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

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Abstract

We investigate a new family of explicit two–stage methods for the numerical integration of scalar autonomous ODEs. We show that it is possible to obtain formulae of order three with only two evaluations per step. Moreover, we can obtain A–stable and L–stable methods of order three from the preceding family. Finally we compare the new methods with other conventional methods, to show that they perform better, carrying out some numerical experiments.

1 Introduction.

Our aim in the present work is to develop new explicit A–stable methods of order three, involving two function evaluations per step, for the scalar autonomous problem

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

It is well–known that an explicit two–stage Runge–Kutta method cannot have order greater than two when applied to (1) (see [2], pp. 173–178). Moreover, none of them is A–stable (the stability function of all such methods is a polynomial) ([2], pp. 198–203).

The explicit two–stage methods we get, can be shown as a generalization of the explicit two–stage R–K methods (for scalar autonomous problems) that provide better order and linear stability results. For our methods, 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–stable methods of order three. In fact, as a first example, we can obtain an

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A–stable explicit two–stage method of order three, whose stability function is given by the $(2,2)$–Padé approximation to the exponential function (see [1], pp. 50–51). Furthermore, we can get an L–stable method, with associated stability function given by the $(1,2)$–Padé approximation to the exponential.

We can generalize the previous idea and obtain explicit s–stage A–stable methods 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 shall restrict our attention to two–stage methods.

Finally we compare the new methods with other methods of Runge–Kutta type, to show that they perform better when applied to the problem (1), carrying out some numerical experiments.

2 Construction of the new methods.

We 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

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

In the above expression it is possible to consider $r \in \mathbb{Z}$. However, it is easily seen that for any $r < 0$ we can obtain an equivalent formulae of the preceding family of methods, multiplying the numerator and the denominator of $F(x,y)$ by the factor $x^{-r}y^{-r}$.

Obviously, there is no loss of generality in assuming that the polynomials $N(x,y)$ and $D(x,y)$ do not have common factors.

The family of methods we have just defined, can be shown as a generalization of the explicit two–stage Runge–Kutta methods (for the problem 1). In fact, taking $r = 0$ in (4) we get all the R–K formulae as a subfamily of our methods.

3 Consistency of the methods.

It is well-known that consistency is a necessary condition for a numerical process to be convergent. So we are interested in studying the consistency of the methods given by (2).

A single–step method for problem (1) takes the form

$$y_{n+1} = y_n + h\Phi(y_n, h)\,. \tag{5}$$

The numerical method (5) is said to be consistent with the differential equation (1) if

$$\Phi(y, 0) = f(y)\,. \tag{6}$$

For our methods Φ is given by

$$\Phi(y,h) = F(k_1,k_2)\,, \tag{7}$$

where F is defined as in (4), but now

$$k_1 = f(y)\,, \quad k_2 = f(y + hc_2k_1)\,. \tag{8}$$

Taking $h = 0$ we have $k_1 = k_2 = f(y)$, and from the fact that F is an homogeneous function we get

$$\Phi(y,0) = F(f(y), f(y)) = \frac{N(1,1)}{D(1,1)} f(y)\,. \tag{9}$$

Thus we obtain the consistency condition

$$\frac{N(1,1)}{D(1,1)} = 1\,. \tag{10}$$

It follows that we must take $D(1,1) \neq 0$ so that the consistency condition holds. From now on, and without loss of generality, we can also assume that $N(1,1) = D(1,1) = 1$ holds for any consistent method of our family.

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

4 A useful notation.

We want to simplify the study of the order of consistency and the linear stability properties of our methods. So we will introduce new notations in order to obtain a better expression of our formulae. We define

$$s = \frac{k_2 - k_1}{c_2k_1}\,, \tag{11}$$

where $c_2 \neq 0$ and k_1, k_2 are given by (3). Note that s depends on the choice of the parameter c_2. In terms of s, any consistent method of the preceding family takes the form

$$y_{n+1} = y_n + hk_1G(s)\,, \tag{12}$$

where G is given by

$$G(s) = \frac{P(s)}{Q(s)} = \frac{1 + \sum_{i=1}^{n} n_i s^i}{1 + \sum_{i=1}^{d} d_i s^i}\,, \tag{13}$$

with P and Q not having common factors. It is easy to show that 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 (12) (the opposite is also true). Since (11) implies $k_2/k_1 = 1 + c_2s$, we have

$$F(k_1,k_2) = k_1F\left(1, \frac{k_2}{k_1}\right) = k_1F(1, 1 + c_2s) = k_1G(s)\,. \tag{14}$$

In the same manner we have from (11) that

$$k_1 G(s) = k_1 G\left(\frac{k_2 - k_1}{c_2 k_1}\right) = F(k_1, k_2)\,, \tag{15}$$

holds.

It is easily seen that n and d (in 13) 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 $d = \max\{i = 0, 1, \ldots, r/D_i \neq 0\}$. Obviously, we also have $n_0 = d_0 = 1$ in (13) from the condition $N(1,1) = D(1,1) = 1$.

It is a simple task to show that $s = O(h)$ and therefore we have that $s^k = O(h^k)$ for any given $k \in \mathbb{N}$. This implies that when we consider 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 (12) with $n = d = k$.

5 Attainable order for the methods.

We will investigate the order of consistency of any explicit two–stage method given by (12). As is usual with other single–step methods, we begin considering the local truncation error T_{n+1} of a consistent formula of our family at the point x_n, that is

$$T_{n+1} = y(x_{n+1}) - y(x_n) - hk_1 G(s)\,, \tag{16}$$

where now k_1, k_2 and s are given by

$$k_1 = f(y(x_n))\,, \quad k_2 = f(y(x_n) + hc_2 k_1)\,, \quad s = \frac{k_2 - k_1}{c_2 k_1}\,, \tag{17}$$

and G is defined by (13).

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

To show that some methods of the family attain order three, it suffices to consider the subfamily we get when taking $n = d = 2$ in the expression (13) of function G (as we have shown in the last section), and we will do so in the later.

Now we consider the Taylor's expansion of $y(x_{n+1}) = y(x_n + h)$

$$y(x_{n+1}) = y(x_n) + hf + \frac{h^2}{2} f f_y + \frac{h^3}{6}[f f_y^2 + f^2 f_{yy}] + O(h^4)\,, \tag{18}$$

where f, f_y and f_{yy} are all evaluated at the point $y(x_n)$. If we expand $s = s(h)$ as a function of h (note that s depends on c_2 through expression (11)), we obtain

$$s = hf_y + \frac{h^2}{2} c_2 f f_{yy} + O(h^3)\,, \tag{19}$$

and it is clear that $s = O(h)$. Now from (16), (18) and (19) we get

$$\begin{aligned} T_{n+1} = \frac{h^2}{2}(1 - 2(n_1 - d_1)) f f_y \quad + \quad & \frac{h^3}{6}[(1 - 6((n_2 - d_2) - d_1(n_1 - d_1))) f f_y^2 \\ & + (1 - 3c_2(n_1 - d_1)) f^2 f_{yy}] + O(h^4)\,, \end{aligned} \tag{20}$$

and therefore a consistent method must satisfy the following conditions in order to have order three

$$\begin{aligned} n_1 - d_1 &= \frac{1}{2}, & (21)\\ (n_2 - d_2) - d_1(n_1 - d_1) &= \frac{1}{6}, & (22)\\ c_2(n_1 - d_1) &= \frac{1}{3}. & (23) \end{aligned}$$

Any consistent method satisfying (21) has, at least, order two.

It is easy to check that the above system has many solutions. In fact, we get a two–parameter family of solutions given in terms of d_1 and d_2 by

$$c_2 = \frac{2}{3}, \quad n_1 = \frac{1}{2} + d_1, \quad n_2 = \frac{1}{6} + \frac{1}{2}d_1 + d_2. \tag{24}$$

It is a simple task to show that no two-stage method of our family has order greater than three (it suffices to take $n = d = 3$ in (13) and expand to an higher order the above expressions).

From (24) we have that any three order method of the subfamily we get taking (n=d=2) in (13) takes the form (in terms of the parameters d_1 and d_2)

$$y_{n+1} = y_n + hk_1 G(s), \tag{25}$$

where

$$G(s) = \frac{1 + \dfrac{1+2d_1}{2}s + \dfrac{1+3d_1+6d_2}{6}s^2}{1 + d_1 s + d_2 s^2}, \tag{26}$$

and k_1, k_2 and s are given as usually by

$$k_1 = f(y_n), \quad k_2 = f\left(y_n + \frac{2}{3}hk_1\right), \quad s = \frac{3(k_2 - k_1)}{2k_1}. \tag{27}$$

In order to get the general form of a three order method of our family (without the restriction $n = d = 2$) it suffices to take in the above expressions

$$G(s) = \frac{1 + \dfrac{1+2d_1}{2}s + \dfrac{1+3d_1+6d_2}{6}s^2 + \displaystyle\sum_{i=3}^{n} n_i s^i}{1 + d_1 s + d_2 s^2 + \displaystyle\sum_{i=3}^{d} d_i s^i}, \tag{28}$$

in place of (26). This follows from the fact that $s = O(h)$.

6 A first example.

As a first example, we can take $d_i = 0$ and $n_{i+2} = 0$ for $i \geq 1$. The resulting three order formula is given by

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

where k_1 and s are defined through (27).

Let us consider the problem

$$y' = 1 - y^2\,, \quad y(0) = 0\,, \tag{30}$$

with true solution given by $y(x) = (e^{2x} - 1)/(e^{2x} + 1)$. When we apply method (29) to this problem for a range of values of x and h, we get the Table 1 of errors.

Table 1: Errors for our method of order three.

$\lvert\text{error}\rvert$	$h = 0.1$	$h = 0.05$	$h = 0.025$	$h = 0.0125$
$x = 1.0$	$0.6267D-05$	$0.8245D-06$	$0.1057D-06$	$0.1338D-07$
$x = 3.0$	$0.5719D-05$	$0.6606D-06$	$0.7936D-07$	$0.9725D-08$
$x = 5.0$	$0.2464D-06$	$0.2846D-07$	$0.3419D-08$	$0.4189D-09$
$x = 7.0$	$0.7107D-08$	$0.8215D-09$	$0.9868D-10$	$0.1209D-10$
$x = 9.0$	$0.1776D-09$	$0.2054D-10$	$0.2468D-11$	$0.3022D-12$

Now we consider the two–stage Heun method of order two (an example of an explicit two–stage Runge–Kutta formula), that is

$$y_{n+1} = y_n + h\left(\frac{1}{4}k_1 + \frac{3}{4}k_2\right)\,, \tag{31}$$

where

$$k_1 = f(y_n)\,, \quad k_2 = f\Bigl(y_n + \frac{2}{3}hk_1\Bigr)\,. \tag{32}$$

Note that Heun's method makes use of the same evaluations as our method (k_1 y k_2 are the same in both methods). When we apply Heun's formula to problem (30) we obtain Table 2 of errors.

Table 2: Errors for Heun's formula of order two.

$\lvert\text{error}\rvert$	$h = 0.1$	$h = 0.05$	$h = 0.025$	$h = 0.0125$
$x = 1.0$	$0.7298D-03$	$0.1745D-03$	$0.4267D-04$	$0.1055D-04$
$x = 3.0$	$0.1532D-03$	$0.3540D-04$	$0.8534D-05$	$0.2096D-05$
$x = 5.0$	$0.5758D-05$	$0.1309D-05$	$0.3142D-06$	$0.7706D-07$
$x = 7.0$	$0.1611D-06$	$0.3615D-07$	$0.8645D-08$	$0.2118D-08$
$x = 9.0$	$0.4002D-08$	$0.8866D-09$	$0.2114D-09$	$0.5175D-10$

The two preceding tables show that our method perform better. Moreover, if we consider the three–stage Heun's method of order three, that is

$$y_{n+1} = y_n + h\left(\frac{1}{4}k_1 + \frac{3}{4}k_3\right)\,, \tag{33}$$

where now

$$k_1 = f(y_n)\,, \quad k_2 = f\Bigl(y_n + \frac{1}{3}hk_1\Bigr)\,, \quad k_3 = f\Bigl(y_n + \frac{2}{3}hk_2\Bigr)\,, \tag{34}$$

and we apply it to problem (30), we get Table 3. So our first method performs more or less as the three order Heun's method (from an error and order point of view), but it makes use of less function evaluations per step (see Figures 1 and 2).

Table 3: Errors for Heun's method of order three.

$\lvert\text{error}\rvert$	$h = 0.1$	$h = 0.05$	$h = 0.025$	$h = 0.0125$
$x = 1.0$	$0.6910D-05$	$0.8471D-06$	$0.1045D-06$	$0.1298D-07$
$x = 3.0$	$0.6283D-05$	$0.7298D-06$	$0.8793D-07$	$0.1079D-07$
$x = 5.0$	$0.2568D-06$	$0.2975D-07$	$0.3578D-08$	$0.4387D-09$
$x = 7.0$	$0.7298D-08$	$0.8451D-09$	$0.1016D-09$	$0.1245D-10$
$x = 9.0$	$0.1811D-09$	$0.2097D-10$	$0.2521D-11$	$0.3090D-12$

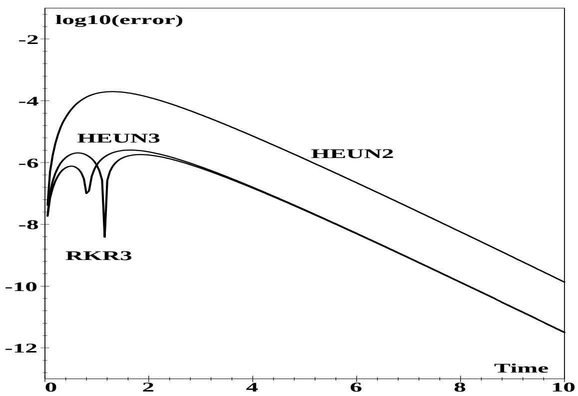

Figure 1: $y'=1-y^2$, $y(0)=0$, $h=0.05$, $t\in[0,10]$.

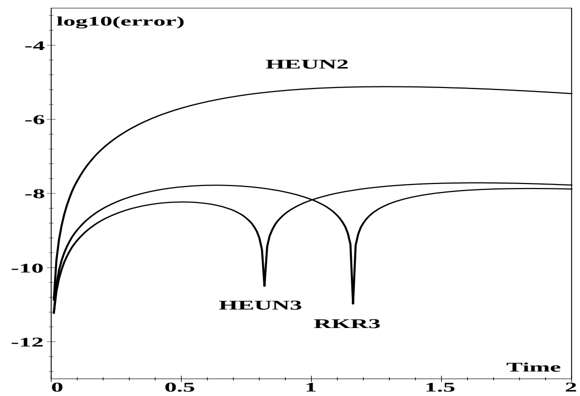

Figure 2: $y'=1-y^2$, $y(0)=0$, $h=0.01$, $t\in[0,2]$.

7 Linear stability properties.

When we apply a consistent method of our family to the scalar test equation

$$y' = \lambda y\,, \quad \lambda \in \mathbb{C}\,, \tag{35}$$

we get

$$y_{n+1} = R(z)\, y_n\,, \tag{36}$$

where $R(z)$ is the associated stability function (with $z = h\lambda$). When applied to the test equation, we have from (11) that $s = h\lambda$, and therefore $R(z)$ is

$$R(z) = 1 + zG(z) = 1 + z\,\frac{1 + \sum_{i=1}^{n} n_i z^i}{1 + \sum_{i=1}^{d} d_i z^i}\,. \tag{37}$$

The stability function $R(z)$ for a three order method takes the form

$$R(z) = 1 + z\,\frac{1 + \frac{1+2d_1}{2} z + \frac{1+3d_1+6d_2}{6} z^2 + \sum_{i=3}^{n} n_i z^i}{1 + d_1 z + d_2 z^2 + \sum_{i=3}^{d} d_i z^i}\,. \tag{38}$$

When we take $d_1 = -1/2$, $d_2 = 1/12$ and $n_i = d_i = 0$ for $i \geq 3$, the resulting stability function is given by

$$R(z) = \frac{12 + 6z + z^2}{12 - 6z + z^2}\,, \tag{39}$$

that is, the $(2,2)$–Padé approximation to e^z. So we get a first example of an A–stable explicit two–stage method of order three

$$y_{n+1} = y_n + hk_1 \left(\frac{12}{12 - 6s + s^2} \right)\,, \tag{40}$$

that is

$$y_{n+1} = y_n + h \left(\frac{16\,(k_1)^3}{31\,(k_1)^2 - 18\,k_1\,k_2 + 3\,(k_2)^2} \right)\,. \tag{41}$$

It is also easy to obtain L–stable methods of order three. For example, taking $d_1 = -2/3$, $d_2 = 1/6$ and $n_i = d_i = 0$ for $i \geq 3$, we get that the associated stability function is given by the $(1,2)$–Padé approximation to e^z

$$R(z) = \frac{6 + 2\,z}{6 - 4\,z + z^2}\,, \tag{42}$$

from which we get the L–stable formula

$$y_{n+1} = y_n + h\,k_1 \left(\frac{6 - s}{6 - 4\,s + s^2} \right)\,. \tag{43}$$

It is also possible to construct an L–stable method of order three, with associated stability function given by the $(1,3)$–Padé approximation to e^z (see [3]). Moreover, for a given rational function $R(z)$ we can get methods of the family (2), whose stability function is $R(z)$ (see [4]).

8 More numerical experiments.

We consider the problem

$$y' = 1000(1 - y)\,, \quad y(0) = 0\,, \tag{44}$$

whose solution is given by $y(x) = 1 - e^{-1000x}$. This problem is a particular case of a family of scalar equations of Prothero and Robinson, given by

$$y' = \lambda(y - g(x)) + g'(x)\,. \tag{45}$$

Applying the last two methods to the preceding problem, we get Tables 4 and 5. From these tables it is clear that both methods perform well, even when we take great steps. Obviously the L–stable method works better for this problem.

9 Non–linear stability considerations.

The study of the non–linear stability properties of the methods is very difficult. The rational functions of the stages involved in our formulae complicate the study of such properties from a theoretical point of view. So we will consider some numerical experiments with non–linear test problems of the form $y'(x) = f(y(x))$, 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

Table 4: Errors for the A–stable method.

$\lvert\text{error}\rvert$	$h = 0.5$	$h = 0.25$	$h = 0.125$	$h = 0.0625$
$x = 1.0$	$0.9531D + 00$	$0.8253D + 00$	$0.4639D + 00$	$0.4633D - 01$
$x = 2.0$	$0.9085D + 00$	$0.6811D + 00$	$0.2152D + 00$	$0.2146D - 02$
$x = 3.0$	$0.8659D + 00$	$0.5621D + 00$	$0.9986D - 01$	$0.9944D - 04$
$x = 4.0$	$0.8253D + 00$	$0.4639D + 00$	$0.4633D - 01$	$0.4607D - 05$
$x = 5.0$	$0.7866D + 00$	$0.3829D + 00$	$0.2149D - 01$	$0.2134D - 06$

Table 5: Errors for the L–stable method.

$\lvert\text{error}\rvert$	$h = 0.5$	$h = 0.25$	$h = 0.125$	$h = 0.0625$
$x = 1.0$	$0.1556D - 04$	$0.3661D - 08$	$0.2740D - 14$	$0.1993D - 24$
$x = 2.0$	$0.2420D - 09$	$0.1341D - 16$	$0.7510D - 29$	$0.0000D + 00$
$x = 3.0$	$0.3766D - 14$	$0.4908D - 25$	$0.0000D + 00$	$0.0000D + 00$
$x = 4.0$	$0.5859D - 19$	$0.1926D - 33$	$0.0000D + 00$	$0.0000D + 00$
$x = 5.0$	$0.9115D - 24$	$0.0000D + 00$	$0.0000D + 00$	$0.0000D + 00$

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 will consider the stiff problem

$$y' = (y-1)(y-1001)\,, \quad y(0) = a\,, \tag{46}$$

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

$$y(x) = 1 + \frac{1000(a-1)e^{-1000x}}{(a-1)e^{-1000x} + 1001 - a}\,. \tag{47}$$

It is easy to show that the true solutions are contractive for $a < 501$, and after a short transient they are virtually identical to the steady–state solution $y(x) = 1$ (the solution of (47) with $a = 1$).

When we apply the A–stable formula to this problem with fixed step $h = 0.1$ for a range of values of the parameter a we get Figures 3 and 4. Figure 3 shows that the numerical solutions we get taking values of $a = 5, 10, 15$ have a contractive behaviour. However, from Figure 4 it is clear that for $a = -10, -5, 0$ the numerical solutions do not have this 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 obtain Figures 5 and 6. Now Figure 5 shows that the numerical solutions we get with the L–stable method, from the values $a = 100, 200, 300$ are contractive. Taking $a = -15, -10, -5$, the resulting solutions (see Figure 6) do not have this property.

Numerical experiments with a wide range of values of a and h show that taking $1 < a < 501$, the numerical solutions are contractive for both methods. For fixed h and a (with $1 < a < 501$), the L–stable method is better than the A–stable from a qualitative point of view (the numerical solutions for the L-stable formula go faster to the steady–state solution).

When we consider $a < 1$ the situation changes and both methods have numerical solutions that are not contractive in general. In fact, taking $a << 0$ some solutions cross the steady–state solution (as can be shown in Figures 4 and 6) or even go away from this solution.

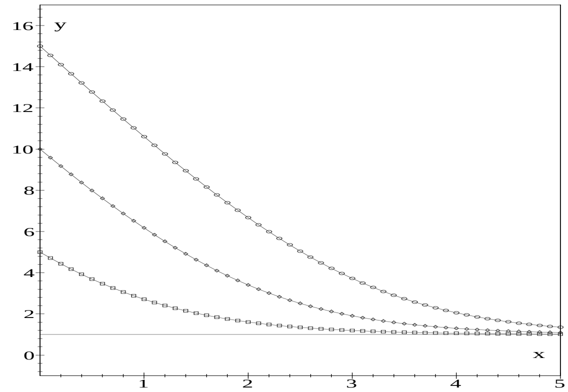

Figure 3: $y' = (y-1)\,(y-1001)\,,\ \ y(0) = a\,,$ $h = 0.1\,,\ \ x \in [0,5]$. Numerical solutions for $a = 5, 10, 15$ with the A–stable method.

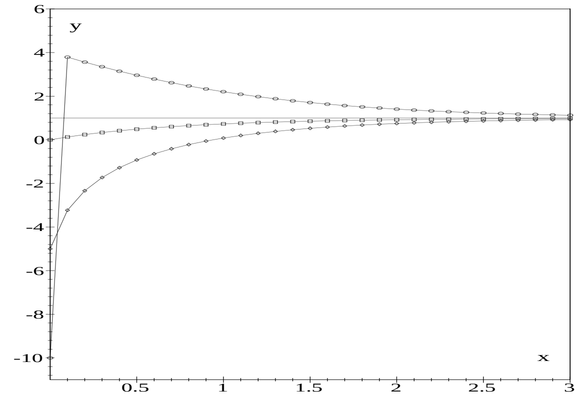

Figure 4: $y' = (y-1)\,(y-1001)\,,\ \ y(0) = a\,,$ $h = 0.1\,,\ \ x \in [0,3]$. Numerical solutions for $a = -10, -5, 0$ with the A–stable method.

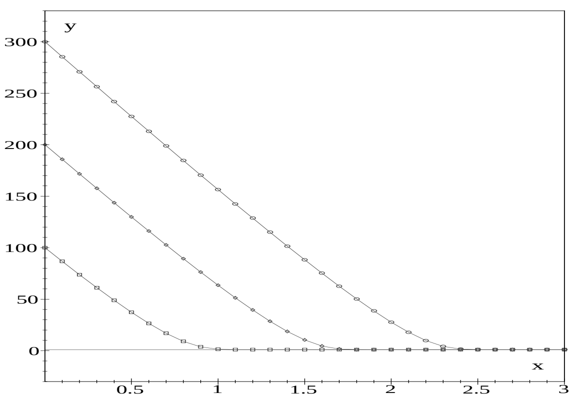

Figure 5: $y' = (y-1)\,(y-1001)\,,\ \ y(0) = a\,,$ $h = 0.1\,,\ \ x \in [0,3]$. Numerical solutions for $a = 100, 200, 300$ with the L–stable method.

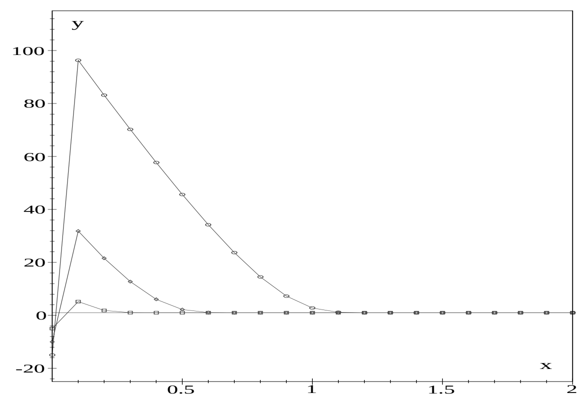

Figure 6: $y' = (y-1)\,(y-1001)\,,\ \ y(0) = a\,,$ $h = 0.1\,,\ \ x \in [0,2]$. Numerical solutions for $a = -15, -10, -5$ with the L–stable method.

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