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A NEW FAMILY OF EXPLICIT TWO–STAGE METHODS OF ORDER THREE FOR THE SCALAR AUTONOMOUS IVP*

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Abstract

In this work, we propose a new family of explicit two–stage formulae for the numerical integration of scalar autonomous ODEs. For scalar autonomous problems, these methods can be seen as a generalization of the explicit two–stage Runge–Kutta ones, that provides better order and stability results. In fact, we show that it is possible to obtain formulae of order three with only two evaluations per step. It is also possible to get A–stable and L–stable methods of order three from the preceding family, without losing the explicitness of the formulae. Finally we carry out some numerical experiments.

1 Introduction.

We consider the scalar autonomous problem

$$y' = f(y)\,, \quad y(x_0) = y_0\,, \quad f : \mathbb{R} \to \mathbb{R}\,. \tag{1}$$

From Butcher's theory we know that a Runge–Kutta method which has order k for a scalar initial value problem may have order less than k when applied to a problem involving a system of differential equations. However, when $k \leq 3$, any Runge–Kutta method has the same order applied to systems as it has when applied to the scalar autonomous problem (see for example [1], pp. 173–175).

The Butcher theory also shows that an s–stage explicit Runge–Kutta method cannot have order greater than s ([1], pp. 176–178). Therefore, an explicit two–stage Runge–Kutta method cannot have order greater than two when applied to (1).

Taking advantage of the structure of the problem (1), we obtain new explicit methods of order three and only two evaluations per step. Our methods can be seen as a generalization of the explicit Runge–Kutta methods (for scalar autonomous problems), that provides better order and stability results with the same number of stages.

Moreover, the stability function of all the explicit Runge–Kutta formulae is a polynomial, and so, none of them is A–stable ([1], pp. 198–200).

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Many unconventional classes of methods have been proposed in the literature (see for instance [2], pp. 171–186), looking for better stability properties. Some of them, the so called linear multistep methods with variable matrix coefficients, make use of variable matrix coefficients that in practice are taken to be an approximation to $-\partial f/\partial y$, for the purpose of achieving good stability properties, but at the cost of being linearly implicit (see [3], pp. 39–45). Other methods, the so called nonlinear methods, have good stability properties (A–stability or L–stability) without losing the explicitness of the resulting formulae. However, such methods have many problems involving the level of local accuracy. In fact, most of these methods fail when the solution goes through a zero (losing their order), due to strange local truncation errors.

Our methods do not have this kind of problems. The local truncation errors associated to our formulae, are of the same form as those associated to any Runge–Kutta method. In fact, the stages are given as in the Runge–Kutta ones, but the resulting formulae involve rational functions of the stages. At the cost of losing the linearity in the final formulae, we get many free parameters that allow us to obtain a family of three order methods, whose stability function is given by a rational function. Special choices of such parameters provide A–stable and L–stable formulae with associated stability function given by Padé approximations to the exponential, retaining the order three.

We also get methods that minimize the local truncation error (in fact, those methods applied to (1) when f is linear, show order four).

We can generalize the preceding idea and obtain explicit s–stage A–stable methods for the problem (1) of order greater than s. For example, it is possible to get explicit three-stage A–stable formulae for problem (1), of order five. However, in the present work we restrict our attention to two–stage methods.

Finally we show that the new methods perform well when applied to the problem (1), carrying out some numerical experiments.

2 The new family of methods.

Let us consider the family of explicit two–stage methods for problem (1), defined by

$$y_{n+1} = y_n + hF(k_1, k_2)\,, \tag{2}$$

where k_1 and k_2 given by

$$k_1 = f(y_n)\,, \quad k_2 = f(y_n + hc_2k_1)\,, \tag{3}$$

with $c_2 \neq 0$. $F(x, y)$ is some rational function given in terms of the quotient of two homogeneous polynomials $N(x, y)$ and $D(x, y)$ with degrees $r+1$ y r respectively, for some $r \in \mathbb{N}$. So $F(x, y)$ takes the form

$$F(x, y) = \frac{N(x, y)}{D(x, y)} = \frac{\displaystyle\sum_{i=0}^{r+1} N_i x^{r-i+1} y^i}{\displaystyle\sum_{i=0}^{r} D_i x^{r-i} y^i}\,. \tag{4}$$

Obviously, we can assume that the polynomials $N(x, y)$ and $D(x, y)$ do not have common factors, without loss of generality.

Taking $r = 0$ in (4), we get all the explicit two–stage Runge–Kutta formulae (for problem 1) as a subfamily of our methods.

It is easily seen that the consistency condition for such a method reads

$$\frac{N(1,1)}{D(1,1)} = 1\,. \tag{5}$$

Therefore, we must take $D(1,1) \neq 0$ so that the consistency condition holds. There is no loss of generality in assuming that $N(1,1) = D(1,1) = 1$ holds for any consistent method of our family.

From the previous assumptions we get uniqueness in the representation of the consistent methods. In what follows, we restrict our attention to consistent methods of our family.

Now we introduce new notations, in order to obtain a better expression of our formulae that greatly simplifies the study of the order of consistency and the linear stability properties. We define

$$s = \frac{k_2 - k_1}{c_2 k_1}\,, \tag{6}$$

where k_1, k_2 are given by (3). Note that s depends on the parameter c_2. In terms of s, any consistent method of the preceding family takes the form

$$y_{n+1} = y_n + hk_1 G(s)\,, \tag{7}$$

where G is given by

$$G(s) = \frac{P(s)}{Q(s)} = \frac{1 + \sum_{i=1}^{n} n_i s^i}{1 + \sum_{i=1}^{d} d_i s^i}\,, \tag{8}$$

with P and Q not having common factors. Any consistent method defined in terms of k_1 and k_2 through (2) can be but in terms of s in an only way, and the resulting formula takes the form (7). We have that $n_0 = d_0 = 1$ in (8), from the condition $N(1,1) = D(1,1) = 1$. In fact, (6) implies $k_2/k_1 = 1 + c_2 s$, and therefore

$$F(k_1, k_2) = k_1 F\left(1, \frac{k_2}{k_1}\right) = k_1 F(1, 1 + c_2 s) = k_1 G(s)\,. \tag{9}$$

It is easily seen that n and d (in 8) are given in terms of N_i, D_i, and r (in 4) by $n = \max\{i = 0, 1, \ldots, r+1 / N_i \neq 0\}$ and $d = \max\{i = 0, 1, \ldots, r / D_i \neq 0\}$. For more details, see [4].

3 Order of the methods.

Now we investigate the order of consistency of any consistent method (7), by considering the associated local truncation error T_{n+1} at the point x_n, that is

$$T_{n+1} = y(x_{n+1}) - y(x_n) - hk_1 G(s)\,, \tag{10}$$

where now k_1, k_2 and s are given by

$$k_1 = f(y(x_n))\,, \quad k_2 = f(y(x_n) + hc_2 k_1)\,, \quad s = \frac{k_2 - k_1}{c_2 k_1}\,, \tag{11}$$

and G is defined by (8).

We suppose that f is smooth enough in order to give sense to all the derivatives that appear in what follows.

If we expand $s = s(h)$ as a function of h, we obtain

$$s = hf_y + \frac{h^2}{2} c_2 f f_{yy} + O(h^3)\,, \tag{12}$$

where f, f_y and f_{yy} are all evaluated at the point $y(x_n)$. So it is clear that $s = O(h)$. From this fact, we can see that when considering the equations related to order lower or equal to $k+1$, it suffices to consider the parameters n_i and d_i with $i \leq k$, that is, we can restrict our attention to formulae given by (7) with $n = d = k$.

A consistent method of the preceding family must satisfy the following conditions in order to be of order three

$$\begin{aligned} n_1 - d_1 &= \frac{1}{2}\,, && (13) \\ (n_2 - d_2) - d_1\,(n_1 - d_1) &= \frac{1}{6}\,, && (14) \\ c_2\,(n_1 - d_1) &= \frac{1}{3}\,. && (15) \end{aligned}$$

Any consistent method satisfying (13) has, at least, order two. The above system has a family of solutions given in terms of the parameters d_1 and d_2 by

$$c_2 = \frac{2}{3}\,, \quad n_1 = \frac{1}{2} + d_1\,, \quad n_2 = \frac{1}{6} + \frac{1}{2}d_1 + d_2\,. \tag{16}$$

The free parameters d_i and n_i with $i \geq 3$ can be arbitrarily chosen. From (16) we have that any three order method of the family takes the form

$$y_{n+1} = y_n + hk_1 G(s)\,, \tag{17}$$

where

$$G(s) = \frac{1 + \dfrac{1+2d_1}{2}s + \dfrac{1+3d_1+6d_2}{6}s^2 + \displaystyle\sum_{i=3}^{n} n_i s^i}{1 + d_1 s + d_2 s^2 + \displaystyle\sum_{i=3}^{d} d_i s^i}\,, \tag{18}$$

and k_1, k_2 and s are given by

$$k_1 = f(y_n)\,, \quad k_2 = f\left(y_n + \frac{2}{3}hk_1\right)\,, \quad s = \frac{3(k_2 - k_1)}{2k_1}\,. \tag{19}$$

A consistent formula of the family must satisfy the following additional conditions in order to be of order four

$$\begin{aligned} (n_3 - d_3) - d_1\,(n_2 - d_2) + (d_1^2 - d_2)\,(n_1 - d_1) &= \frac{1}{24}\,, && (20) \\ c_2\,[(n_2 - d_2) - d_1\,(n_1 - d_1)] &= \frac{1}{6}\,, && (21) \\ c_2^2\,(n_1 - d_1) &= \frac{1}{4}\,, && (22) \end{aligned}$$

It is a simple task to show that no two-stage method of our family has order four, but we can make use of the free parameters to obtain three order methods with some interesting properties. For example, we may try to minimize the local truncation error.

4 Optimal methods with respect to the local truncation error.

The local truncation error of any three order method of the family is

$$T_{n+1} = \left(\frac{1 - 24\,(n_3 - d_3) + 12\,d_2 + 4\,d_1}{24}\,f f_y^3 + \frac{1}{18}\,f^2 f_y f_{yy} + \frac{1}{216}\,f^3 f_{yyy}\right) h^4 + O(h^5)\,, \tag{23}$$

and so it is not possible to attain order four, since two error coefficients are constant. However, it seems reasonable to use the free parameters to remove the variable coefficient since this will reduce the overall magnitude of the principal error term. Setting

$$n_3 = \frac{1 + 4\,d_1 + 12\,d_2 + 24\,d_3}{24}\,, \tag{24}$$

we get formulae that can be seen as optimal with respect to the local truncation error.

5 Looking for good linear stability properties.

Applying a consistent method of our family to the linear scalar test equation

$$y' = \lambda y\,, \quad \lambda \in \mathbb{C}\,, \tag{25}$$

we get

$$y_{n+1} = R(z)\, y_n\,, \tag{26}$$

where $R(z)$ is the associated stability function, with $z = h\lambda$. When applied to the test equation, we have from (6) that $s = h\lambda$, and therefore $R(z)$ is

$$R(z) = 1 + zG(z)\,, \tag{27}$$

with G given by (8).

Taking $c_2 = 2/3$, $d_1 = -1/2$, $d_2 = 1/12$ and $n_i = d_i = 0$ for $i \geq 3$ in (18) we obtain a three order method whose stability function is given by

$$R(z) = \frac{12 + 6z + z^2}{12 - 6z + z^2}\,, \tag{28}$$

that is, the $(2,2)$–Padé approximation to e^z. The method takes the form

$$y_{n+1} = y_n + hk_1 \left(\frac{12}{12 - 6s + s^2} \right)\,. \tag{29}$$

So we have an first example of an A–stable explicit two–stage method of order three. Moreover, it belongs to the family of optimal methods with respect to the local truncation error (see 24), and therefore when applied to the linear problem $y' = \alpha\, y + \beta$, shows order four.

It is also easy to obtain L–stable methods of order three. For example, from the values $c_2 = 2/3$, $d_1 = -3/4$, $d_2 = 1/4$, $d_3 = -1/24$, $n_i = 0$ for $i \geq 3$ and $d_i = 0$ for $i \geq 4$ in (18), we get a three order method whose stability function is given by the $(1,3)$–Padé approximation to e^z, that is

$$R(z) = \frac{24 + 6z}{24 - 18z + 6z^2 - z^3}\,. \tag{30}$$

The resulting formula is optimal with respect to the local truncation error, and takes the form

$$y_{n+1} = y_n + hk_1 \left(\frac{24 - 6s + s^2}{24 - 18s + 6s^2 - s^3} \right)\,. \tag{31}$$

It is also possible to construct an L–stable method of order three, having the $(1,2)$–Padé approximation to e^z as stability function (see [4]). Moreover, for a given rational function $R(z)$ we can obtain formulae of the family (2), whose stability function is $R(z)$ (see [5]).

6 A numerical experiment with a stiff non–linear problem.

The theoretic study of the non–linear stability properties of the formulae is very difficult, due to the rational functions of the stages involved in our methods. So we consider a numerical experiment with a non–linear stiff problem, $y'(x) = f(y(x))$, in which f is one–sided Lipschitz continuous with one–sided Lipschitz constant 0. We know that if u and v are two solutions to such a problem with initial values given at x_0, then for any $x \geq x_0$, $|u(x) - v(x)| \leq |u(x_0) - v(x_0)|$ holds. We want to see if the numerical solutions obtained from our methods have a similar behaviour.

We consider the stiff problem

$$y' = -y\sqrt{y^2 + 10000}\,, \quad y(0) = a\,, \tag{32}$$

whose solution is given in terms of the initial condition a by

$$y(x) = \frac{200\, a\left(100+\sqrt{a^2+10000}\right)\, e^{100\,x}}{\left(100+\sqrt{a^2+10000}\right)^2\, e^{200\,x} - a^2}\,. \tag{33}$$

It is easy to show that the true solutions are contractive, and after a short transient they are virtually identical to the steady–state solution $y(x) = 0$ (the solution of (33) when $a = 0$).

When we apply the A–stable formula to this problem with fixed step $h = 0.1$ for a range of values of a we get Figure 1. The numerical solutions we obtain do not have a contractive behaviour. However, it is clear that the numerical solutions have a good qualitative behaviour.

Applying the L–stable method to the same problem, for a range of values of a and with fixed step $h = 0.1$, we get Figure 2. Now the numerical solutions are contractive, at least for x big enough. In fact, when $|a| < 70$ (with fixed step $h = 0.1$) they seem to be contractive for $x \geq 0$.

For fixed h and a, the L–stable method is better than the A–stable from a qualitative point of view (the numerical solutions go faster to zero and show a better contractivity behaviour).

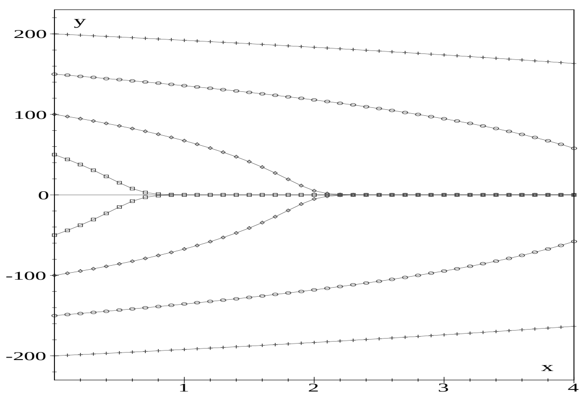

Figure 1: $y' = -y\,(y^2+10000)^{1/2}$, $y(0) = a$, $h = 0.1$, $x \in [0,4]$. Numerical solutions for $a = -200, -150, -100, -50, 50, 100, 150, 200$ with the A–stable method.

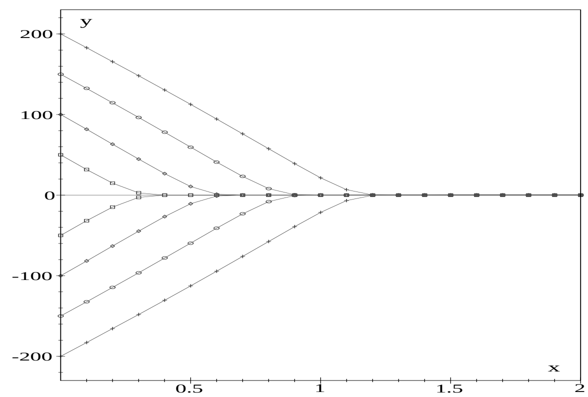

Figure 2: $y' = -y\,(y^2+10000)^{1/2}$, $y(0) = a$, $h = 0.1$, $x \in [0,2]$. Numerical solutions for $a = -200, -150, -100, -50, 50, 100, 150, 200$ with the L–stable method.

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