ON THE STABILITY OF PREDICTOR-CORRECTOR METHODS BETWEEN ADAMS AND BACKWARD DIFFERENCE FORMULA

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ABSTRACT

The predictor-corrector methods take the upper hand in decreasing the number of function evaluations and of derivative evaluations as well comparing to the Runger-Kutta methods and various linear multistep methods. The stability however is a traditional disease of a high order method. This problem is also the case to the predictor-corrector method. The paper discusses on the matter of stability of the k-step Adams predictor-correct method and that of the predictor-corrector methods constructed on the basis of k-step Adams-Brashfort for the predictor and the k-step or (k+1)-step backward difference formula (BDF) for the corrector with low *k*, say $k \le 6$. The reason to consider the BDF corrector is from the fact of having a large portion of the absolute stability region for those methods (with $k \le 6$) competing to other Adams-Moulton correctors. Some awkward performances of the predictor-corrector to the stiffness are also discussed and a modified algorithm is also developed to treat the poor performance of the absolute stability region of a predictor-corrector method by constructing its stability polynomial on the basis of the recurrence equation obtain form the pair of difference equations describing the predictor and corrector. On that construction, we can be able to sketch the region by the boundary locus method.

Keywords: linear multistep method; k-step Adams predictor-corrector; backward difference formula; stiffness; absolute stability region.

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VỀ TÍNH ỔN ĐỊNH CỦA PHƯƠNG PHÁP DỰ BÁO - HIỆU CHỈNH HỌ ADAMS VÀ HỌ SAI PHÂN LÙI

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TÓM TẮT

Phương pháp dự báo - hiệu chỉnh có ưu điểm trong việc giảm đáng kể số lượng tính toán giá trị hàm số và đạo hàm so sánh với phương pháp đơn bước kiểu Runge-Kutta truyền thống cũng như so với nhiều phương pháp đa bước khác. Tính ổn định là một vấn đề truyền thống đối với các phương pháp khi xét ở bậc cao. Bài báo này đề cập đến tính ổn định, và so sánh chúng, của phương pháp với k-bước dự báo kiểu Adams-Brashfort và (k+1)-bước hiệu chỉnh kiểu Adams-Moulton hay kiểu sai phân lùi (BDF) với $k \le 6$. Lý do đề cập đến kiểu hiệu chỉnh BDF ở đây có nguồn gốc từ thực tế rằng một hiệu chỉnh BDF tạo ra một miền ổn định tuyệt đối lớn, với $k \le 6$, so với hiệu chỉnh kiểu Adams-Moulton. Một số nhược điểm của các phương pháp dự báo - hiệu chỉnh này khi áp dụng cho các bài toán stiff cũng được đề cập trong bài báo cùng với một thuật toán cải tiến cho các phương pháp này được phát triển để khắc phục phần nào nhược điểm đó. Đóng góp lớn nhất của bài báo là phương pháp xây dựng đa thức ổn định dựa vào phương trình sai phân mô tả phương pháp dự đoán và phương pháp hiệu chỉnh. Dựa vào đa thức này, phương pháp tập hợp đường bao được áp dụng để mô tả trực quan miền ổn định của phương pháp.

Từ khóa: phương pháp đa bước; k-bước Adams dự báo - hiệu chỉnh; công thức sai phân lùi; bài toán stiff; miền ổn định tuyệt đối.

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1. Introduction

Consider the initial-value problem

$$y' = f(t, y), a \le t \le b, y(a) = \alpha.$$
(1)

The numerical solution to the problem are derived in many approaches including the linear one step and the linear multistep method. The predictor-corrector methods are interested subject among various multistep methods. In fact, these are center of the linear multistep kind as the reason originated for a multi-step method in taking full advantage of function evaluation. The awkward issue, especially in dialing with the stiffness, of the Adam predictor-corrector family lies in the size of their absolute stability region. Estimating how large these regions are can be expected as an explanation for this.

In this circumstance, the hope is not ended by taking a replacement of a BDF corrector to the Adams-Moulton corrector in expecting a considerable enlargement of the absolute stability reason. This is not unreasonable prospect. (See [1]-[5])

For purposes of comparison, we need to estimate the absolute stability region for a kstep Adams-Brashfort predictor with a k'-step Adams-Moulton corrector (denoted by ABk-AMk') and a k-step Adams-Brashfort predictor with a k'-step BDF corrector (denoted by ABk-BDFk'). Two considerations of k' taken into account are k' = k and k' = k+ 1. The following results can be found in some texts (e.g. [6], [7]).

Theorem 1. For the k-step Adams-Brashfort predictor

$$w_{i+1}^* = w_i + h \sum_{j=0}^{k-1} a_{k-j-1} f(t_{i-j}, w_{i-j})$$

and the implicit linear (k' - 1)-step corrector

$$w_{i+1} = \sum_{j=0}^{k'-1} b_{k'-j-1} w_{i-j} + \\ \tilde{a}_{k'-1} h f(t_{i+1}, w_{i+1}^*) + \\ h \sum_{j=0}^{k'-2} \tilde{a}_{k'-j-2} f(t_{i-j}, w_{i-j})$$

with the local truncation error are $\tau_{i+1}^*(h), \tau_{i+1}(h)$, respectively. Then the local

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truncation error of the Adams predictorcorrector is

 $\sigma_{i+1} = \tau_{i+1} + h\tau_{i+1}^* \tilde{a}_{k'-1} f_y(t_{i+1}, \xi_{i+1}), (2)$ for some ξ_{i+1} between 0 and $h\tau_{i+1}^*(h)$. Here, we infer the terms $\sigma_{i+1}, \tau_{i+1}, \tau_{i+1}^*$ as functions of the step-size *h*. The approximated values $w_i's$ produced by the method of $y(t_i)$ are obtained after some conventional one-step methods to generate the first k - 1 or k' - 1initial values such as Runge-Kutta method of the same order. The implicit linear method here is in the general form.

2. Derivation of the absolute stability region to the pece ABk-AMk' and ABk-BDFk' predictor-corrector

We first construct the scheme by which the local error presents and processes for some interested predictor-correct method in PECE mode. The 4-step Adams-Brashfort predictor of these methods is

$$w_{i+1}^* = w_i + \frac{h}{24} [55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) + 37f(t_{i-2}, w_{i-2}) - 9f(t_{i-3}, w_{i-3})],$$
(5)
with $\tau_{i+1}^*(h) = \frac{251}{720} h^4 y^{(5)}(\xi).$

The 3-step and 4-step Adames-Moulton correctors respectively are

$$w_{i+1} = w_i + \frac{h}{24} [9f(t_{i+1}, w_{i+1}^*) + 19f(t_i, w_i) - 5f(t_{i-1}, w_{i-1}) + f(t_{i-2}, w_{i-2})], \quad (6)$$
with $\tau_{i+1}(h) = \frac{-9}{720} h^4 y^{(5)}(\xi)$, and
$$w_{i+1} = w_i + \frac{h}{720} [251f(t_{i+1}, w_{i+1}^*) + 646f(t_i, w_i) - 264f(t_{i-1}, w_{i-1}) + 106f(t_{i-2}, w_{i-2}) - 19f(t_{i-3}, w_{i-3})], \quad (7)$$
with $\tau_{i+1}(h) = \frac{-3}{160} h^5 y^{(6)}(\xi)$.

The 3-step and 4-step BDF correctors respectively are

$$w_{i+1} = \frac{18}{11}w_i - \frac{9}{11}w_{i-1} + \frac{2}{11}w_{i-2} + \frac{6h}{11}f(t_{i+1}, w_{i+1}^*)$$
(8)

with $\tau_{i+1}(h) = \frac{3}{22}h^3 y^{(4)}(\xi)$, and

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$$w_{i+1} = \frac{48}{25} w_i - \frac{36}{25} w_{i-1} + \frac{16}{25} w_{i-2} - \frac{3}{25} w_{i-3} + \frac{12h}{25} f(t_{i+1}, w_{i+1}^*)$$
(9)
with $\tau_{i+1}(h) = \frac{12}{125} h^4 y^{(5)}(\xi).$

From (5) to (9), the intermediate point ξ are between the smallest and the largest mesh point appeared in the corresponding formula.

To conduct the stability characteristic polynomials of these methods, we apply the predictor-corrector scheme to the test equation

$$y' = \lambda y, y(a) = \alpha, a \le t \le b.$$
(10)

Let do this for AB4-BDF4 first and follow the same pattern for various other.

The equation (10) with the predictor (5) and the assumption that the previous four approximations are exact gives

$$w_{i+1}^* = w_i + \frac{\lambda h}{24} (55w_i - 59w_{i-1} + 37w_{i-2} - 9fw_{i-3}).$$
(11)

With the same assumption, the corrector (9) applied to (10) delivers

$$w_{i+1} = \frac{48}{25}w_i - \frac{36}{25}w_{i-1} + \frac{16}{25}w_{i-2} - \frac{3}{25}w_{i-3} + \frac{12\lambda h}{25}w_{i+1}^*.$$
 (12)

Substitute (11) into (12) and set $z = \lambda h$ and check the difference equation for $w_i = \gamma^i$ to obtain

$$\gamma^{4} - \frac{1}{50} (96 + 24z + 55z^{2})\gamma^{3} + \frac{1}{50} (72 + 59z^{2})\gamma^{2} - \frac{1}{50} (32 + 37z^{2})\gamma + \frac{1}{50} (6 + 9z^{2}) = 0.$$
(13)

The left-hand side, $P(\gamma, z) = \rho(\gamma) + z\sigma_1(\gamma) + z^2\sigma_2(\gamma)$, of (13) is defined as the stability polynomial for the method, [2], [3].

The stability polynomials of AB4-BDF3, AB4-AM3, AB4-AM4 are derived respectively as

$$\gamma^{4} - \frac{1}{44} (72 + 24z + 55z^{2})\gamma^{3} + \frac{1}{44} (36 + 59z^{2})\gamma^{2} - \frac{1}{44} (8 + 37z^{2})\gamma + \frac{9}{44} z^{2}, \quad (14)$$

$$\gamma^{4} - \frac{1}{192} (192 + 224z + 165z^{2})\gamma^{3} + \frac{1}{192} (40z + 177z^{2})\gamma^{2} - \frac{1}{192} (8z + 111z^{2})\gamma + \frac{9}{64}z^{2}, \quad (15)$$

$$\gamma^{4} - \left(1 + \frac{299}{240}z + \frac{2761}{3456}z^{2}\right)\gamma^{3} + \left(\frac{11}{30}z + \frac{14809}{17280}z^{2}\right)\gamma^{2} - \left(\frac{53}{360}z + \frac{9287}{17280}z^{2}\right)\gamma + \frac{19}{720}z + \frac{251}{1920}z^{2}, \quad (16)$$



Figure 1. The absolute stability region of the AB4-BDF4



Figure 2. The absolute stability region of the AB4-BDF3



Figure 3. The absolute stability region of the AB3-AM3



Figure 4. *The absolute stability region of the AB4-AM4* For depicting the absolute stability region, the *Root Condition* will be invoked [1], [6]. The *boundary locus method* will be applied to these

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stability polynomials [8]. Figures 1-4 describes the absolute stability regions to the methods 13-16 respectively in (z, γ) -plane. These regions are marked in green. So that, according to the Root Condition, for any z inside theses domain, the corresponding stability polynomial has all (complex) roots γ with the magnitude does not exceed one, and for whose the magnitude one is simple root.

We also see that, the expectation of having a large absolute stability region as we possess for the BDF now comes to an end when replacing the Adams-Moulton correctors by the BDF correctors. Inversely, such regions have been contracted by a little with this replacement however.

The result in Theorem 1 enables us to estimate the local truncation error of these method. Theoretically, the AB4-AM4 ranks the first in the highest order of accuracy (with local truncation error of order $O(h^5)$), then it is followed by the AB4-BDF4 and AB4-AM3 (of which the order are $O(h^4)$) and the last in the rank is AB4-BDF3 (whose the order is $O(h^3)$). The AB4-AM4 has the optimal order following the result in [9], Theorem 3.2.

The BDF correctors even probably provide larger absolute stability regions which maybe accounts for their applicability in dialing with a larger class of the stiff equations can show the less effective, or less accurate comparing to the Adams correctors. Even the AB4-AM3 and AB4-BDF4 are of the same order, the experimental results indicates the favor of the Adams corrector.

For the consistency and zero-stability of these methods, it is straightforward from the first characteristic polynomials $\rho(\gamma)$ of such methods are so. For example, for AB4-AM4, the consistency is the case since.

$$\sum_{j=0}^{3} b_{3-j} = 1,$$

and the zero-stability is inferred from the fact that the first characteristic polynomial

$$\rho(\gamma) = \gamma^4 - \frac{48}{25}\gamma^3 + \frac{36}{25}\gamma^2 - \frac{16}{25}\gamma + \frac{3}{25}$$

has four (complex) roots with modulus less than 1 except for the root 1. That is, this polynomial fulfills the Root Condition. Therefore, it is stable. (See [1], [6], [8]) From this fact, the following theorem is straightforward.

Theorem 2. The ABk-AMk' and ABk-BDFk' are convergent.

Indeed, we have known that (see, for example, [1], [2]) the zero-stability and the convergent are equivalent under the condition of the consistency. The above methods are both zero-stable and consistent, they are convergent anyway.

3. The modified P(EC)^mE algorithm

The abovementioned methods can be improved their accuracy with m iterations to get a $P(EC)^m E$ mode. The following algorithm is introduced with m iterations to generate the approximated value $w_{i+1} = w_{i+1}^{(m)}$ for $y(t_{i+1})$ by applying the corrector difference equation m times. However, we control the number of iteration by the maximum iteration M. This even a little change in the scheme could lead to a fairly good improvement and an avoidance of out of control repetition. Here, we only construct the algorithm for the 3-step Adams-Moulton corrector, we call it the 3-step ABM modified method, denoted by $P(EC)^{M}E$. The other algorithms can be conducted similarly. This algorithm is presented in Matlab code. The convergence of this mode is undoubted. However, the barrier for its accuracy is inevitable since the iterated values converge in fact to the solution of the difference equation used to iterate the corrector values rather than to $y(t_{i+1})$. (See Theorem 3.2, [9]) An unreasonable increment in the number of

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iterations m or decrement could lead the error to increase.

INPUT the function f(t, y), the interval [a, b], the initial value y(a) = a, the tolerance tol > 0 desired for the error estimate obtained from the iterations, the number of iterations M.

OUTPUT the approximation w_i to the solution $y(t_i), \forall i = 0, 1, ..., n$.

Algorithm

```
Function
out=ABM Modification(f,a,b,alpha,
N,tol,M)
% N is the number of mesh points
% alpha is the initial value
% tol is the tolerance used to
control the iteration
% M is the desired maximum number
of iterations
syms z(s);
format long;
8-----STEP 1-----
h=(b-a)/N;
t0=a;
w0=alpha;
t=[t0];
w = [w0];
8-----STEP 2-----
% Generate the starting values by
Runge-Kutta method
for i=1:3
k1=h*f(t0,w0);
k2=h*f(t0+0.5*h,w0+0.5*k1);
k3=h*f(t0+0.5*h,w0+0.5*k2);
k4=h*f(t0+h,w0+k3);
w0=w0+(k1+2*k2+2*k3+k4)/6;
t0=t0+h;
t = [t, t0];
w = [w, w0];
end
8-----STEP 3-----
```

```
for i=4:N
                    t0=t0+h;
                    wp=w(i)+h*(55*f(t(i),w(i))-
59 \pm f(t(i-1), w(i-1)) + 37 \pm f(t(i-1)) + 37 \pm f(t))
2),w(i-2))-9*f(t(i-3),w(i-3)))/24;
                     FLAG=0;
                     count=1;
                     while (FLAG==0) & (count<M)</pre>
w0=w(i)+h^{*}(9^{*}f(t0,wp)+19^{*}f(t(i),w(
i)) - 5 * f(t(i-1), w(i-1)) + f(t(i-1)) + f(t(i-1)) + f(t(i-1))) + f(t(i-1)) + f(t(i-1))) + f(t(i-1)) + f(t(i-1))) + f(t
2),w(i-2)))/24;
                                          if abs(w0-wp)<tol</pre>
                                                                FLAG=1;
                                                               break
                                          else wp=w0;
                                                                count=count+1;
                                          end
                     end
                     t=[t,t0];
                     w = [w, w0];
end
eqn=diff(z,s)==f(s,z);
inc=z(a) == alpha;
as=dsolve(eqn,inc);
out=[t',w',double(subs(as,s,a:h:b)
)', abs (w-
double(subs(as,s,a:h:b)))'];
end
%-----END-----
```

4. Comparison through numerical examples

The efficiency of the above techniques is performed to see the conclusion about their stability.

Example: Consider the equations

$$y' = y - t^{2} + 1, y(0) = \frac{1}{2}, 0 \le t \le 2, (17)$$

$$\begin{cases} y' = 5e^{5t}(y - t)^{2} + 1 \\ y(0) = -1, t \in [0, 1] \end{cases}$$
(18)
$$(y' = -20y + 20 \operatorname{cost} - \operatorname{cin} t$$

$$\begin{cases} y = -20y + 20\cos t - \sin t \\ y(0) = 0, t \in [0,2] \end{cases}$$
(19)

$$\begin{cases} y' = -20(y - t^2) + 2t \\ y(0) = 1/3, t \in [0, 1] \end{cases}$$
(20)

by AD4-AM5, AD4-AM4, AD4-DD15, AD4-DD14, $F(EC) = E$ modification					
Equation	AB4-AM3	AB4-AM4	AB4-BDF3	AB4-BDF4	ABM_Modified
(17)	4.9×10^{-4} ,	9.2×10^{-5} ,	1.5× 10 ⁻² ,	2.5×10^{-3} ,	1.51×10^{-3} ,
N=6,10, 15	1.0×10^{-4} ,	3.9× 10 ⁻⁵ ,	6.3× 10 ⁻³ ,	7.25×10^{-4} ,	1.01×10^{-4} ,
	2.85×10^{-5}	8.2×10^{-6}	2.5×10^{-3}	2.1×10^{-4}	2.86×10^{-5}
(18)	21.845,	7.628,	394.675,	594.29,	8.6×10^{-4} ,
N=6, 10, 20	4.74×10^{-5} ,	6× 10 ⁻⁵ ,	4.1×10^{-4} ,	5.1×10^{-3} ,	1.35×10^{-4} ,
	4.12×10^{-6}	2.6×10^{-6}	6.36×10^{-5}	3.62×10^{-5}	4.12×10^{-6}
(19)	2.1×10^{9} ,	1.1×10 ⁹ ,	5.08×10^{10} ,	2.8×10^{10} ,	3.38×10^{20} ,
N=8, 30, 50,	0.57,	0.0105,	10 ⁶ ,	1.05×10^{6} ,	1.05×10^{-4} ,
100	2.27×10^{-8} ,	1.63×10^{-8} ,	1.16×10^{-6} ,	2.7×10^{-7} ,	2.27×10^{-8}
	6.94×10^{-10}	4.23×10^{-10}	5.86×10^{-8}	4.26×10^{-9}	6.94×10^{-10}
(20)	0.27, 0.0257,	0.204,	3.58×102,	2.8×10^2 ,	3.98×10^{-4} ,
N= 10, 15,	$1.47 imes 10^{-4}$,	0.00372,	43.53,	53.54,	1.65×10^{-4} ,
20, 100	1.53×10^{-12}	7.5×10^{-6} ,	0.0409,	0.08,	1.15×10^{-5}
		6.45×10^{-13}	4.13×10^{-11}	1.05×10^{-11}	1.53×10^{-12}

Table 1. The absolute errors produced by AB4-AM3, AB4-AM4, AB4-BDF3, AB4-BDF4, $P(EC)^{M}E$ modification

With N is the number of mesh points, so the step-size h = (b - a)/N. Since the above techniques are convergent, the error decreases as N increase. The poor performance for insufficient small step-sizes when applied to the stiff equation (18)-(20) show the aukward of these methods for the stiffness, especially when the transient in (19) and (20) are stronger. Table 1 shows this point. The experimental results also show that the Adams correctors are superior to the BDF ones. This is identical to the size of the absolute stability regions for the corresponding method as shown in Figures 1-4. These results also show that for a fairly small step-size, the $P(EC)^M E$ modified produces a supperior results for both stiff and non-stiff problems [5].

5. Conclusion

Using the above strategy of analyzing the stability of a predictor-corrector method, we can be able to figure out the applicability and the efficiency of the method intended to use for a particular problem keeping in mind that there is no best scheme for solving all initial value problem numerically, but the best one depends on each problem.

The modification we make here for these predictor-corrector methods even improves the

approximation, its speed of convergence is not so high as expected comparing to that of a conventional corrector when the step-size is very small. The reason for this probably comes from the round-off error produced when the repetitions of the corrector are performs.

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