EPS & EPUS Step-size Control for Linear Multistep Method

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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:

\[
\frac{dQ_0}{dh} = Q_2 \\
\frac{dQ_2}{dh} = q(h)
\]

where

\[
Q_2(h) = \int_0^h (h-s)q(s)ds \quad \text{for } h \geq 0 \text{ and }
\]

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

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

The control of the step size for the multistep linear methods used for solving 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 with the following ODEs:

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\[ Q_s(h) = \int_0^h (h - s)q(s)ds \quad \text{for } h \geq 0 \]

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

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

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

by an expression of the form

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

Obtained by

\[ \frac{dQ}{dh} = q(h) \]

\[ Q(a) = Q_a \]

and its transformed analogue

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

\[ h(Q_a) = a \]

in this paper we consider the 2D system of the form:
\[ \frac{dQ_1}{dh} = Q_2 \]
\[ \frac{dQ_2}{dh} = q(h) \]

where \( Q_i(h) = \int_0^h (h-s)q(s)ds \) 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 \( P_{ij} \) is the \( (i-1) \)-th degree polynomial defined by the function values \( \{f_i \equiv f(t_i, \tilde{y}_i)\} \) 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 \( \tilde{y}_{n+1}^P \), 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
\[ P_{k+1,n+1}(t) = P_{k,n+1}(t) + \prod_{i=0}^{k-1} (t-t_{n-i}) f^P[t_{n+1},\ldots,t_{n+k+1}] \]

By the expression of the form
\[ f^P[t_{n+1},\ldots,t_{n-k+1}] \int \prod_{i=1}^{k-2} (t-t_{n-i}) dt \]

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

2.3- EPS Stepsize Control:

Define
\[ Q_i(h) = \int_0^h (h-s)q(s)ds \quad \text{for } h \geq 0 \]

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 \( \varepsilon \) 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:
\[ \sup_{0 < h \leq \varepsilon} |Q_i(h)f^P[t_{n+1},\ldots,t_{n+k+1}]| = \varepsilon \quad \text{........... (1)} \]

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 monotonicity of \( Q_i(h) \) for \( h \geq 0 \) it then suffices to solve:

\[ Q_i(h^*) = \lambda^* \quad \text{............ (2)} \]

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

2.4- A Numerical Approach

To solve (2), differentiating with respect to \( h \) we note, however, that
\[ Q'_i(h) = \int_0^h q(s)ds \]
and

\[ Q_1^*(h) = q(h). \]

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

\[
\begin{align*}
\frac{dQ_1}{dh} &= Q_2 \\
\frac{dQ_2}{dh} &= q(h)
\end{align*}
\]

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

\[
\begin{align*}
\frac{dh}{dQ_1} &= \frac{1}{Q_2(h)} \\
\frac{dQ_2}{dQ_1} &= \frac{q(h)}{Q_2(h)}
\end{align*}
\]

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:

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

writing

\[
\tilde{Q}_1(h) = \begin{cases} Q_1(h) / h & : h > 0 \\ 0 & : h = 0 \end{cases}
\]

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

\[
\tilde{Q}_1(h^*) = \lambda^*
\]
where \( \lambda^* \in \left| \int f^p [t_n, t_{n-1}, \ldots, t_{n-k}] \right| \).

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
\[ Q_1(h) = \int_0^h Q_2(s) ds = \int_0^h Q_1'(s) ds < h \max_{s \in [0,h]} Q_1'(s) = h Q_1'(h) \]
\[ Q_2(h) = \int_0^h q(s) ds = \int_0^h Q_2'(s) ds < h \max_{s \in [0,h]} Q_2'(s) = h Q_2'(h) \]

for \( h \geq 0 \), and thus
\[ 0 \leq \lim_{h \to 0} \tilde{Q}_1(h) = \lim_{h \to 0} \frac{1}{h} Q_1(h) \leq \lim_{h \to 0} Q_1'(h) = 0 \]

Differentiating
\[ \tilde{Q}_1'(h) = D_h \{ h^{-1} Q_1(h) \} \]
\[ = -\frac{1}{h^2} Q_1(h) + \frac{1}{h} Q_1'(h) \]
\[ = \frac{1}{h^2} [-Q_1(h) + hQ_1'(h)] \]

and using the result (7)
\[ Q_1(h) < h Q_1'(h) \]
\[ Q_2(h) < h Q_2'(h) \]

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 Hopital's rule:
Given

\( Q'_1(h) / h = Q_2(h) / h = r_1(h) \)

\( Q'_2(h) / h = Q_2(h) / h = r_1(h) \)

\[
 r_1(h) = \frac{\hbar}{k-2} \sum_{i=1}^{k-2} (s - t_n - t_{n-1}) ds
\]

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

this implies

\[
 \tilde{Q}'_1(0) = \frac{1}{2} r_1(0) \quad \text{and} \quad \tilde{Q}'_2(0) = \frac{1}{2} r_2(0)
\]

which is strictly positive. Defining

\[
 F_1(x, y) = \begin{cases} 
 -\frac{y}{x} + r_1(x) & : x > 0 \\
 1 & : x = 0 \\
 \frac{1}{2} r_1(x) & : x = 0 
\end{cases} \quad \text{and} \quad F_2(x, y) = \begin{cases} 
 -\frac{y}{x} + r_2(x) & : x > 0 \\
 1 & : x = 0 \\
 \frac{1}{2} r_2(x) & : x = 0 
\end{cases}
\]

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

\[
 \tilde{Q}'_1(h) = F_1(h, \tilde{Q}_1(h)) \quad \text{and} \quad \tilde{Q}'_2(h) = F_2(h, \tilde{Q}_2(h))
\]

\[
 \tilde{Q}_1(0) = 0 \quad \text{and} \quad \tilde{Q}_2(0) = 0
\]

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

The above, and the coordinate reversed equation,

\[
 h'_1(\tilde{Q}_1) = \frac{1}{F_1(h(\tilde{Q}_1), \tilde{Q}_1)} \quad \text{and} \quad h'_2(\tilde{Q}_2) = \frac{1}{F_1(h(\tilde{Q}_2), \tilde{Q}_2)} \quad \text{h}(0) = 0
\]
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 \( \tilde{h}^* > 0 \) but introduces a trivial root at \( \tilde{h}^* = 0 \). Our representation
\( \lambda^* = Q_1(\tilde{h}^*) \) 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:

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