y_n}, \qquad y_o \text{ given}$$

has the solution

$$y_n = \frac{(1 + k\lambda)^n y_o}{1 + y_o((1 + k\lambda)^n - 1)}. \tag{28}$$

The iteration is defined as long as

$$(1+k\lambda)^n \neq \frac{y_o - 1}{y_o}. \tag{29}$$

Proof: A proof by induction shows that (24) leads to

$$\begin{aligned} y_n &= \frac{(1+k\lambda)^n y_o}{1 + y_o k\lambda \sum_{i=0}^{n-1}(1+k\lambda)^i} \\ &= \frac{(1+k\lambda)^n y_o}{1 + y_o((1+k\lambda)^n - 1)}. \end{aligned} \tag{30}$$

The iteration is defined as long as the denominator of (24) is non-zero, i.e. as long as (29) is satisfied. ◇

It should be noted that the actual iterations produce versions (27) and (30) of the solutions. Versions (25) and (28) are chosen in the formulation of the theorems because they are more concise, and more convenient for the analysis of the properties of the schemes. Though both versions are mathematically the same, they might be different in their sensitivity to rounding errors.

Solution (28) is given by Mickens [11, (2.4.37)] for the case $\lambda = 1$ in a slightly different formulation. He derived it by introducing $x_k = 1/y_k$ and then solving the difference equation for x_k.

We now discuss the aproximation of the differential equation by the difference equations.

If we replace in (25) $(1-k\lambda)^n$ by $(e^{-k\lambda})^n = e^{-\lambda kn} = e^{-\lambda t_n}$, we get $u(t_n)$, i.e. the exact solution at $t_n = nk$ in formulation (18). If we replace in (28) $(1+k\lambda)^n$ by $e^{k\lambda n} = e^{\lambda t_n}$, we get $u(t_n)$, i.e. the exact solution at $t_n = nk$ in formulation (17). Thus the quality of the approximation of the solutions of the differential equation by the solutions of the difference equations is completely governed by the quality of approximation of $e^{\pm\lambda k}$ by the first two terms of its Taylor expansion, $1 \pm \lambda k$.

$1 + \lambda k$ is a qualitatively correct approximation to $e^{\lambda k}$ as long as $1 + k\lambda > 0$, i.e. as long as $k\lambda > -1$.
$1 - \lambda k$ is a qualitatively correct approximation to $e^{-\lambda k}$ as long as $k\lambda < 1$. This confirms

that (23)

$$y_{n+1} = y_n + k\lambda y_n(1 - y_{n+1}) \tag{31}$$

gives qualitatively correct aproximations for $k\lambda > -1$, and that (21)

$$y_{n+1} = y_n + k\lambda y_{n+1}(1 - y_n) \tag{32}$$

gives qualitatively correct approximations for $k\lambda < 1$. For $|\lambda k| > 1$, one of the schemes gives the correct dynamic behavior of the approximated differential equation, and its adjoint gives stability *and global attractivity* to the unstable steady state. The difference scheme (20)

$$y_{n+1} = y_n + \frac{k\lambda}{2}(y_n(1 - y_{n+1}) + y_{n+1}(1 - y_n)) \tag{33}$$

gives qualitatively correct approximations when both components of it do so, i.e. for $|\lambda k| < 1$, and even in a larger λk interval: up to $|\lambda k| = 2$. It produces oscillatory trajectories and thus wrong dynamic behavior for $|\lambda k| \geq 2$, but the stability of both fixed points is correct for all λk [10, 19]. More details are given in [7, 10]. The papers by Twizell, Wang and Price [18, 19] contain errors which are corrected in [7, 10].

Scheme (31) treats the solution $\tilde{u} = 1$ implicitly, and this is favorable for $\lambda > 0$ since $\tilde{u}(t;\lambda) \equiv 1$ is stable then. For $\lambda < 0$, $\bar{u}(t;\lambda) \equiv 0$ is stable, and thus scheme (32) is favorable. In their favorable cases, the two schemes have all advantages of fully implicit schemes. In addition, they give good approximations of the blow-up solutions then.

Note that conditions (26) or (29) need not be violated directly. Since we are dealing with discrete equations, the denominators can change sign without hitting zero. The blow-up time can thus be passed unvoluntarily. This is detected by a sudden sign change of the iterates. Twizell et al found that there are for given λk 'forbidden initial values' since they nullify the denominator of the scheme. In the light of our analysis, it should be stated that for certain given initial values there are forbidden λk-values: they are forbidden, because the time step is already of the size of the blow-up time of the solution for that initial value.

How do the continuous and the discrete blow-up times compare?
We consider scheme (32) for $k\lambda < 0$ and $u_o > 1$. It seems reasonable to consider for given λ only those k for which it happens that there is an N such that $1 - \lambda k(1 - y_N) = 0$, i.e.

for which blow-up actually happens. Then we get from (19) and (22) that

$$(1-k\lambda)^N = \frac{u_o}{u_o - 1} = e^{-\lambda T}. \tag{34}$$

To get a rough idea what (34) actually means, we make further simplifications:
$\lambda = -1,\ N = 1,\ u_o > 2$. Then

$$t_1 = k = \frac{1}{u_o - 1} < 1 \tag{35}$$

and

$$\begin{aligned} T &= \ln \frac{u_o}{u_o - 1} \\ &= \ln(1+k) \\ &= k - \frac{k^2}{2} + \frac{k^3}{3} - + \ldots . \end{aligned} \tag{36}$$

Thus t_1 is too large, and the error is of order k^2.
Better approximations of the blow-up can be obtained by using this scheme with a standard step size control, or with a nonlinear transformation as discussed by Stuart and Floater [17]. Note that their function $H(u)$ satisfies
$H(u) = u/f(u)$ if $f(u) \propto u^m$ as $u \to \infty$ and
$H(u) = 1/f(u)$ if $f(u) \propto e^u$ as $u \to \infty$.
We can thus expect that $H(u) = 1/f'(u)$ will be the right choice in the general case, and that their method will simplify considerably when used in combination with scheme (13). This will be dealt with in [10].

3 Exact difference schemes

In this section we compare the exact schemes we found in Mickens' book with the corresponding schemes obtained by using (13). For deriving the exact schemes, Mickens used a-priori knowledge about the solution of the differential equations. Application of our method (13) does not require such knowledge.

The list contains:

the reference number in the book,
the differential equation,
the exact scheme, and
the difference scheme obtained by using (13).
For more transparence, we use u_j for the time iterates in Mickens' schemes and y_j for the time iterates in our schemes.

The schemes obtained with (13) are second order accurate and self-adjoint up to their order of accuracy [10]. Mickens' schemes are sometimes self-adjoint, sometimes not. We did not change that. Because of this, our schemes seem to differ more from Mickens' schemes than they actually do.

Schemes adjoint to each other always have the same order of accuracy, and the first term in the error expansion is same size, with opposite sign. Consequently, self-adjoint schemes have always an even order of accuracy [8]. If a scheme is exact, its adjoint is also exact. The arithmetic mean of the two is then self-adjoint and exact.

(3.3.5) The differential equation

$$\dot{u} = -\lambda u \tag{37}$$

has the exact scheme [11, (3.3.5)]

$$\frac{u_{n+1} - u_n}{(1 - e^{-\lambda k})/\lambda} = -\lambda u_n. \tag{38}$$

Using (13), we obtain

$$\frac{y_{n+1} - y_n}{k} = -\lambda (y_n + y_{n+1})/2. \tag{39}$$

We note that

$$k = (1 - e^{-\lambda k})/\lambda + k\left(\frac{\lambda k}{2!} - \frac{(\lambda k)^2}{3!} + - \ldots\right). \tag{40}$$

(3.3.32)

$$\begin{aligned} \dot{u} &= u^2 && (41) \\ \frac{u_{n+1} - u_n}{k} &= u_n u_{n+1} && (42) \\ \frac{y_{n+1} - y_n}{k} &= y_n y_{n+1} && (43) \end{aligned}$$

This example was discussed in the introduction.

(3.3.27)

$$\begin{aligned}
\dot{u} &= \lambda_1 u - \lambda_2 u^2 && (44)\\
\frac{u_{n+1} - u_n}{(e^{\lambda_1 k} - 1)/\lambda_1} &= \lambda_1 u_n - \lambda_2 u_{n+1} u_n && (45)\\
\frac{y_{n+1} - y_n}{k} &= \lambda_1 (y_n + y_{n+1})/2 - \lambda_2 y_{n+1} y_n && (46)
\end{aligned}$$

In the case $\lambda_1 = \lambda_2 = \lambda$ this leads to

$$\frac{y_{n+1} - y_n}{k} = \frac{\lambda}{2}(y_n(1 - y_{n+1}) + y_{n+1}(1 - y_n)), \qquad (47)$$

the arithmetic mean of schemes (21) and (23). It was considered in section 2. A comparison with (38) and (42) shows that it is the linear term in eq. (44) that introduces the error when applying scheme (13).

(3.3.42)

$$\begin{aligned}
\dot{u} &= -u^3 && (48)\\
\frac{u_{n+1} - u_n}{k} &= -\frac{2u_{n+1}^2 u_n^2}{u_{n+1} + u_n} && (49)\\
\frac{y_{n+1} - y_n}{k} &= +y_n^3/2 - 3y_n^2 y_{n+1}/2 && (50)\\
&= \frac{-2y_n^3 y_{n+1} + y_n^4 - 3y_n^2 y_{n+1}^2}{2(y_{n+1} + y_n)} && (51)
\end{aligned}$$

Note that $(-2 + 1 - 3)/2 = -2$. Thus the error of scheme (51) is governed by the size of $|y_{n+1}/y_n - 1|$, and it is a very good approximation to (49) whenever $y_{n+1}/y_n \approx 1$ (no additional condition on k !).

(3.3.41)

$$\begin{aligned}
\dot{u} &= -u/2 + 1/(2u) && (52)\\
\frac{u_{n+1} - u_n}{1 - e^{-k}} &= -\frac{u_n^2}{u_{n+1} + u_n} + \frac{1}{u_{n+1} + u_n} && (53)\\
\frac{y_{n+1} - y_n}{k} &= -\frac{y_{n+1} + y_n}{4} + \frac{3}{4\ y_n} - \frac{y_{n+1}}{4\ y_n^2} && (54)
\end{aligned}$$

$$= -\frac{y_n^2 + y_{n+1}^2 + 2y_n y_{n+1}}{4(y_{n+1}+y_n)} + \frac{3 + 2y_{n+1}/y_n - (y_{n+1}/y_n)^2}{4(y_{n+1}+y_n)} \tag{55}$$

Note that $(1+1+2)/4 = 1$ and $(3+2-1)/4 = 1$. Thus (55) is a qualitatively correct approximation if $y_{n+1}/y_n \approx 1$ and if k is small enough so that the higher order terms in (40), $\lambda = 1$, do not cause qualitative changes.

(3.3.11)

$$\ddot{u} = -\omega^2 u \tag{56}$$

$$\frac{u_{n+1} - 2u_n + u_{n-1}}{\frac{4}{\omega^2}\sin^2\frac{k\omega}{2}} = -\omega^2 u_n \tag{57}$$

To apply formula (13), we transform (56) into a first order system and get:

$$\begin{aligned} \frac{y_{n+1} - y_n}{k} &= \frac{v_{n+1} + v_n}{2} \\ \frac{v_{n+1} - v_n}{k} &= -\omega^2 \frac{y_{n+1} + y_n}{2} \; . \end{aligned} \tag{58}$$

To get a second order difference equation from this, we evaluate (58) both centered in $n + \frac{1}{2}$ (as written down) and in $n - \frac{1}{2}$, subtract one from the other, devide by k, eliminate the vs and get

$$\frac{y_{n+1} - 2y_n + y_{n-1}}{k^2} = -\omega^2(y_{n-1} + 2y_n + y_{n+1})/4. \tag{59}$$

We note that

$$k^2 = \frac{4}{\omega^2}\sin^2\frac{k\omega}{2} + k^2\left(\frac{2k^2}{3!} - \left(\frac{2}{5!} + \frac{1}{36}\right)\left(\frac{k\omega}{2}\right)^4 + - \ldots\right). \tag{60}$$

(3.5.16) and (7.3.19)

$$u_t = u u_{xx} \tag{61}$$

has the special solutions

$$u(x,t) = \left(\frac{\alpha}{2}x^2 + \beta_1 x + \beta_2\right)/(\alpha_1 - \alpha t) \; . \tag{62}$$

No exact scheme is known, but two 'best schemes': best according to the principles formulated in [11, p. 85]. They are

$$\frac{u_m^{n+1} - u_m^n}{\Delta t} = u_m^{n+1}\,\frac{u_{m+1}^n - 2u_m^n + u_{m-1}^n}{\Delta x^2} \quad \text{and} \tag{63}$$

$$\frac{u_m^{n+1} - u_m^n}{\Delta t} = u_m^n\,\frac{u_{m+1}^{n+1} - 2u_m^{n+1} + u_{m-1}^{n+1}}{\Delta x^2} \; . \tag{64}$$

Scheme (13) produces the arithmetic mean of the two adjoint schemes:

$$\frac{y_m^{n+1}-y_m^n}{\Delta t} = \frac{1}{2}\left(y_m^{n+1}\,\frac{y_{m+1}^n - 2y_m^n + y_{m-1}^n}{\Delta x^2} + y_m^n\,\frac{y_{m+1}^{n+1} - 2y_m^{n+1} + y_{m-1}^{n+1}}{\Delta x^2} \right) . \tag{65}$$

4 Symplectic schemes

W. Kahan considered in his (unpublished) lecture notes on 'unconventional numerical methods' the first order system

$$\begin{aligned} \dot{u} &= \alpha u + \beta u v, \qquad u(0) = u_o \\ \dot{v} &= \gamma v + \delta u v, \qquad v(0) = v_o \end{aligned} \tag{66}$$

with given constants $\alpha, \beta, \gamma, \delta$, and gave the following nonstandard difference scheme for it:

$$\begin{aligned} \frac{u_{n+1}-u_n}{k} &= \frac{\alpha}{2}(u_{n+1}+u_n) + \frac{\beta}{2}(u_{n+1}v_n + u_n v_{n+1}) \\ \frac{v_{n+1}-v_n}{k} &= \frac{\gamma}{2}(v_{n+1}+v_n) + \frac{\delta}{2}(u_{n+1}v_n + u_n v_{n+1}) . \end{aligned} \tag{67}$$

The axes $u = 0$ and $v = 0$ are invariant under (66). In the case

$$\alpha < 0, \quad \beta > 0, \quad \gamma > 0, \quad \delta < 0 \tag{68}$$

this is a simplified predator (u) and pray (v) Lotka-Volterra system. For positive u and v the dynamical system (66) has one equilibrium point, $\bar{u} = -\alpha/\beta > 0, \quad \bar{v} = -\gamma/\delta > 0$. Point $(\bar{u}, \bar{v})$ has neutral stability, and thus the trajectories of system (66) with positive initial values (u_o, v_o) are closed curves around $(\bar{u}, \bar{v})$. The Jacobian in $(\bar{u}, \bar{v})$ has two conjugate purely imaginary eigenvalues.

When such a system is approximated numerically, it is not sufficient that the Jacobian of the discrete model has conjugate complex eigenvalues of modulus 1 in $(\bar{u}, \bar{v})$: Examples are known for which this condition is satisfied, but the discrete trajectories spiral (inwards or outwards) instead of being closed curves. In the case of system (67), however, the discrete trajectories are closed curves. Sanz-Serna [16] explained that this is so because system (67) is symplectic with respect to a noncanonical Hamiltonian. M.J. Gander [6] then showed that the following scheme for system (66) ($\alpha = \delta = 1,\ \beta = \gamma = -1$) is symplectic as well:

$$\begin{aligned} \frac{u_{n+1} - u_n}{k} &= u_n - u_n v_n \\ \frac{v_{n+1} - v_n}{k} &= -v_n + u_{n+1} v_n \quad . \end{aligned} \tag{69}$$

It is easy to check that system (67) is the system we obtain by applying formula (13) to system (66).

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