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Global extrapolation procedures for special and general initial value problems.

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ABSTRACT

Two- and three- grid global extrapolation procedures are considered for the special and general initial value problems of arbitrary order q. Extrapolation formulas are developed for consistent numerical methods of arbitrary order p .

The global extrapolations of a number of existing numerical methods are considered and tested on three problems from the literature.

1. THE SPECIAL INITIAL VALUE PROBLEM

1.1 Introduction

Consider the special initial value problem of order q given by

(1) $y^{(q)}(t) = f(t,y)$; $y^{(r)}(t_0) = z_r$, $r = 0,1,\ldots,q^{-1}$

and suppose that the solution is sought at time $t = T < \infty$.

The interval of integration will be divided, first of all, into N sub-intervals each of width h so that $Nh = T - t_0$, giving a discretization or grid G_1 consisting of the N+1 points $t_{n,,1} = t_0 + nh$ (n = 0 ,1, . . . ,N). The theoretical solution of (1) at $t = t_{n,1}$ is clearly $y(t_{n,1})$ and the notation $y_{n,1}$ will be used to denote the solution of an approximating method at the same point t_{n+1} of $t_{n,1}$ of G_1 $(n = 0,1,\ldots.,N)$.

The application of a convergent numerical method M to find the solution yields, at the point $T = t_{N,1}$ of G_1 the *magnified error function* (Lapidus and Seinfeld [5; p.242], Henrici [3; p.80]) or the *global error* (Verwer and de Vries [10]) in the form

(2) $\varepsilon_{N,1} = C_{p+q}\, h^p y^{(p+q)}(T) + c_{p+q+2}\, h^{p+2} y^{(p+q+2)}(T) + c_{p+q+4}\, h^{p+4} y^{(p+4)} y^{(p+q+4)}(T) + \ldots.,$

where $p \geq 1$ is the *order* of the numerical method and C_{p+q} is its *error constant.* The term in h^p in (2) gives the time component of the principal part of the local truncation error when M is associated with the solution of a time-dependent partial differential equation.

1.2 Global extrapolation using two discretizations

Suppose now that the interval of integration is divided into 2N sub-intervals each of width $\frac{1}{2}h$ giving a discretization G_2 consisting of the 2N+1 points $t_{i,2} = t_0 + \frac{1}{2}ih$ $(i = 0, 1,\ldots, 2N)$. Clearly the points $t_{r,2}$ (r=0,2,4,….,2N) of G_2 are coincident with the points $t_{n,1} = t_0 + nh$ (n = 1 ,2,. . . ,N) of G_1 . The notation $y_{i,2}$ will be used to denote the solution of the method M at the points $t_{i,2}$ (i = 0,1 , . . . ,2N) of the grid G_2

The application of M to find the solution at the point $T = t_{2N,2}$ of G_2 generates the global error

$$(3) \qquad \varepsilon_{2N,2} = 2^{-p} c_{p+q} h^p y^{(p+q)}(T) + 2^{-p-2} c_{p+q+2} h^{p+2} y^{(p+q+2)}(T) + 2^{-p-4} c_{p+q+4} h^{p+4} y^{(p+q+4)}(T) + \dots ,$$

which, like $\varepsilon_{N,1}$ is $0(h)^p$ so that $y_{N,1}$ and $y_{2N,2}$ are both approximations of order p to y(T).

Consider, now, the approximation

$$(4) \qquad y^{(E)} = \alpha y_{2N,2} + (1-\alpha) y_{N,1}$$

and the associated global error

$$(5) \qquad \varepsilon^{(E)} = \alpha \varepsilon_{2N,2} + (1-\alpha)\varepsilon_{N,1}.$$

It is easy to show that the term in h^p in (5) vanishes when the parameter a takes the value

$$(6) \qquad \alpha = 2^p/(2^p - 1) \quad \text{with} \quad 1-\alpha = 1/(1-2^p).$$

The *global extrapolation* carried out using the two discretizations $G_1$and G_2 has thus produced an approximation $y^{(E)}$ defined by (4), which is of order p+2 provided α takes the value given by (6).

1.3 Numerical results

The global extrapolation procedure described in §1.2 was tested on the following problem

Problem 1. This problem is given by

$$y_1' = y_2 \qquad ; \quad y_1(0) = 1,$$
$$y_2' = -\frac{y_2}{t} + y_1^3 - 3y_1^5 \qquad ; \quad y_2(0) = 0.$$

The problem has a singularity in y_2'; therefore, a fully implicit method must be used to obtain the solution. Noting that the problem has the vector form $\underline{y}'(t) = \underline{f}(t, \underline{y})$, the solution was obtained using the first order backward Euler method

$$\underline{y}(t+h) - \ell \underline{f}\left(t+h, \underline{y(t+h)}\right) = \underline{y(t)} ,$$

the Newton-Raphson method for an algebraic system (of order 2) being employed to compute $\underline{y}(t+h)$.

The problem has theoretical solution

$$y_2(t) = \left(1+t^2\right)^{-\frac{1}{2}} , \quad y_2(t) = -t\left(1+t^2\right)^{-\frac{3}{2}}$$

and the maximum error moduli at time t = 0.25 are given in Table 1. It may be seen from Table 1 that the errors relating to one grid are decreasing by a factor of 2 (approximately) as h is successively halved, while the errors following global extrapolation of the solution are decreasing by a factor of 4 (approximately).

1.4 Global extrapolation using three discretizations

Suppose, finally, that the interval of integration is divided into 3N subintervals each of width $\frac{1}{3}h$ giving a discretization G_3 consisting of the 3N+1 points $t_{j,3} = t_0 + \frac{1}{3} jh \; (j = 0,1,\ldots,3N)$. It is clear that the points $t_{s,3} \; (s = 0,3,6,\ldots 3N)$ of G_3 are coincident with the points $t_{n,1} \; (n = 0,1,\ldots,N)$ of the original grid G_1. The notation $y_{j,3}$ will be used to denote the solution of the numerical method M at the points $t_{j,3} \; (j = 0,1,\ldots,3N)$ of G_3.

The application of M to find the solution at the point $T = t_{3N,3}$ of G_3 gives a third approximation to y(T) and generates the global error

(7) $$\varepsilon_{3N,3} = 3^{-p} c_{p+q} h^p y^{(p+q)}(T) + 3^{-p-2} c_{p+q+2} y^{(p+q+2)}(T) + 3^{-p-4} c_{p+q+4} y^{(p+q+4)}(T) + \dots ,$$

Which, like $\varepsilon_{N,1}$ and $\varepsilon_{2N,2}$ is $0(h^p)$, so that the third approximation to y(T), given by $y_{3N,3}$, is also of order p.

Considering the approximation

(8) $$y^{(E)} = \alpha y_{3N,3} + \beta y_{2N,2} + (1-\alpha-\beta)\, y_{N,1}$$

and the resulting global error

(9) $$\varepsilon^{(E)} = \alpha\varepsilon_{3N,3} + \beta\varepsilon_{2N,2} + (1-\alpha-\beta)\,\varepsilon_{N,1}.$$

where α and β are parameters, it may be shown that the terms in h^p and h^{p+2} in (9) vanish when

(10) $$\alpha = 3^{p+3} / \left(5 + 3^{p+3} - 2^{p+5}\right), \beta = -2^{p+5} / \left(5 + 3^{p+3} - 2^{p+5}\right)$$

with, consequently, $1-\alpha-\beta = 5 / \left(5 + 3^{p+3} - 2^{p+5}\right)$.

This global extrapolation, which uses the three discretizations G_1, G_2 and G_3, has produced an approximation $y^{(E)}$ defined by (8) which is of order p+4 provided α and β take the values in (10).

1.5 Numerical results using the three-grid extrapolation.

Problem 2 (Stiefel and Bettis [7]). This is the "almost periodic" problem given by

$$z''(t) + z(t) = 0.001e^{it} \quad ; \quad z(0) = 1 \;, z'(0) = 0.9995i \;, \; z(t) \in \mathbb{C}.$$

The analytic solution of this problem is given by

$$u(t) = \cos t + 0.0005t \sin t \,, u \in \mathbb{R} \,,$$

$$v(t) = \sin t - 0.0005t \cos t \,, v \in \mathbb{R} \,,$$

$$z(t) = u(t) + iv(t)$$

and represents the motion of the point z(t) on a perturbation of a circular orbit. The distance of this point from the centre of the orbit at time t is given by $\gamma(t) = \{u^2(t)+v2(t)\}^{\frac{1}{2}}$ and the error modulus $|E(\gamma)|$ of the computed value of γ was determined at $t = 40\pi$ for the three-discretization extrapolations of the fourth order method based on the (2,2) padé approximant of Twizell and Khaliq [8], the fourth order method of Cash [l] and the sixth order method of Cash [l].

The computed results were found using the time steps $h = \frac{\pi}{4}, \frac{\pi}{5}, \frac{\pi}{6}$, $\frac{\pi}{9}$ and $\frac{\pi}{12}$ (on the first discretization G_1); the results for the two fourth order methods are given in Table 2 and for Cash's sixth order method in Table 3. The solution at the first time step for every numerical experiment was computed using the second order Taylor series approximation.

It is not the purpose of the present paper to compare the relative merits of the methods developed in [1,8]. The aim of the paper is to show that global extrapolation, as detailed above, increases the order of the method being used. It is clear from the two tables that this aim has been achieved for all three methods tested on Problem 2.

Problem 3 (Van Dooren [9]). This is the nonlinear Duffing equation

$$y''(t) + y(t) + y^3(t) = F \cos \Omega t \; ; \; y(0) = A \; , \; y'(0) = 0$$

with F = 0.002, Ω=1.01 and A = 0.200426728067 (Chawla and Rao [2]).

This problem was solved using the second order P-stable method based on the (1,1) padé approximant [8] and the more accurate second order method based on the (1,2) padé approximant [8] which, using the notation of Lambert and Watson [4], has periodicity interval $H^2 \in (0,7.2)$.

The global extrapolation procedure using three discretizations was also carried out, increasing the orders of each of the two numerical methods to six.

The step size h was given the values $\pi/5, \pi/10, \pi/20$, and $\pi/40$ and the solution computed at time $t = 40\pi$. Van Dooren [9] gives the solution of Problem 3 in the form

$$y(t) = \sum_{i=0}^{4} a_{2i+1} \cos[(2i+1)\Omega t], \tag{16}$$

where

$a_1 = 0.200179477536$, $a_3 = 0.000246946143$,

$a_5 = 0.000000304014$, $a_4 = 0.000000000374$, $a_5 = 0.0$,

noting that the order of (16) is nine, with a precision of the coefficients of 10^{-12}.

The errors using the two numerical methods with one and three grids are given in Tabel 4 where, for comparison purposes, the results of chawla and Rao [2] relating to their sixth order method $M_6(0)$ are reproduced,

It is seen from Table 4 that the order of the two methods based on the (1,1) and (1,2) padé approximants [8] are duly increased by the global extrapolation procedure of §1.4. The results using the (1,1) method with three discretizations are inferior to those of Chawla and Rao [2], while those using the (1,2) method with three discretizations are better than those in [2]. particularly for the value h = $\pi/5$.

2. THE GENERAL INITIAL VALUE PROBLEM

Consider now the general initial value problem of order q given by

$$y^{(q)}(t) = f\left(t, y(t), y'(t), y''(t), \ldots, y^{(q-1)}(t)\right) \; ; \qquad y^{(r)}(t_0) = z_r, r = 0,1,\ldots,q-1 \tag{11}$$

and suppose, again, that the solution is sought at time $t = T < \infty$.

As in §1, the interval of integration will be divided into subintervals in three ways giving rise to the same three grids G_1, G_2, G_3.

The application of a convergent numerical method M to find two approximations $y_{N,1}$ and $y_{2N,2}$ yields the global errors

(12) $$\varepsilon_{N,1} = c_{p+q} h^{p+q} y^{(p+q)}(T) + c_{p+q+1} h^{(p+q+1)} y^{(p+q+1)}(T) + c_{p+q+2} h^{p+q+2} y^{(p+q+2)}(T) +$$

and

(13) $$\varepsilon_{2N,2} = 2^{-p} c_{p+q} h^{p} y^{(p+q)}(T) + 2^{-p-1} c_{p+q+1} h^{p+q+1} y^{(p+q+1)}(T) + 2^{-p-2} c_{p+q+2} h^{p+q+2} y^{(p+q+2)}(T) + \ldots$$

respectively, where, as in §1, p is the order of M.

Considering, now, the approximation $y^{(E)}$ of (4) and the associated global error given by (5), it is easy to show that the term in h^p in (5) vanishes when the parameter α takes the value given by (6). The global extrapolation procedure involving the two discretizations G_1 and G_2 described in §1.2 for the special initial value problem (1), is therefore valid for the general initial value problem (11) but, this time, the order of the extrapolation is only p+1.

The application of M on the third grid G_3 generates the approximation $y_{3N,3}$ and the associated global error function

(14) $$\varepsilon_{3N,3} = 3^{-p} c_{p+q} h^{p} y^{(p+q)}(T) + 3^{-p-1} c_{p+q+1} h^{p+q+\bar{1}} y^{(p+q+1)}(T) + 3^{-p-2} c_{p+q+2} h^{p+q+2} y^{(p+q+2)}(T) + \ldots$$

Considering the approximation $y^{(E)}$ of (8) and the associated global error given by (9), it may be shown that the terms in and h^p h^{p+1} and in (9) vanish when the parameters α and β take the values

(15) $$\alpha = 3^{p+1} / \left(1 + 3^{p+1} - 2^{p+2}\right) \quad \text{and} \quad \beta = -2^{p+2} / \left(1 + 3^{p+1} - 2^{p+2}\right)$$

so that $1 - \alpha - \beta = 1 / \left(1 + 3^{p+1} - 2^{p+2}\right)$. The three-discretization extrapolation of the general initial value problem (11) is thus only of order p+2, compared with p+4 for the special problem (1).

Putting p =q =1 and using the two grids G_1 and G_2 gives the second order global extrapolation procedure for parabolic equations outlined by Verwer and de Vries [10], while using all three grids G_1, G_2 and G_3 with p = q = 1 gives the third order algorithm of those authors. Putting p = 2 and q = 1 gives the values of the parameters α and β associated with the stable, two- or three-discretization global extrapolations of the well-known Crank-Nicolson method.

It may also be seen that, putting p=q=N=1 in the above analysis, and using G_1 and G_2, gives the parameter α for the L_0-stable second order l*ocal extrapolation* method of Lawson and Morris [6] which was based on the well-known fully implicit first order method for parabolic equations. The local extrapolation of the well-known Crank-Nicolson method for parabolic equations is also described by the above procedure (using G_1 and G_2) with q=N=1 and p = 2; this local extrapolation has a stability restriction.

Table 1. Maximum error moduli for Problem 1 using the first order fully implicit method.

Grids	1	2
Order	1	2
h=1/16	0.56E-2	0.25E-3
h=1/32	0.29E-2	0.62E-4
h=1/64	0.15E-2	0.15E-4
h=1/128	0.76E-3	0.38E-5

Table 2. Error moduli for problem 2 using two fourth order methods [1, 8]

Method	(2,2)padé [8]		Cash[1]	
Girds	1	3	1	3
Order	4	8	4	8
h=π/4	0.43E-2	0.21E-5	0.46E-2	0.25E-5
h=π/5	0.13E-2	0.32E-6	0.14E-2	0.38E-6
h=π/6	0.53E-3	0.63E-7	0.56E-3	0.76E-7
h=π/9	0.88E-4	-0.85E-9	0.94E-4	0.13E-8
h=π/12	0.27E-4	0.79E-10	0.28E-4	0.52E-10

Table 3. Error moduli for Problem 2 using the sixth order method of Cash [1]

Grids	1	3
Order	6	10
h=π/4	0.24E-4	0.11E-8
h=π/5	0.49E-5	0.14E-9
h=π/6	0.14E-5	0.26E-10
h=π/9	0.11E-6	0.62E-12
h=π/12	0.18E-7	0.46E-13

Table 4. Error moduli for problem 3

Method	(1,1)padé [8]		(1,1)padé [8]		Chawla and Rao [2]
Girds	1	3	1	3	1
Order	2	6	2	6	6
h=π/5	0.36E-1	0.20E-1	0.87E-1	0.77E-4	0.14E-2
h=π/10	0.14	0.28E-1	0.23E-1	0.12E-5	0.22E-4
h=π/20	0.35E-1	0.41E-5	0.58E-2	0.19E-7	0.34E-6
h=π/40	0.87E-1	0.54E-7	0.15E-2	0.52E-8	0.54E-8

REFERENCES

1. J.R. Cash, "Efficient P-stable methods for periodic initial value problems", *BIT* 24 (1984), 248-252.
2. M,M. Chawla and P.S. Rao, "High-accuracy P-stable methods for y"=f(t,y)", *IMA J. Numer. Anal.* 5 (1985), 215-220.
3. P. Henrici, *Discrete Variable* Methods *in Ordinary Differential Equations,* John Wiley and Sons, New York (1962).
4. J.D. Lambert and I.A. Watson, "Symmetric multistep methods for periodic initial value problems", *J. Inst. Maths. Applies*. 18 (1976), 189-202.
5. L. Lapidus and J.H. Seinfeld, *Numerical Solution of Ordinary Differential Equations*, Academic Press, New York (1971).
6. J.D. Lawson and J.LI. Morris, "The extrapolation of first order methods for parabolic partial differential equations. I", *SINUM* 15 (1978), 1212-1224.
7. E. Stiefel and D.G. Bettis, "Stabilization of Cowell's methods", *Numer. Math.* 13 (1969), 154-175.
8. E.H. Twizell and A.Q.M. Khaliq, "Multiderivative methods for periodic initial value problems", *SINUM* 21 (1984), 111-122.
9. R. Van Dooren, "Stabilization of Cowell's classical finite difference methods for numerical integration", *J. comput Phys*. 16 (1974), 186-192.
10. J.G. Verwer and H.B. de Vries, "Global extrapolation of a first order splitting method", *SISCC* 6 (1985), 771-780.