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Hybrid Predictors and Correctors for Solving a Special Class of Second Order Differential Equations

by

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Abstract

Hybrid predictors and correctors of order k + k' + 1 are constructed for the numerical solution of second order differential equations not containing the first derivative explicitly. These methods are based on both explicit (k'=k-1) and implicit (k'=k) linear k-step methods.

§1. Introduction

The numerical solution of the special class of second order differential equations

$$(1)\qquad \begin{aligned} y''(x) &= f(x,y(x)),\\ y(x_0) &= y_0,\\ y'(x_0) &= y_0', \end{aligned}$$

via Runge-Kutta type method was discussed by e.g., Collatz [2, p. 61], de Vogelaere [11] and Scraton [10]. Linear k-step methods of the form

$$(2)\qquad \sum_{j=0}^{k} \alpha_j y_{n+j} = h^2 \sum_{j=0}^{k'} \beta_j f_{n+j}$$

for the solution of (1) were discussed by e.g., Henrici [6, p. 289] and Lambert [7, p. 252]. The direct application of methods of class (2) to problem (1), rather than the application of a conventional linear multistep method to an equivalent first-order system is usually recommended (see Ash [1]).

A rigid theory of the stability and convergence of general multistep methods was developed by Dahlquist [3, 4] and Henrici [6, p. 307].

Definition 1: The method (2) is said to be zero-stable if no root of the first characteristic polynomial

$$(3)\qquad \rho(\xi) = \sum_{j=0}^{k} \alpha_j \xi^j$$

CONGRESSUS NUMERANTIUM, 46 (1985), pp. 241-248

has modulus greater than one, and if every root of modulus one has multiplicity not greater than two.

Definition 2: The method (2) has order p if the linear difference operator

(4) $$L[y(x);h] = \sum_{j=0}^{k} \alpha_j \underline{y}(x+jh) - h^2 \sum_{j=0}^{k'} \beta_j \underline{y}''(x+jh),$$

where y(x) is an arbitrary function, can be expanded in Taylor's series as follows

(5) $$L[y(x);h] = C_{p+2} h^{p+2} y^{(p+2)}(x) + 0(h^{p+3})$$

and $C_{p+2} \neq 0$. The number C_{p+2} is called the error constant.

Definition 3: A method (2) is said to be consistent if it has order at least one.

One can easily show that for a consistent method

(6) $$\rho(1) = \rho'(1) = 0,$$

(7) $$\rho''(1) = 2\sigma(1),$$

where

(8) $$\sigma(\xi) = \sum_{j=0}^{k'} \beta_j \xi^j$$

is called the second characteristic polynomial.

Theorem (Henrici [6, p. 307]):

The order p of a zero-stable method (2) cannot exceed k + 2. A necessary and sufficient condition for p = k + 2 is that k be even, that all roots of $\rho(\xi)$ have modulus one, and that $\sigma(\xi)$ be determined by

(9) $$\sigma(\xi) = \sum_{j=0}^{k'} C_j (\xi-1)^j$$

and C_j are the coefficients in the expansion of

(10) $$\frac{\rho(\xi)}{(\log\xi)^2} = \sum_{j=0}^{\infty} C_j (\xi-1)^j.$$

Since stability is a necessary condition for convergence, the last theorem restricts the order of multistep methods for larger k. Although $p = k + k' - 1$ could actually be attained, one has to confine oneself to the use of methods of order $k + 1$ (or $k + 2$) to have convergence.

The approach to a relaxation of the previous theorem is discussed by Neta and Lee [8]. One includes in (2), the second derivative at a single offstep point x_{n+r}, with a real $r \notin I_k := \{0,1,\ldots,k\}$, usually noninteger.

For a given ρ, the generalized k-step method with a σ of degree k' is of order $p \geq k' + 3$. Such correctors with the necessary predictors for $k \leq 10$ were constructed by Neta [9] for Störmer-Cowell type methods. In [8], it was shown that methods of maximal order ($p=k+k'+1$) exist. The purpose of this note is to construct explicit and implicit maximal order correctors of step $k \leq 10$ if exist. We also construct predictors of the same or higher order. The general form of the corrector is

$$(11) \qquad y_{n+k} + \sum_{i=0}^{k-1} \alpha_i y_{n+i} = h^2 \sum_{i=0}^{k'} \beta_i f_{n+i} + h^2 \beta_r f_{n+r}$$

and the predictor

$$(12) \qquad y_{n+r} + \sum_{i=m_1}^{k-1} \alpha_i^p y_{n+i} + \alpha_{r-1}^p y_{n+r-1} = h^2 \sum_{i=m_1}^{k-1} \beta_i^p f_{n+i} + h^2 \beta_{r-1}^p f_{n+r-1}$$

where m_1 may take the value of -1. Note that this predictor is using the values y_{n+r-1}, f_{n+r-1}. These values are available after the first application of this hybrid method ($n > 0$). This idea is new and may replace the necessity of taking m_1 equal to -2. For implicit method one requires also a predictor for y_{n+k}.

$$(13) \qquad y_{n+k} + \sum_{i=m_3}^{k-1} \alpha_i^e y_{n+i} + \alpha_r^e y_{n+r} = h^2 \sum_{i=m_3}^{k-1} \beta_i^e f_{n+i} + h^2 \beta_r^e f_{n+r},$$

where m_3 may take the value of -1. Note that this predictor is using the values y_{n+r}, f_{n+r}. This form of predictor is different from the one suggested in [8, 9].

In the next section we construct the maximal order correctors.

In Section 3 we give the predictors.

§2. Corrector methods

In this section we construct explicit and implicit correctors of order $k + k' + 1$. We follow the method described in [8] for constructing such correctors. We choose r such that the k homogeneous linear equations for $a_2, \ldots, a_k, \beta_r$,

$$(14) \qquad \sum_{i=0}^{k-2} a_{i+2}\delta_{j-i} - \binom{r}{j}\beta_r = 0 \qquad j = k' + 1, k' + 2, \ldots, k' + k$$

have a nontrivial solution. The number δ_ℓ are given in Table 1 [8] and the a_i's relate to α_i's via

$$(15) \qquad \rho(\xi) = \sum_{i=2}^{k} a_i(\xi-1)^i.$$

The determinant of (14) is a polynomial of degree $k' + k$ in r which has the $k' + 1$ zeros $r = 0, 1, \ldots, k'$, leading to $\beta_r \neq 0$ and all $a_i = 0$. The remaining real zeros, if any, could be tested as to whether they produce a stable ρ or not. The necessary condition for stability is given in [8]

$$(16) \qquad \frac{k}{2} < r < \begin{cases} \infty & \text{if } k' = k \\ k & \text{if } k' = k - 1. \end{cases}$$

Using this method we found there exists no explicit method of step $7 \leq k \leq 10$ and no implicit method of step $5 \leq k \leq 10$. In all these cases we found that all remaining zeros r were complex. For explicit methods with step $k = 4, 5$ the only real zero was $r = k$, i.e., $r \in I_k$, which is not admissible.

The only four methods are given in Table 1. The results obtained using quadruple precision.

§3. Predictors

In this section we first discuss the predictors for y_{n+r} and then the predictors for y_{n+k} required for implicit methods only. The predictors suggested in the literature (Gragg and Stetler [5], Neta and

Lee [8] and Neta [9]), require the knowledge of y_{n-1} and even y_{n-2}. Clearly, the problem is for $n < 2$. Here we suggest to use y_{n+r-1} instead of y_{n-2}, thus remedying those cases for which one requires y_{n-2}. The value of y_{n+r-1} is available to the user for $n > 1$. We

k	3	3	4	6
k'	2	3	4	5
p	6	7	9	12
error constant	.19506961-2	-.40974629-3	.10237162-3	-.26351551-3
α_0	.33974596	.21955646	.12005172	.44073883
α_1	.32050807	.56088708	.85814015	-.23561119-1
α_2	-.1660254+1	-.17804435+1	-.10764355+1	-.24600533+2
α_3	1.	1.	-.90175640	.16340591+2
α_4	-	-	1.	.40010967+2
α_5	-	-	-	-.33168203+2
α_6	-	-	-	1.
r	.27320508+1	.30998512+1	.39578900+1	.52609010+1
β_r	.14433757	-.17060250	.47587450	.22793114+1
β_0	-.24519053-1	.19037446	-.47607846	-.24788779+1
β_1	-.58384716-1	.42966196	-.24184615	-.32420131
β_2	.10283122+1	.10399476+1	.46318699	-.73093719+1
β_3	-	.88414818-1	.51181710	-.19288598+2
β_4	-	-	.7775689-1	-.33695301+2
β_5	-	-	-	-.10898672+1

Table 1

write the predictors as follows:

$$y_{n+r} + \sum_{i=m_1}^{k-1} \alpha_i^p y_{n+i} + \alpha_{r-1}^p y_{n+r-1} = h^2 \sum_{i=m_1}^{k-1} \beta_i^p f_{n+i} + h^2 \beta_{r-1}^p f_{n+r-1}$$

where m_1 may take the value of -1.

The coefficients α_i^p, β_i^p, $i = m_1, \ldots, k-1$, α_{r-1}^p, β_{r-1}^p, the order p and the error constant are given in Table 2 for all methods.

Note that for 3-step method we need values at x_{n-1} and x_{n+r-1} to be able to construct a method of order higher than 6. The 6th-order method, using only values at x_{n-1}, has an error constant larger than the corrector and order equal to that of the corrector. For the 4-step method we constructed two methods of order 10, one uses the values at x_{n-1} and x_{n+r-1} and the other using the values at x_{n-1} and x_{n-2}. As mentioned before, the first one can be used for $n > 1$ whereas the second can be used only after $n > 2$. The 6-step, 12th-order method requires only values at x_{n+r-1}.

Now, we turn to the predictor for y_{n+k}. Since y_{n+r} is computed we can utilize it to obtain y_{n+k}. The predictors are of the form

$$y_{n+k} + \sum_{i=m_3}^{k-1} \alpha_i^e y_{n+i} + \alpha_r^e y_{n+r} = h^2 \sum_{i=m_3}^{k-1} \beta_i^e f_{n+i} + h^2 \beta_r^e f_{n+r}$$

Since y_{n+r}, f_{n+r} increase the number of free parameters by 2, it was possible to take $m_3 = -1$. We also were able to obtain predictors of order higher than correctors. This alleviated the problem created by the relatively large error constants of predictors compared to correctors. If we take $m_3 = 0$ the number of parameters is not enough to obtain a method of order $k + k' + 1$.

k	3	3	4	4	6
k'	2	3	4	4	5
p	6	8	10	10	12
C_{p+2}	.15345044-2	.37799083-3	.33457995-3	.45316620-4	.24939624-7
α^p_{r-1}	-	-.16367041+3	-	.43155998+3	-.27870041+1
α^p_{-2}	-	-	.89183517	-	-
α^p_{-1}	.16495722	-.34707085+1	.48225668+2	-.20987953+1	-
α^p_0	.41805548+1	-.17210929+2	.97142753+2	-.21742056+2	-.65123495-2
α^p_1	-.81239305+1	.29591150+2	-.29265853+3	.53587174+1	-.11831175
α^p_2	.27784184+1	.15376090+3	.97484840+2	.45688822+2	-.22584136
α^p_3	-	-	.47913432+2	-.45976667+3	.32949617
α^p_4	-	-	-	-	.28451133+1
α^p_5	-	-	-	-	-.10369400+1
β^p_{r-1}	-	.15573287+2	-	-.55893549+2	.37920207
β^p_{-2}	-	-	.38973204-2	-	-
β^p_{-1}	-.54985740-2	-.16795316	.40910386+1	-.87317361-1	-
β^p_0	.58522790	-.53312061+1	.62017857+2	-.39967164+1	-.23807188-3
β^p_1	.37430479+1	-.21107539+2	.16583176+3	-.26064624+2	-.15269409-1
β^p_2	.98662380	-.24422142+2	.61918294+2	-.38785414+2	-.15557853
β^p_3	-	-	.41169635+1	.44601261+2	-.44728515
β^p_4	-	-	-	-	-.54763223
β^p_5	-	-	-	-	.96975979-1

Table 2

k	3	4
k'	3	4
p	8	10
error constant	-.49880214-3	-.47842068-6
α_r^e	.13941424+1	-.11071926+1
α_{-1}^e	.35465085+1	.15454834-1
α_0^e	.14205646+2	.13557671
α_1^e	-.36517468+2	-.13269980
α_2^e	.16371171+2	-.26371860
α_3^e	-	.35257943
β_r^e	.11444377	.57198711-2
β_{-1}^e	.17609964	.66125882-3
β_0^e	.52155324+1	.27989375-1
β_1^e	.17504634+2	.15770493
β_2^e	.44443744+1	.15303799
β_3^e	-	-.16592532-1

Table 3

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