EPS & EPUS Step-size Control for Linear Multistep Method

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Received on: 09/11/2004 **Accepted on: 27/12/2004**

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

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

Keywords: Ordinary differential equation, Adam-Bashforth-Moulton formula.

السيطرة على حجم الخطوة التكاملية المتعددة الخطوات الخطية

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تاريخ استلام البحث: 2004/11/9 **تاريخ قبول البحث: 2004/12/27**

الملخص

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

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

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

حيث

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

و

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

الكلمات المفتاحية: **المعادلات التفاضلية الاعتيادية، صيغة أدم –مولتن –باشفورث.**

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

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

by an expression of the form

$$f^P[t_{n+1},\ldots,t_{n-k+1}]\int_{t_n}^{t_{n+1}}\prod_{i=0}^{k-1}(t - t_{n-i})dt$$ 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 ≥ 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 $\{t_j, t_{j-1}, \ldots, t_{j-i+1}\}$ .Such formulae are usually used in predictor - corrector pairs [5]. Denoting the Adams-Bashforth estimate $\tilde{y}^P_{n+1}$, 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 , $\tilde{y}^c_{n+1}$ for $y(t_{n+1})$ .we refer to this as the corrector (C_{K+1}) .The resulting Adam-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

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

By the expression of the form

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

where $f^{P}[t_{n+1},\ldots,t_{n-k+1}]$ here denotes the (k+1)-st Newton divided difference through the points

$$\{(t_i, y_i), (t_{n+1}, y^{p}_{p+1}) : i = n,\ldots,n-k+1\}$$

2.3- EPS Stepsize Control:

Define

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

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 $\in$ 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:

$$\sup_{0 \prec h \leq h^*} \left| Q_1(h) f^{p}[t_{n+1,}t_n,\ldots,t_{n-k+1}] \right| = \in \qquad \ldots\ldots\ldots. (1)$$

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

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

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

$$Q_1(h^*) = \lambda^* \qquad \ldots\ldots\ldots. \ldots..(2)$$

for (assuming $f[t_n,\ldots,t_{n-k}] \neq 0)$, $\lambda^* = \in / \left| f[t_n, t_{n-1},\ldots,t_{n-k}] \right|$.

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

$$\frac{dQ_1}{dh} = Q_2 \qquad \frac{dQ_2}{dh} = q(h) \qquad \textbf{..................(3)}$$

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

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

$$\frac{dh}{dQ_1} = \frac{1}{Q_2(h)} \qquad \frac{dQ_2}{dQ_1} = \frac{q(h)}{Q_2(h)}, \qquad \textbf{..................(4)}$$

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 $[Q_1(a), \lambda]$ provides a simple direct expression for the required stepsize $h^* = h(\lambda^*)$. 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:

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

writing

$$\tilde{Q}_1(h) = \begin{cases} Q_1(h)/h & : \mathrm{h} \succ 0 \\ 0 & : \mathrm{h} = 0 \end{cases} \qquad ....\ ....\ ....\ ..(5)$$

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

$$\tilde{Q}_1(\tilde{h}^*) = \lambda^* \qquad ....\ ....\ ....(6)$$

where $\lambda^* = \in / \left| f^{\,p}[t_n, t_{n-1}, ..., t_{n-k}] \right|$.

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

$$Q_1(h) = \int_0^h Q_2(s)ds = \int_0^h Q_1^{/}(s)ds \prec h.\max_{s\in[0,h]} Q_1^{/}(s) = h.Q_1^{/}(h)$$

$$Q_2(h) = \int_0^h q(s)ds = \int_0^h Q_2^{/}(s)ds \prec h.\max_{s\in[0,h]} Q_2^{/}(s) = h.Q_2^{/}(h) \qquad \text{……….(7)}$$

for $h \geq 0$, and thus

$$0 \leq \lim_{h\to 0} \tilde{Q}_1(h) = \lim_{h\to 0} \frac{1}{h} Q_1(h) \leq \lim Q_1^{/}(h) = 0$$

Differentiating

$$\tilde{Q}_1^{/}(h) = D_h\left\{h^{-1}.Q_1(h)\right\}$$

$$= - \frac{1}{\mathrm{h}^2}.Q_1(h) + \frac{1}{h}.Q_1^{/}(h)$$

$$= \frac{1}{\mathrm{h}^2}[-Q_1(h) + hQ_1^{/}(h)]$$

and using the result (7)

$$Q_1(h) \prec h.Q_1^{/}(h)$$

$$Q_2(h) \prec h.Q_2^{/}(h) \qquad \text{……………….(8)}$$

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 $\lim_{h\to 0} \frac{1}{h^2} Q_1(h)$ & $\lim_{h\to 0} \frac{1}{h^2} Q_2(h)$ respectively we note by Hopitats rule :

$$\frac{1}{h^2}Q_1(h)\Big|_{h=0} = \lim_{h\to 0}\frac{Q_1^{/}(h)}{2h} \quad \&$$

$$\frac{1}{h^2}Q_2(h)\Big|_{h=0} = \lim_{h\to 0}\frac{Q_2^{/}(h)}{2h}$$

Given

$$Q_1^{/}(h)/h = Q_2(h)/h = r_1(h)$$

$$Q_1^{/}(h)/h = Q_2(h)/h = r_1(h)$$

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

$$\tilde{Q}_1^{/}(0) = \frac{1}{2}r_1(0) \qquad \& \qquad \tilde{Q}_2^{/}(0) = \frac{1}{2}r_2(0)$$

which is strictly positive . Defining

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

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

$$\tilde{Q}_1^{/}(h) = F_1(h, \tilde{Q}_1(h)) \qquad \text{and} \qquad \tilde{Q}_2^{/}(h) = F_2(h, \tilde{Q}_2(h))$$
$$\tilde{Q}_1(0) = 0 \qquad\qquad \tilde{Q}_2(0) = 0$$

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 $\lambda^*\tilde{h}^* = Q_1(\tilde{h}^*)$ is equivalent for $\tilde{h}^* \succ 0$ but introduces a trivial root at $\tilde{h}^* = 0$ .our representation $\lambda^* = \tilde{Q}_1(\tilde{h}^*)$ 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 :

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

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

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

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

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