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THE RKFHB4 METHOD FOR
DELAY - DIFFERENTIAL EQUATIONS

by

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ABSTRACT

A method for the numerical solution of initial value problems for systems of retarded delay-differential equations is described. It uses a variable step Runge-Kutta Fehlberg 4/5 method combined with fourth degree Hermite-Birkhoff interpolation, which makes the usual local error estimator asymptotically correct. To obtain good numerical stability, the basic interpolation is modified for small delays. The possible initial discontinuities are algorithmically treated by using a very short stepsize in the critical step, and to this end the stepsize control has been somewhat modified. Numerical examples are included.

INTRODUCTION

In recent years, there has been growing interest in models for dynamical systems where the rate of change depends on the whole history of the system and not only, as in ordinary differential equations, on the present state vector. Such models arise in many fields of applications, [13].

The method described here is applicable to initial value problems for systems of retarded delay-differential equations on a finite interval $[t_0, T]$

$$\begin{cases} \dot{y}(t) = f(t, y(t), y(t-\tau_1), \dots, y(t-\tau_m)), & t \geq t_0 \\ y(s) = g(s), & s \leq t_0 \\ \tau_i = \tau_i(t), & i = 1, 2, \dots, m \end{cases} \quad (1)$$

where $y, f \in R^n$ and $\tau_i \geq 0$, hence the term retarded. Dots denote differentiation

w.r.t. t , $\dot{} = \frac{d}{dt}$. As an example, consider the single equation with a constant delay

$$\begin{cases} \dot{y}(t) = qy(t-\tau) & t \geq 0 \\ y(s) = 1 & s \leq 0 \end{cases}$$

which, for $q = -1.5$, $\tau = 1$, has the solution graphed below.

It exemplifies the smoothing property of retarded equations: the jump in $\dot{y}$ at $t=0$ is inherited as a jump in $\dot{y}$ at $t=\tau$, and generally, $y^{(k)}$ is discontinuous at $t=(k-1)\tau$, $k=1,2,\dots$. Only for special initial functions g the solution is smooth for all $t \geq 0$.

Because of these discontinuities, much work has concentrated on low-order methods such as generalizations of Euler's method, [2], [1]. For problems with smooth solutions, higher order methods have been studied. The class of problems

$$\dot{y}(t) = f(t, y(t), y(\alpha(t)))$$

$$y(t_0) = y_0$$

where the function α is such that $t_0 \leq \alpha(t) \leq t$ for all t in $[t_0, T]$, has been discussed by Stetter [14] and Feldstein [6]. Owing to the conditions on α there are no initial jumps. Tavernini [16] suggests one-step methods and obtains a fourth order method with six evaluations per step of the derivatives.

The use of extrapolation to obtain higher accuracy was advocated by Feldstein for the class of problems above, and for more general functional differential equations by Cooke and List, [1]. They assume that the positions and magnitudes of the jumps can be calculated in advance, and are able to correct for the jumps to

make the extrapolation work. A similar idea is exploited by Zwerkina [17], who designed Adams-type multistep methods with corrections for jump discontinuities.

ONE-STEP METHODS WITH INTERPOLATION FOR VOLTERRA FUNCTIONAL DIFFERENTIAL EQUATIONS

The retarded delay-differential equation (1) is a member of the more general class of Volterra functional differential equations

$$\begin{cases} \dot{y}(t) = (Vy)(t) & t \geq t_0 \\ y(s) = g(s) & s \leq t_0 \end{cases} \quad (2)$$

Here, V is a Volterra functional, i.e. $(Vy)(t)$ depends on values of $y(r)$ for $r \leq t$ only. An existence - uniqueness theorem for the initial value problem (2) was given by Driver, [4].

THEOREM

If g is continuous for all $s \leq t_0$, V satisfies the Lipschitz condition

$$\|(Vy_1)(t) - (Vy_2)(t)\| \leq L \max_{s \leq t} \|y_1(s) - y_2(s)\|$$

for continuous functions y_1 and y_2 , and $(Vy)(t)$ is continuous in t , then there is a unique, continuous solution of (2) on $[t_0, t_0 + H)$ for sufficiently small H .

To display more explicitly the dependence of $(Vy)(t)$ on $y(t)$ we shall write (2) in the form

$$\begin{cases} \dot{y}(t) = f(y(t), z(t)) & t \geq t_0 \\ z(t) = (Fy)(t) \\ y(s) = g(s) & s \leq t_0 \end{cases} \quad (3)$$

where we now assume that F is a Lipschitz continuous Volterra functional, and f is Lipschitz continuous in both arguments.

The numerical method generates a sequence y_i , $i = 0, 1, 2, \dots$, which approximate the exact solution $y(t_i)$ on the grid

$$t_N < \dots < t_{-1} < t_0 < t_1 < t_2 < \dots < t_K = T$$

(K and N are integers)

We need a numerical approximation $\tilde{F}$ to F . When the method steps from t_j to t_{j+1} we

have available y_k , $k \leq j$, so $(Fy)(t)$ is approximated by $(\tilde{F}Y)(t)$, where Y^T denotes the super-vector $(y_{-N}^T, y_{-1}^T, y_0^T, \dots, y_K^T)$. Now we can define a onestep method with interpolation for (3):

Apply a onestep method for ordinary differential equations to (3), now assuming that $z(t)$ is a known function of t ; then we get

$$y_{n+1} = y_n + (t_{n+1} - t_n) \phi(y_n, z)$$

Here we have used the notation of Henrici [11] for the increment function ϕ . In the sequel, for brevity of notation, we assume that the grid is equidistant with step h ; the results can be modified for variable stepsize in exactly the same manner as for ordinary differential equation, see [11].

We apply the onestep method with interpolation $(\phi, \tilde{F})$ to (3) by the prescription

$$\begin{cases} y_{n+1} = y_n + h \phi(y_n, \tilde{z}) + p_n, & n \geq 0 \\ \tilde{z}(t) = (\tilde{F}Y)(t) \\ y_j = g(t_j) + w_j & j \leq 0 \end{cases}$$

where p_n are local perturbations arising in computation, such as rounding errors, and w_j are errors in the starting values. We then have the following convergence result:

THEOREM

If 1) $\tilde{F}$ is Lipschitz continuous in the sense

$$\|(\tilde{F}U)(t) - (\tilde{F}V)(t)\| \leq \tilde{L}(d) \max_{k \leq j} \|u_k - v_k\| \quad (4)$$

for $t \leq t_j + d$

2) ϕ is consistent, hence convergent, for ordinary differential equations and, as $h \rightarrow 0$,

3) $w_j \rightarrow 0$

4) $p_n/h \rightarrow 0$

5) $\|(Fy)(t) - (\tilde{F}Y)(t)\| \rightarrow 0$

then the method $(\phi, \tilde{F})$ converges.

Remark 1. Note that a certain amount of extrapolation is involved in the condition

(4) on $\tilde{F}$; for most Runge Kutta methods we need $d = h$.

Remark 2. $\tilde{F}$ is applied to a function u rather than a sequence U by the trivial

discretization $u_k := u(t_k)$.

Proof Define the exact increment function Δ by

$$\begin{cases} y(t_{j+1}) = y(t_j) + h \Delta(y(t_j), z) \\ z(t) = (Fy)(t) \end{cases}.$$

Putting $e_j = y(t_j) - y_j$ we get

$$\begin{cases} e_{j+1} = e_j + h[\Delta(y(t_j), z) - \phi(y_j, \tilde{z})] - p_j, & j \geq 0 \\ e_j = -w_j, & j \leq 0 \end{cases}$$

Denoting the local error of ϕ used on (4) by

$$hr'_j = h(\phi(y(t_j), z) - \Delta(y(t_j), z))$$

and the interpolation error in step j by

$$r''_j(t) = (Fy)(t) - (\tilde{F}y)(t)$$

we have, after some adding and subtracting,

$$\begin{aligned} \|e_{j+1}\| \leq & \|e_j\| + h(L_1 \|e_j\| + L_2 (\max_{t_j \leq s \leq t_j+d} \|r''_j(s)\| + \\ & + \tilde{L} \max_{l \leq j} \|e_l\|)) + \|p_j\| + h \|r'_j\|, \quad j \geq 0 \end{aligned}$$

$$\|e_j\| = \|w_j\|, \quad j \leq 0$$

Here, we have used the Lipschitz constants L_1 and L_2 of ϕ w.r.t. first and second arguments, resp. Thus, $\|e_j\|$ is bounded by the increasing sequence (for $j \geq 0$).

$$v_j = \|w_j\|, \quad j \leq 0$$

$$v_{j+1} = (1 + h a_1) v_j + h a_2 \max_{l \leq j} v_l + R_j, \quad j \geq 0$$

$$= (1 + h a) v_j + R_j$$

where $a_1 = L_1$, $a_2 = L_2 \tilde{L}$, and R_j is an upper bound for

$$\|p_j\| + h (\|r'_j\| + L_2 \max_{t_j \leq s \leq t_j+d} \|r''_j(s)\|).$$

Thus, putting $hR = \max_j R_j$, $w = \max_{j \leq 0} \|w_j\|$, we have

$$\|e_j\| \leq R \left(e^{a(t_j - t_0)} - 1 \right) / a + w e^{a(t_j - t_0)}$$

which proves convergence.

QED.

If the solution y and the function f are smooth enough we can use higher order methods ϕ and more accurate functionals $\tilde{F}$. If the local error of ϕ is $\mathcal{O}(h^{p+1})$, and the interpolation error is $\mathcal{O}(h^q)$, the global error is of order $h^{p \min q}$. Thus, the classical Runge Kutta method with third degree polynomial interpolation gives $\mathcal{O}(h^4)$ error with four evaluations per step, as noted by Stetter [14].

The error bound obtained in this way is much too pessimistic, especially for stable problems. It can be sharpened for this case by the use of logarithmic norms, as in Dahlquist [3].

ASYMPTOTIC ERROR ESTIMATES

A better error estimate can be found if there exists an asymptotic expansion in powers of h of the global error. Several workers have established the existence for special methods of one or a few terms, [8], [6].

But for equations with true delay-terms, there is no such infinite expansion if one uses polynomial interpolation. The reason for this is seen by a simple example. Consider Euler's method with stepsize h for

$$\dot{y}(t) = qy(t-\tau), \tau \text{ constant} \tag{5}$$

where we take as approximation to $y(t-\tau)$ the value y_k at the nearest gridpoint t_k which is less than or equal to $t-\tau$. Then, the interpolation error $r''(t, h) = y(t-\tau) - y(t_k)$ is $\mathcal{O}(h)$, so the global error is $\mathcal{O}(h)$, but

$$\lim_{h \rightarrow 0} r''(t, h)/h \neq 0,$$

even if the solution $y(t)$ is smooth.

In the table below, we have solved (5) over $[0, 1]$ by this method with stepsizes $h = 2^{-N}$, $N = 2(1)8$, $\tau = 0.7$, and q and the initial function chosen to make $e^{-0.5t}$ the exact solution. The second column shows the global error at $t = 1$ divided by h .

N	$(\text{error}/h) \cdot 10^4$
2	574
3	197
4	-581
5	-192
6	578
7	193
8	-578

The periodicity is explained by the fact that the interpolation error is proportional to $h \cdot \text{fractional part of } (\tau/h) = h \cdot (7 \cdot 2^N) \bmod 10$.

If we use higher order interpolation, however, there will be at least one term of an asymptotic expansion in powers of h of the global error. The proof is given in detail in [12], with consideration of the difference equation for the remainders, which are indicated by $\mathcal{O}(h^{p+1})$ here.

THEOREM

Assume, that the exact solution y and the function f are sufficiently differentiable. Then, if the local error of ϕ is of order $p+1$ and the interpolation error is of order q , and $q \geq p+1 \geq 2$,

$$\|y(t_j) - y_j\| = h^p e(t_j) + \mathcal{O}(h^{p+1})$$

where $e(t)$ satisfies the linear, nonhomogenous Volterra functional equation

$$\begin{aligned} \dot{e} &= (V'(y))(t)e + \varphi(t), \quad t \geq 0 \\ e(s) &= 0 \quad s \leq 0 \end{aligned}$$

Here, $V'(y)$ is the Fréchet derivative of V along the exact solution $y(t)$, $\varphi(t)$ is the principal error function of ϕ used on (3), and we have ignored the initial errors w_j and the local perturbations p_j .

Proof We make use of Stetter's theorem [15]. For the local error = residual when $y(t)$ is substituted into the numerical scheme, we have

$$h(\Delta(y(t_j), Fy) - \phi(y(t_j), \tilde{F}y)) = h[h^p \varphi(t_j) + \mathcal{O}(h^{p+1}) + Q_j]$$

where $\|Q_j\| = \|\phi(y(t_j), Fy) - \phi(y(t_j), \tilde{F}y)\| = \mathcal{O}(h^q) = \mathcal{O}(h^{p+1})$,

thus the local error has an expansion to at least one term.

It remains to show the stability in the sense of [15] of the inhomogenous, linearized, discretized problem, i.e.,

$$\begin{cases} u_{j+1} - u_j - h \tilde{\phi}' U = \rho_j, & j \geq 0 \\ u_j = 0 & j \leq 0 \end{cases}$$

where $\tilde{\phi}'$ is the Fréchet derivative of $\phi(u_j, \tilde{F}U)$ evaluated at $u_j = y(t_j)$. Under our assumptions of differentiability and Lipschitz continuity we get for $x_j = \|u_j\|$

$$\begin{cases} x_{j+1} \leq x_j + h L(h) \max_{k \leq j} x_k + \|\rho_j\|, & j \geq 0 \\ x_j = 0, & j \leq 0 \end{cases}$$

and, putting $k^* = (t-t_0)/h$, assuming this is an integer,

$$\begin{aligned} x_{k^*} &\leq h^{-1} \max_{k \leq k^*} \|\rho_k\| \cdot \left(e^{L(h)(t-t_0)} - 1 \right) / L(h) = \\ &= O(h^{-1}) \max_{k \leq k^*} \|\rho_k\| \end{aligned}$$

which is the necessary bound on the solution. Here, $L(h)$ is the norm of the linear operator $\tilde{\phi}'$. It can be bounded in terms of h , and the Lipschitz constants for f and $\tilde{F}$, and tends to $L_1 + L_2 \tilde{L}$ as $h \rightarrow 0$.

Note also that linearization and discretization do not, in general, commute exactly for Runge Kutta methods owing to the off-step derivative calculations. The remaining conditions for the application of Stetter's theorem are easily seen to be satisfied. QED.

The functional $\tilde{F}$ can use also the approximate values of $\dot{y}$ which are calculated anyway in integrating the differential system. The theorems hold after the obvious modifications; one only has to use majorizing recursions for 2-vectors of norms instead of scalars. Thus we can use Hermite-Birkhoff interpolation, which was suggested by Fox [8], and has, compared with Newton interpolation, smaller error constant and less sensitivity to rapid variation of the distance between gridpoints..

Remark. Delay-differential equations with state-dependent delays, say

$$\dot{y}(t) = f(t, y(t), y(t-\tau))$$

$$\tau = \tau(t, y(t))$$

are not covered by the results here, because the functional is not Lipschitz continuous.

But there is still a unique, continuous solution, and under suitable assumptions on τ , and on the interpolation method, the theorems still hold. This generalization is carried through in [12].

THE RKFHB4 METHOD

Our program uses the Runge Kutta Fehlberg 4/5 method and fourth degree Hermite--

Birkhoff interpolation. We shall discuss the treatment of the initial discontinuities and the stability of the method when used on the test equation with delay

$$\dot{y}(t) = qy(t-\tau)$$

DISCONTINUITIES, STEPSIZE REGULATION

The algorithmic treatment of differential equations with discontinuities is discussed e.g. in [7] and [9]. The difficulty is to find the point, say t^* , where the switch from one smooth right hand side to another occurs. For the clever treatment of discontinuities, therefore, the differential system is assumed given in the form

$$\dot{y}(t) := \underline{\text{if}} \psi(t,y) \geq 0 \underline{\text{then}} f_1(t,y) \\ \underline{\text{else}} f_2(t,y);$$

and the user is required to supply the function ψ explicitly. Then, some root-finding technique can be used to obtain t^* to the desired accuracy.

To save the user from this extra work, we choose instead the brute force method of letting the normal error estimator discover the jumps.

The stepsize control suspects that there is a point of discontinuity t^* in $[t_j, t_j + h']$ if h' is the second unsuccessful stepsize tried to step from t_j . To determine when t^* has been passed, we save an upper bound $\bar{t} = t_j + h'$ on t^* (we assume integration in the positive t -direction). Over the interval $[t_j, t_j + h']$ the normal error / unit step criterion is now replaced by error per step criterion with smaller tolerance, no increase in stepsize is allowed, and whenever a step to, say $t_j + h''$, fails, $\bar{t}$ is set to $t_j + h''$ and the stepsize is halved. When the point $\bar{t}$ has been passed, the stepsize is allowed to increase, and we first try a step of length h' .

For smooth solutions, the stepsize control works like for ordinary differential equations, since the $\mathcal{O}(h^4)$ -part of the global error comes from φ , and not from interpolation. However, when the error tolerance, say ε , is not very stringent, the asymptotic theory is not really valid, and therefore the stepsize is additionally monitored so that the maximal interpolation error over any step is approximately bounded by ε .

STABILITY FOR SMALL DELAYS

To discuss the stability we first give the exact definition of the basic interpolation (later to be modified), for a single equation, to avoid double indices. In the derivative calculations when the method steps from t_j to t_{j+1} , $y(t-\tau)$ is computed as $Q_j(t-\tau)$, where Q_j is the fourth degree polynomial which satisfies

$$Q_j(t_k) = y_k, \quad k = l^*-1, l^*, l^*+1$$

$$\dot{Q}_j(t_k) = d_k, \quad k = l^*, l^*+1$$

where $t_l < t-\tau \leq t_{l+1}$, and $l^* = \min(l, j-1)$.

The choice of l^* instead of l gives an explicit method even for small τ . The d_k are the approximate $\dot{y}$ -values at the gridpoints, i.e., for

$$\dot{y}(t) = f(t, y(t), y(t-\tau)),$$

$$d_k := f(t_k, y_k, Q_{k-1}(t_k - \tau)).$$

If $\tau < h$ the intermediate stage derivative calculations imply extrapolation. This has adverse effects on the stability.

Consider the test equation with delay (5). As $\tau \rightarrow 0$, this tends to $\dot{y}(t) = q y(t)$. The length of the intersection of the stability region in hq -plane with the real axis is only about 0.16 for the RKFHB4 method with basic interpolation, if $\tau \ll h$. But the stability interval of the Runge Kutta Fehlberg 4/5 method is approximately $(-3, 0]$.

One way of improving the situation is to allow the approximation to $y(t-\tau)$ to use also the current value of y ,

$$y(t-\tau) \approx Q_j(t-\tau) + \omega(\tau, h)(y(t) - Q_j(t)) = R_j(t, \tau, h)$$

If we choose the continuous function $\omega(\tau, h)$ such that $\omega(0, h) = 1$, then $R_j(t, 0, h) = y(t)$, and the discretization of

$$\dot{y}(t) = f(t, y(t), y(t-\tau)) \quad \text{for } \tau = 0$$

and

$$\dot{y}(t) = f(t, y(t), y(t))$$

will become the same, and the stability region will be the same for $\tau \rightarrow 0$ as for the testequation without delay.

As criteria for the choice of $\omega(\tau, h)$ we have used the accuracy and stability when the method is applied to the testequation with delay. To make ω simple to compute, we choose

$$\omega = \omega(\theta), \quad \text{where } \theta = \tau/h$$

and require

$$\omega(0) = 1$$

$$\omega(\theta) = 0, \quad \text{if } \theta \geq 1$$

since no extrapolation is necessary when $\theta > 1$.

ACCURACY

Let q and τ be such that $e^{\lambda t}$ is a solution of (5), thus $q = \lambda e^{\lambda \tau}$. Let $y_n = 1$, and $y_{n-1}, y_{n-2}, \dot{y}_{n-1}, \dot{y}_n$ have exact values. Then

$$y_{n+1} = e^{\lambda h} + C(\lambda h)^{p+1} + \mathcal{O}(h^{p+2})$$

with $p=4$. To calculate the error constant C , we used the symbolic manipulation system REDUCE [10]. The result is

$$C(\omega) = (1 - 5\omega - 60\omega^3)/49920$$

$|C(1)| = 1/780$ is the maximum value of $|C|$. Thus any ω between 0 and 1 is acceptable for accuracy reasons, since for the non-delayed parts of the system the error constants are of this magnitude.

STABILITY

By the stability region S of the method we mean that set of values of (qh, θ) for which the numerical solutions are bounded. S can be represented graphically by a set of stability regions in qh -plane, one for each θ -value. To make computer plots of these, one observes that the RKFHB4 method applied to the test equation gives a linear recursion

$$X_{n+1} = A(qh, \theta) X_n$$

for the vectors $X_n = (y_n, d_n, y_{n-1}, d_{n-1}, y_{n-2}, d_{n-2})^T$. A is a 6×6 complex matrix. Thus, the interior $\underline{S}$ of S is given by

$$\underline{S} = \{(qh, \theta) \mid \text{spectral radius of } A \text{ less than } 1\}$$

By plotting $\underline{S}$ instead of S we neglect some boundary points - for instance, the origin $qh=0$! We now choose $\omega(\theta)$ to obtain the largest $\underline{S}$, by inspecting the stability plots. It turns out that the optimal ω for each θ , say ω_{opt} , is a decreasing function of θ , and that

$$\omega = (1 - \theta)^3$$

is close-to-optimal.

Note that the stability region of the differential equation is bounded (except for $\tau=0$). If $q\tau \in D$ (see the figure) all solutions are bounded. D is bounded by the curve

$$|q\tau| = \arg(q\tau) - \pi/2$$

and its mirror image in the real line

NUMERICAL EXAMPLES

The following two problems have been run with error tolerance $\varepsilon = 10^{-N}$, $N = 1(1)8$, and the maximal error e in the first component over the range and the number NFC of function evaluations were recorded.

Problem 1
$$\begin{cases} \dot{y}_1 = y_2 \\ \dot{y}_2 = -y_1/2 - 1/2 + y_1^2(t/2 - \pi/4) \end{cases}$$

$$\begin{cases} y_1(s) = \sin s \\ y_2(s) = \cos s \end{cases} \quad s \leq 2$$

over $[2, 20]$. The exact solution is $y_1(t) = \sin t$

Problem 2
$$\begin{cases} \dot{y} = qy(t-\tau) & t \geq 0 \\ y(s) = 1 & s \leq 0 \end{cases}$$

over $[0, 7]$.

$q = -1.5$, $\tau = 1$, makes the unsmooth solution barely asymptotically stable. The stability limit is $q\tau = -\pi/2$.

The exact solution is a polynomial of degree k over $[(k-1)\tau, k\tau]$. Putting

$$y(t) = y_k(t) = \sum_{j=0}^{k+1} a_{kj} (t-k\tau)^j, \quad t \in [k\tau, (k+1)\tau]$$

$$y_{-1}(t) = 1$$

and substituting in the differential equation, one obtains a recurrence for the a_{kj} which allows stable computation of $y(t)$.

The results are presented in log-log graphs of e^{-1} (continuous line) and ε^{-1} (broken line) versus NFC . Also the slope expected for a fourth order method has been indicated.

One hopes for proportionality between e and ε , the quotient e/ε being determined by the stability of the differential system and the length of the integration range. The behaviour deviates from this for small N , both because the asymptotic theory is not valid, and because the influence of the choice of starting stepsize is greater since the total number of steps is low. For the problem with discontinuities, the graph is more erratic, and it is perhaps recommendable to run such problems with different ε and compare the results.

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