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Variable Step-size Variable Formula Stiffly Stable Linear 3-step Methods

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Abstract: In this paper we developed the variable step size variable formula stiffly stable linear 3-step methods which are suitable for stiff problems (see [1]). Particular emphasis is given to develop methods with large region of instability in the right half plane which are suitable for stiff systems with the capability of detecting unstable behavior of a problem.

1. Introduction

The unpredictable behavior of solutions of differential equations forces the numerical integration to proceed with step-sizes which, in general, must vary from point to point if a prescribed error is to be maintained. Multi-step methods which use equidistant nodes and a fixed method, therefore, are not suitable in practice. If a fixed method is used and the step size is allowed to vary then every change of the step length requires re-computation of starting data which entails a complicated interpolation process. This of course reduces the efficiency of these integration methods. For this reason, we want to derive linear 3-step methods with variable grids. We are, like in [1], interested in methods which are stiffly stable as well as having a large region of instability in the right half plane.

We recall that on a uniform grid

$$t_n = nh, \qquad n = 0,1,\cdots, \qquad h > 0,$$

a linear multi-step method of step number k (in our case $k = 3$)

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j}$$

is defined by a set of constant coefficients $\{\alpha_j, \beta_j\}$, $\quad j = 0,1,\cdots,k$. We use the normalization

$$\alpha_k = 1.$$

On a variable grid

$$\{ \ t_0, \ t_n = t_0 + \sum_{\nu=0}^{n} h_\nu, \quad n = 1,2,\ldots \quad \}$$

the coefficients α_j, β_j normally depend on n. For practical purposes we like to write the method in the variable step case in terms of the step h_n :

$$\sum_{j=0}^{k} \alpha_{j,n} y_{n+j} = h_n \sum_{j=0}^{k} \beta_{j,n} f_{n+j}$$

where

$$y_{n+j} := y(t_{n+j})$$

$$f_{n+j} := f(t_{n+j}, y_{n+j})$$

$$t_{n+j} := t_n + \sum_{\nu=0}^{j-1} h_{n+\nu}, \quad j = 1,2,\ldots,k$$

with normalization

$$\alpha_{k,n} = 1.$$

In this paper we use $k = 3$ and for simplicity we write α_j, β_j instead of $\alpha_{j,n}, \beta_{j,n}$ keeping in mind that α_j and β_j depend on n, that means, they depend on the variable grids.

Thus we have

(1) $$\sum_{j=0}^{3} \alpha_j y_{n+j} = h_n \sum_{j=0}^{3} \beta_j f_{n+j}$$

where

$$\alpha_3 = 1$$

$$y_{n+j} := y(t_{n+j})$$

$$t_{n+j} := t_n + \sum_{\nu=0}^{j-1} h_{n+\nu}$$

$$= t_n + h_n \sum_{\nu=0}^{j-1} (h_{n+\nu} / h_n), \quad j = 1,2,3$$

We can also write

$$t_{n+j} = t_n + h_n \tau_j,$$

where

$$\tau_0 := 0$$

$$\tau_j := \sum_{\nu=0}^{j-1} (h_{n+\nu} / h_n), \quad j = 1,2,3$$

i.e.

$$\tau_0 = 0$$

$$\tau_1 = h_n / h_n = 1$$

$$\tau_2 = 1 + h_{n+1} / h_n$$

$$\tau_3 = 1 + h_{n+1} / h_n + h_{n+2} / h_n$$

2. Derivation

The associated linear difference operator of (1) is

(2) $$L[y(t); h_n, h_{n+1}, h_{n+2}] = \sum_{j=0}^{3} [\alpha_j y(t + \tau_j h_n) - h_n \beta_j y'(t + \tau_j h_n)]$$

$$= \rho_n - h_n \sigma_n$$

By definition the method is of order 3 if

$$L[y(t); h_n, h_{n+1}, h_{n+2}] \equiv 0 \quad \text{for} \quad y(t) = t^m, \quad m = 0,1,2,3$$

and

$$L[y(t);h_n,h_{n+1},h_{n+2}]\neq 0 \quad \text{for} \quad y(t)=t^4.$$

In general, we can say that the method is of order 3 if

$$L[y(t);h_n,h_{n+1},h_{n+2}]\equiv 0$$

for all continuously differentiable functions $y(t)$ whose fourth and higher derivatives are identically zero and

$$L[y(t);h_n,h_{n+1},h_{n+2}]\neq 0$$

for any continuously differentiable function whose fourth derivative is not identically zero.

Thus applying (2) to the test functions

$$y(t)=1$$
$$y(t)=t-t_n$$
$$y(t)=(t-t_n)^2$$
and
$$y(t)=(t-t_n)^3$$

respectively, we obtain,

(3)
$$\begin{aligned}
&\sum_{j=0}^{3}\alpha_j=0\\
&\sum_{j=0}^{3}\alpha_j(t+\tau_j h_n-t_n)=h_n\sum_{j=0}^{3}\beta_j\\
&\sum_{j=0}^{3}\alpha_j(t+\tau_j h_n-t_n)^2=2h_n\sum_{j=0}^{3}(t+\tau_j h_n-t_n)\beta_j\\
&\sum_{j=0}^{3}\alpha_j(t+\tau_j h_n-t_n)^3=3h_n\sum_{j=0}^{3}(t+\tau_j h_n-t_n)^2\beta_j
\end{aligned}$$

(3) is true for any t in the interval. Taking $t=t_n$ and using $\tau_0=0$ we obtain,

(4)
$$\begin{aligned}
&\alpha_0+\alpha_1+\alpha_2+\alpha_3=0\\
&\tau_1\alpha_1+\tau_2\alpha_2+\tau_3\alpha_3=\beta_0+\beta_1+\beta_2+\beta_3\\
&\tau_1^2\alpha_1+\tau_2^2\alpha_2+\tau_3^2\alpha_3=2(\tau_1\beta_1+\tau_2\beta_2+\tau_3\beta_3)\\
&\tau_1^3\alpha_1+\tau_2^3\alpha_2+\tau_3^3\alpha_3=3(\tau_1^2\beta_1+\tau_2^2\beta_2+\tau_3^2\beta_3)
\end{aligned}$$

If the method is of order 3 then

$$L[y(t);h_n,h_{n+1},h_{n+2}]=C_4 h_n{}^4 y^{(4)}(t)+O(h_n{}^5)$$

Again using $y(t)=(t-t_n)^4$ we obtain

$$\sum_{j=0}^{3}\alpha_j(t+\tau_j h_n-t_n)^4-4h_n\sum_{j=0}^{3}(t+\tau_j h_n-t_n)^3\beta_j=C_4 h_n{}^4 4!$$

For $t=t_n$ this gives the error constant

$$C_4=(\alpha_1\tau_1{}^4+\alpha_2\tau_2{}^4+\alpha_3\tau_3{}^4)/24-(\beta_1\tau_1{}^3+\beta_2\tau_2{}^3+\beta_3\tau_3{}^3)/6$$

Introducing the parameters

$$a=-(1+\alpha_2)$$
$$b=1+\alpha_1+\alpha_2$$

we get

$$\alpha_2=-1-a$$
$$\alpha_1=a+b$$

and $\alpha_0=-b$

Also we have $\alpha_3=1$.

The equations in (4) now determine $\beta_0,\ \beta_1,\ \beta_2$ if we introduce a free parameter $\beta_3=c$. Thus we obtain the following system of equations:

$$\begin{aligned}\beta_0+\beta_1+\beta_2&=a+b+\tau_2(-1-a)+\tau_3-c\\ 2\beta_1+2\tau_2\beta_2&=a+b+\tau_2{}^2(-1-a)+\tau_3{}^2-2\tau_3 c\\ 3\beta_1+3\tau_2{}^2\beta_2&=a+b+\tau_2{}^3(-1-a)+\tau_3{}^3-3\tau_3{}^2 c\end{aligned}\qquad(5)$$

Keeping (a,b) fixed in G (see Figure 1) and choosing c freely at each step we get unique solution for $\beta_j,\ j=0,1,2$ which as a result, gives a zero-stable method at each step with the variable grids. Thus we obtain zero-stable variable step variable formula methods.

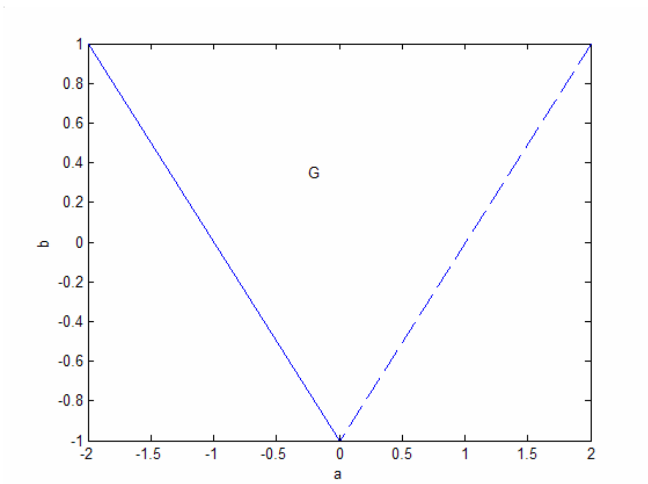

Figure 1

3. Variable step-size variable formula stiffly stable linear 3-step methods with large region of instability in the right half plane

For the assurance of a 3-step LMM to be stiffly stable we take the parameters (a,b) in W (see Figure 2). For details see [1]. We have c as a free parameter in each step of the method. We want to choose carefully so that at each step the formula we get,

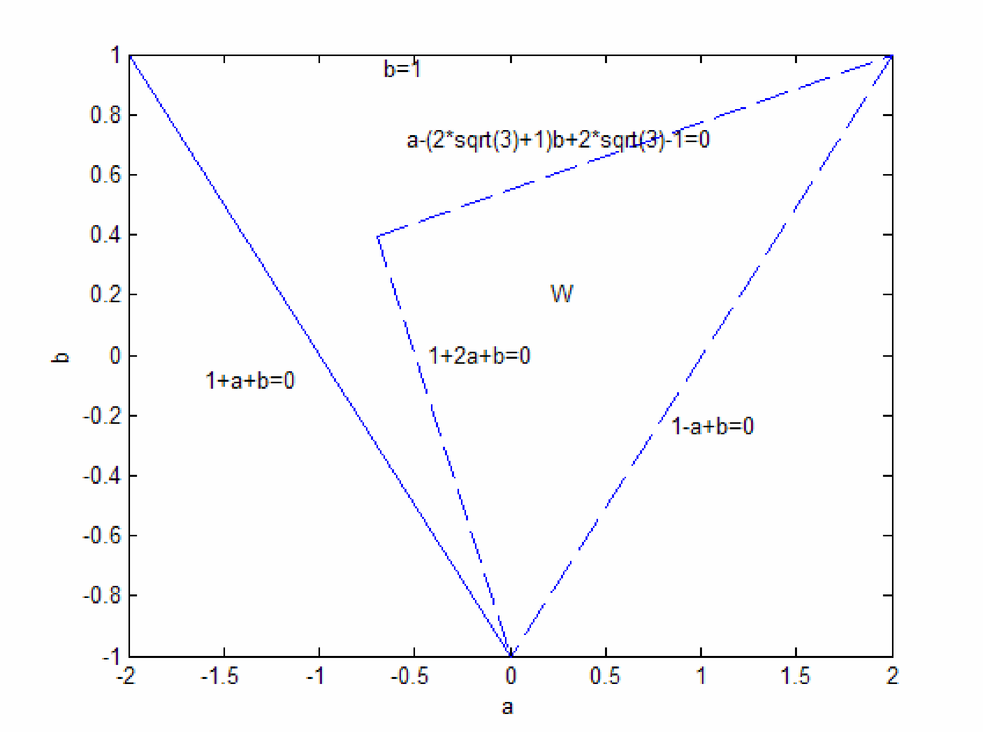

Figure 2

becomes stiffly stable and at the same time it has a large region of instability in the right half plane (see [1]). We can achieve this if we choose $c = \beta_3$ such that

$$\beta_3 - \beta_2 + \beta_1 - \beta_0 > 0$$

and that (6)

$$-\beta_0 + \beta_1 - \beta_2 + \beta_3 =: \varepsilon > 0$$

be small enough to satisfy an inequality like

$$0 < (a-b+11)/24 < c < (a-b+11)/24 + (1-b)(1+2a+b)/(6(1-a+b)).$$

The equations (4) and (6) will give unique solutions of β_j's at each step. The formula thus obtained at each step will have large region of instability in the right half plane and it will be stiffly stable too.

4. Implementation

In this section we describe algorithm using the method of the previous sections. The algorithm is of an experimental nature written in such a way that experiments with different formulas can be easily done. No efforts have been made to make the algorithm computationally efficient. Following is the algorithm:

Step 1: Initialize the problem. Initialize the method by taking the input for the parameter a, b and step size h. Input the accuracy requirement δ. Compute α_j, $j = 0,1,2,3$.

Step 2: Take two steps with step size h with trapezoidal rule.

Step 3: Compute t_i, $i = 1,2,3$ and β_j, $j = 0,1,2,3$ (remember $\beta_3 = c$).

Step 4: Go one step with the method.

Step 5: Compute the approximate local error, compare with δ and decide the new step size h. Repeat from step 2 until t reaches the final time t_1.

5. Test Problem: Methods like BDF which has small region of instability (see Figure 4 in [1]) are some times dangerous to some stiff problems. Lindberg (see [2]) described two test problems in which the eigenvalues changes from large negative values to large positive values. We consider one problem here which is:

$$
\begin{aligned}
y_1' &= 10^4 y_1 y_3 + 10^4 y_2 y_4, & y_1(0) &= 1 \\
y_2' &= -10^4 y_1 y_4 + 10^4 y_2 y_3, & y_2(0) &= 1 \\
y_3' &= 1 - y_3, & y_3(0) &= -1 \\
y_4' &= -y_4 - 0.5 y_3 + 0.5, & y_4(0) &= 0.
\end{aligned}
$$

The exact solution of this problem can be characterized in the following way:

$$
\begin{aligned}
y_3(t) &= 1 - 2e^{-t} \\
y_4(t) &= te^{-t}.
\end{aligned}
$$

If we set $y = [y_1, y_2]^T$, then $y' = A(t)y$ and $y(0) = [1,1]^T$, where

$$
A(t) = 10^4 \begin{bmatrix} 1 - 2e^{-t} & te^{-t} \\ -te^{-t} & 1 - 2e^{-t} \end{bmatrix}.
$$

The eigenvalues of $A(t)$ are

$$
\lambda_{1,2} = 10^4 [(1 - 2e^{-t}) \pm ite^{-t}].
$$

So initially the eigenvalues are -10^4 and approach to 10^4 as $t \to \infty$. So methods like BDF can not detect the instability of these solutions.

The MATLAB subroutine for stiff problems, namely ODE15S, ODE23S, ODE23T, ODE23TB also could not detect them. With these subroutines the solution of this problem is shown in Figure 3.

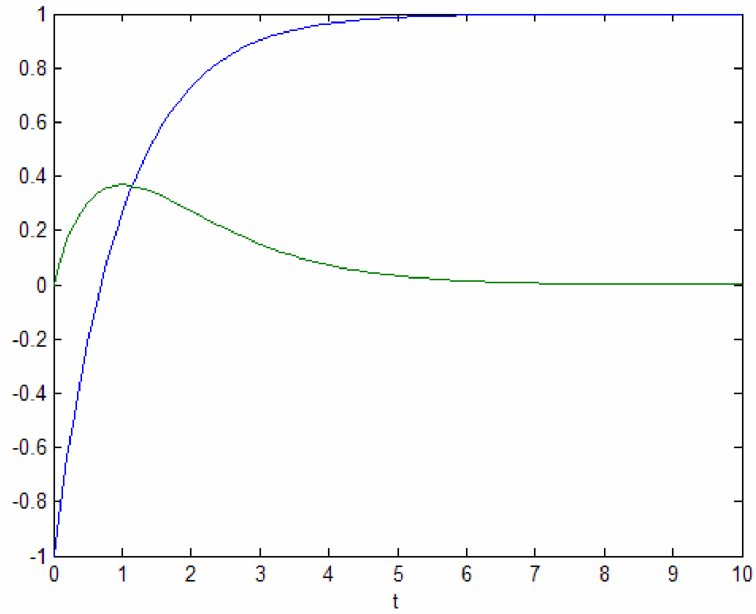

Figure 3

If we use our method we get the solution where the instability is detected.

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Reference:

[1]. G. K. Beg, "Stiffly Stable Linear 3-step Methods", Technical Report#377,(2007), Department of Mathematics & Statistics, King Fahd University of Petroleum and Minerals, KSA.

[2]. B. Lindberg, "On a Dangerous Property of Methods for Stiff Differential Equations", BIT, **14** (1974), pp 430-436.