

EPS & EPUS Step-size Control for Linear Multistep Method

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Received on: 9/11/2004

Accepted on: 27/12/2004

الملخص

في هذا البحث تم السيطرة على حجم الخطوة التكاملية لطرق آدم المتعددة الخطوات الخطية المستخدمة لحل المعادلات التفاضلية الاعتيادية . لقد تم استنتاج نتائج نظرية لصيغة آدم-مولتن-باشفورت باستخدام سيطرات (EPS) و (EPUS). النتائج النظرية المستخلصة اعتمدت على النظام :

$$\frac{dQ_1}{dh} = Q_2$$

$$\frac{dQ_2}{dh} = q(h)$$

حيث

$$Q_1(h) = \int_0^h (h-s)q(s)ds \quad \text{for } h \geq 0$$

و

$$q(s) = \prod_{i=0}^{k-2} (s + t_n - t_{n-i}) = \prod_{i=0}^{k-2} (s + \Psi_i) \quad , \quad \Psi_i = t_n - t_{n-i}$$

ABSTRACT

In this paper we consider step-size control in one class of Adams linear multi-step methods for Ordinary differential equation. Theoretical results are presented for Adam-Bashforth-Moulton formula using both Error-per-step (EPS) & Error-per-Unit -Step (EPUS) controls. These obtained by considering a 2D system of the form:

$$\frac{dQ_1}{dh} = Q_2$$

$$\frac{dQ_2}{dh} = q(h)$$

where $Q_1(h) = \int_0^h (h-s)q(s)ds \quad \text{for } h \geq 0 \quad \text{and}$

$$q(s) = \prod_{i=0}^{k-2} (s + t_n - t_{n-i}) = \prod_{i=0}^{k-2} (s + \Psi_i) \quad , \quad \Psi_i = t_n - t_{n-i}$$

1. INTRODUCTION:

Two of the most popular families of multistep methods are the so-called Adams families, which are based on the exact integrating polynomials. One family (Adams-Bashforth) leads to explicit methods; the other (Adams-Moulton) leads to implicit methods [1],[3].

Linear multi-step methods (LMM) form the basis of a wide range of ODE integrators. Whereas they are often very efficient in advancing the integration, the implementation of suitable stepsize selection strategies can be non-trivial. Given a user specified error-per-step, or error-per-unit-step, a nontrivial polynomial equation must in general be solved, to obtain a suitable step-size h^* for the following step.

Wille' in 1994 [4], Numerical Analysis Report No.247, showed that applied to Predictor -Corrector schemes, one natural error estimate may be obtained by comparing the values yielded by the corrector and predictor Stages

$$P_{k+1,n+1}(t) = P_{k,n+1}(t) + \prod_{i=0}^{k-1} (t - t_{n-i}) f^P[t_{n+1}, \dots, t_{n-k+1}]$$

by an expression of the form

$$f^P[t_{n+1}, \dots, t_{n-k+1}] \int_{t_n}^{t_{n+1}} \prod_{i=0}^{k-1} (t - t_{n-i}) dt \quad \text{Obtained by}$$

$$\frac{dQ}{dh} = q(h)$$

$$Q(a) = Q_a$$

and its transformed analogue

$$\frac{dh}{dQ} = \frac{1}{Q(H(Q))}$$

$$h(Q_n) = a$$

in this paper we consider the 2D system of the form :

$$\frac{dQ_1}{dh} = Q_2$$

$$\frac{dQ_2}{dh} = q(h)$$

where $Q_1(h) = \int_0^h (h-s)q(s)ds$ for $h \geq 0$ and

$$q(s) = \prod_{i=0}^{k-2} (s + t_n - t_{n-i}) = \prod_{i=0}^{k-2} (s + \Psi_i) \quad , \quad \Psi_i = t_n - t_{n-i}$$

2.ADAMS FORMULA:

2.1- Predictor-Corrector Schemes: [4],[2]

Given an ODE

$$y'(t) = f(t, y(t))$$

the k -th order Adams-Bashforth and $(k+1)$ -th order Adams-Moulton

methods to advance a numerical solution $\{\tilde{y}_i \approx y(t_i)\}$ across a step $[t_n, t_{n+1}]$ may be written as

$$\tilde{y}_{n+1} = \tilde{y}_n + \int_{t_n}^{t_{n+1}} P_{k,n}(t) dt$$

and

$$\tilde{y}_{n+1} = \tilde{y}_n + \int_{t_n}^{t_{n+1}} P_{k+1,n+1}(t) dt$$

Respectively, where $P_{i,j}$ is the $(i-1)$ -th degree polynomial defined by the function values $\{\tilde{f}_i \equiv f(t_i, \tilde{y}_i)\}$ at the points $\{t_j, t_{j-1}, \dots, t_{j-i+1}\}$. Such formulae are usually used in predictor - corrector pairs [5]. Denoting the Adams-Bashforth estimate $\tilde{y}_{n+1}^P$, the predictor (P_k), and using this value in the definition of $P_{k+1,n+1}$, by the second formula we obtain a new value, $\tilde{y}_{n+1}^C$ for $y(t_{n+1})$. we refer to this as the corrector (C_{K+1}). The resulting Adams-Bashforth-Moulton scheme may be expressed $P_kEC_{k+1}E$ where E denotes the intervening function evaluations and the subscripts, the order of the equations used.

2.2- An Error Estimate

Applied to the above scheme, one natural error estimate may be obtained by comparing the values by the corrector and predictor stages. That is

$$P_{k+1,n+1}(t) = P_{k,n+1}(t) + \prod_{i=0}^{k-1} (t - t_{n-i}) f^P[t_{n+1}, \dots, t_{n-k+1}]$$

By the expression of the form

$$f^P[t_{n+1}, \dots, t_{n-k+1}] \int_{t_n}^{t_{n+1}} \prod_{i=-1}^{k-2} (t - t_{n-i}) dt$$

where $f^P[t_{n+1}, \dots, t_{n-k+1}]$ here denotes the $(k+1)$ -st Newton divided difference through the points $\{(t_i, y_i), (t_{n+1}, y_{n+1}^P) : i = n, \dots, n - k + 1\}$

2.3- EPS Stepsize Control:

Define

$$Q_1(h) = \int_0^h (h-s)q(s)ds \quad \text{for } h \geq 0$$

and

$$q(s) = \prod_{i=0}^{k-2} (s + t_n - t_{n-i}) = \prod_{i=0}^{k-2} (s + \Psi_i) \quad , \quad \Psi_i = t_n - t_{n-i} .$$

Given a requested step tolerance ϵ and using an EPS error control strategy, to advance a step $[t_n, t_{n+1}]$ we would ideally choose $h^* = t_{n+1} - t_n$ such that:

$$\sup_{0 \leq h \leq h^*} |Q_1(h) f^P[t_{n+1}, t_n, \dots, t_{n-k+1}]| = \epsilon \quad \dots\dots\dots(1)$$

However, since no a priori f-information is known for the desired step , it is usual (assuming a slow variation in $f^{(k)}$) to approximate

$$f^P[t_{n+1}, \dots, t_{n-k+1}] \approx f[t_n, \dots, t_{n-k}]$$

By the monotonicity of $Q_1(h)$ for $h \geq 0$ it then suffices to solve:

$$Q_1(h^*) = l^* \quad \dots\dots\dots(2)$$

for (assuming $f[t_n, \dots, t_{n-k}] \neq 0$), $l^* = \epsilon / |f[t_n, t_{n-1}, \dots, t_{n-k}]|$.

2.4- A Numerical Approach

To solve (2), differentiating with respect to h we note, however, that

$$Q_1'(h) = \int_0^h q(s)ds$$

and

$$Q_1''(h) = q(h).$$

Given this, Q_1 may be redefined in terms of differential equation

$$\begin{aligned}\frac{dQ_1}{dh} &= Q_2 \\ \frac{dQ_2}{dh} &= q(h)\end{aligned}\dots\dots\dots(3)$$

for $h \geq 0$ given $Q=0$ where $Q=[Q_1, Q_2]^T$.

Solving for h^* such that $Q_1(h^*) = l^*$ then reduces to a so-called g-stop problem [3]. Reversing coordinates

$$\begin{aligned}\frac{dh}{dQ_1} &= \frac{1}{Q_2(h)} \\ \frac{dQ_2}{dQ_1} &= \frac{q(h)}{Q_2(h)},\end{aligned}\dots\dots\dots(4)$$

and noting that h is monotone in Q_1 for $Q_1 > 0$, we observe however that given suitable starting values for $(a, Q(a))$, integrating (4) across $[Q_1(a), l]$ provides a simple direct expression for the required stepsize $h^* = h(l^*)$. This is our key advance. The direct solution of (4) in the Adams EPS case is, however, complicated by the singularity at $h=0$. As we now show, this does not occur for EPUS schemes: they are singularity free. Theoretically, it is hoped that equations of the form (4) may also provide insight into how new analytic stepsize estimators can be derived.

2.5-EPUS Stepsize Control

To adapt the above error-per-step strategy to an error-per-unit-step (EPUS) strategy, we merely need replace (1) by an equation of the form:

$$\sup_{0 \leq h \leq h^*} |Q_1(h) f^p[t_{n+1}, t_n, \dots, t_{n-k+1}] / h| = \epsilon$$

writing

$$\tilde{Q}_1(h) = \begin{cases} Q_1(h)/h & : h \neq 0 \\ 0 & : h = 0 \end{cases} \dots\dots\dots(5)$$

we now, following of the EPS case, consider equations of the form

$$\tilde{Q}_1(h^*) = l^* \dots\dots\dots(6)$$

where $l^* = \epsilon / |f^p[t_n, t_{n-1}, \dots, t_{n-k}]|$.

Taking limits, and given that

$$Q_1'(s) = Q_2(s)$$

$$Q_2'(s) = q(s)$$

is strictly positive monotone increasing for $h \geq 0$, it thus follows that $\tilde{Q}_1(h)$ is continuous for all $h \geq 0$.

We note

$$\begin{aligned} Q_1(h) &= \int_0^h Q_2(s)ds = \int_0^h Q_1'(s)ds \quad \mathbf{p} \quad h. \max_{s \in [0, h]} Q_1'(s) = h.Q_1'(h) \\ Q_2(h) &= \int_0^h q(s)ds = \int_0^h Q_2'(s)ds \quad \mathbf{p} \quad h. \max_{s \in [0, h]} Q_2'(s) = h.Q_2'(h) \end{aligned} \quad \dots\dots\dots(7)$$

for $h \geq 0$, and thus

$$0 \leq \lim_{h \rightarrow 0} \tilde{Q}_1(h) = \lim_{h \rightarrow 0} \frac{1}{h} Q_1(h) \leq \lim_{h \rightarrow 0} Q_1'(h) = 0$$

Differentiating

$$\begin{aligned} \tilde{Q}_1'(h) &= D_h \{h^{-1}.Q_1(h)\} \\ &= -\frac{1}{h^2}.Q_1(h) + \frac{1}{h}.Q_1'(h) \\ &= \frac{1}{h^2}[-Q_1(h) + hQ_1'(h)] \end{aligned}$$

and using the result (7)

$$\begin{aligned} Q_1(h) \quad \mathbf{p} \quad h.Q_1'(h) \\ Q_2(h) \quad \mathbf{p} \quad h.Q_2'(h) \end{aligned} \quad \dots\dots\dots(8)$$

it follows that $\tilde{Q}_1'(h)$ is strictly positive and so $Q_1(h) \uparrow$ on $h > 0$. Defining

$$\left. \frac{1}{h^2} Q_1(h) \right|_{h=0} \quad \& \quad \left. \frac{1}{h^2} Q_2(h) \right|_{h=0}$$

as the $\lim_{h \rightarrow 0} \frac{1}{h^2} Q_1(h)$ & $\lim_{h \rightarrow 0} \frac{1}{h^2} Q_2(h)$ respectively we note by Hopitats

rule :

$$\begin{aligned} \left. \frac{1}{h^2} Q_1(h) \right|_{h=0} &= \lim_{h \rightarrow 0} \frac{Q_1'(h)}{2h} \quad \& \\ \left. \frac{1}{h^2} Q_2(h) \right|_{h=0} &= \lim_{h \rightarrow 0} \frac{Q_2'(h)}{2h} \end{aligned}$$

Given

$$Q_1'(h)/h = Q_2(h)/h = r_1(h)$$

$$Q_1'(h)/h = Q_2(h)/h = r_1(h)$$

$$\text{where } r_1(h) = \int_0^h \prod_{i=1}^{k-2} (s - t_n - t_{n-i}) ds$$

$$r_2(h) = \prod_{i=1}^{k-2} (h - t_n - t_{n-i})$$

this implies

$$\tilde{Q}_1'(0) = \frac{1}{2} r_1(0) \quad \& \quad \tilde{Q}_2'(0) = \frac{1}{2} r_2(0)$$

which is strictly positive . Defining

$$F_1(x,y) = \begin{cases} \frac{-y}{x} + r_1(x) & : x \neq 0 \\ \frac{1}{2} r_1(x) & : x = 0 \end{cases} \quad \& \quad F_2(x,y) = \begin{cases} \frac{-y}{x} + r_2(x) & : x \neq 0 \\ \frac{1}{2} r_2(x) & : x = 0 \end{cases}$$

we can then obtain $\tilde{Q}_1(h)$ & $\tilde{Q}_2(h)$ by direct integration :

$$\begin{aligned} \tilde{Q}_1'(h) &= F_1(h, \tilde{Q}_1(h)) & \text{and} & & \tilde{Q}_2'(h) &= F_2(h, \tilde{Q}_2(h)) \\ \tilde{Q}_1(0) &= 0 & & & \tilde{Q}_2(0) &= 0 \end{aligned}$$

thus by (8)&(9) , $\tilde{Q}_1'(h)$ & $\tilde{Q}_2'(h)$ is strictly positive for all $h \geq 0$.

The above, and the coordinate reversed equation,

$$h_1'(\tilde{Q}_1) = \frac{1}{F_1(h(\tilde{Q}_1), \tilde{Q}_1)} \quad , \quad h_2'(\tilde{Q}_2) = \frac{1}{F_1(h(\tilde{Q}_2), \tilde{Q}_2)} \quad , \quad h(0) = 0$$

are therefore singularity free. The validity of the boundary condition $h(0)=0$ relies on the continuity of (5) .re expressing (6) as $l^* \tilde{h}^* = Q_1(\tilde{h}^*)$ is equivalent for $\tilde{h}^* \neq 0$ but introduces a trivial root at $\tilde{h}^* = 0$.our representation $l^* = \tilde{Q}_1(\tilde{h}^*)$ removes this.

CONCLUSION:

Theoretical results are presented for Adam-Bashforth-Moulton formula using both Error-per-step (EPS) & Error-per-Unit -Step (EPUS) controls. These obtained by considering a 2D system of the form :

$$\frac{dQ_1}{dh} = Q_2$$

$$\frac{dQ_2}{dh} = q(h)$$

$$\text{where } Q_1(h) = \int_0^h (h-s)q(s)ds \quad \text{for } h \geq 0 \text{ and}$$

$$q(s) = \prod_{i=0}^{k-2} (s + t_n - t_{n-i}) = \prod_{i=0}^{k-2} (s + \Psi_i) \quad , \quad \Psi_i = t_n - t_{n-i} .$$

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