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A-stable and Stiffly-stable Formulas in Generalized Linear Multistep Methods for Ordinary Differential Equations

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In this paper, generalized linear multistep methods for ODEs whose predictor of off-grid point is an implicit formula are proposed and stability properties are investigated for the methods. Then, it is proved that there exists a family of A-stable methods of order 3 and, furthermore, there exists a unique A-stable one-step method of order 4. Also, it is numerically shown that there exist two families of stiffly stable methods, with orders 5 and 7, respectively.

1. Introduction

The order of accuracy of stable k-step linear multistep methods (LMMs) for solving the initial value problem of the ordinary differential equation (ODE),

$$\begin{cases} \dfrac{dy}{dx} = f(x, y), \\ y(x_0) = y_0, \end{cases}$$

is at most $k+2$, which is about the half of the attainable order with the methods without stability conditions.[3),4)].

In order to overcome the barrier, Gragg & Stetter[5)] and Butcher[1),2)] proposed and developed k-step generalized linear multistep method (GLMM) in the form

$$\begin{cases} \text{(I)}\ \sum_{i=0}^{k} \alpha_i y_{n+i} + h \sum_{i=0}^{k} \beta_i f_{n+i} + h\gamma f_{n+s} = 0, \\ \text{(II)}\ y_{n+s} = \sum_{i=0}^{k} \hat{\alpha}_i y_{n+i} + h \sum_{i=0}^{k} \hat{\beta}_i f_{n+i}, \end{cases} \tag{1.1}$$

with $\alpha_k = -1, \beta_k \neq 0,\ \hat{\alpha}_k = 0,\ \hat{\beta}_k = 0$, where s is a non-integer, h a step size of integration, y_n an approximation to $y(x)$ at $x_n = x_0 + nh$, and $f_n = f(x_n, y_n)$. In fact, their methods possess about $2k$ order and satisfy a zero-stability condition. However, unfortunately these methods never have not a property of A-stability but a property of stiff-stability.

This paper is concerned with a modification to the form of the GLMM formulas (1.1) such that higher stability can be attained. In the formulas (1.1), especially we are very much interested in the case where $\alpha_k = -1, \beta_k \neq 0,\ \hat{\alpha}_k \neq 0$, and $\hat{\beta}_k \neq 0$. Under these assumptions, therefore the formula (II) is implicit with respect to y_{n+k} together with the formula (I). This approach which assumes $\hat{\alpha}_k \neq 0$ and $\hat{\beta}_k \neq 0$ is essentially different from the methods that are proposed and developed by Gragg & Stetter[5)] and Butcher[1),2)].

In this paper, stability properties of GLMM proposed above are mainly investigated: It is proved that there exists a family of A-stable one-step GLMMs with order 3 and, furthermore, there uniquely exists the A-stable one-step GLMM of order 4. It is also shown that there exists a family of stiffly stable two-step GLMMs with order 5 and a family of stiffly stable three-step GLMMs with order 7. In order to verify stability of those methods, also some problems with high stiffness ratio are numerically solved.

For simplification of discussions, the construction of GLMM is accomplished for a scalar ODE, since it is able to apply GLMM to a system of ODEs without any modification. On the other hand, stability analysis for GLMM will be not only done for a scalar ODE, but for a system of ODEs.

2. Generation of Coefficients and Order of GLMM

In this section, we derive the coefficients of GLMM (1.1) and investigate orders of those formulas. For the formula (I) in (1.1), in particular, an optimization of the order is done.

2.1 Associated Difference Operator

Suppose that y is a sufficiently smooth function. Let $y(x_{n+i})$ and $y'(x_{n+i})$ be values of y and its derivative y', respectively, at $x = x_{n+i}$.

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Recall that, for the given data $\{y(x_n),\ldots, y(x_{n+k})\}$ and $\{y'(x_n),\ldots,y'(x_{n+k})\}$, the Hermite interpolation polynomial for y is given as

$$H(x) = \sum_{i=0}^{k} r_i(x)y(x_{n+i}) + \sum_{i=0}^{k} s_i(x)y'(x_{n+i}), \qquad (2.1)$$

where

$$r_i(x) = \{1-2g_i(x_{n+i})(x-x_{n+i})\}\,\ell_i(x)^2,$$
$$s_i(x) = (x-x_{n+i})\ell_i(x)^2,$$
$$g_i(x) = \sum_{p=0}^{k} \frac{1}{x-x_{n+p}},$$
$$\ell_i(x) = \frac{\omega(x)}{(x-x_{n+i})\omega'(x_{n+i})},$$
$$\omega(x) = \prod_{p=0}^{k}(x-x_{n+p}).$$

It is also well-known that its interpolation error $e(x)=y(x)-H(x)$ is given by

$$e(x)=\frac{\omega(x)^2}{(2k+2)!}y^{(2k+2)}(\xi_0), \qquad (2.2)$$

where ξ_0 is an appropriate point belonging to the minimum interval including $\{x, x_n, x_{n+1},\ldots, x_{n+k}\}$. Hereafter we denote this interval by $\hat{I}$.

In order to derive a difference operator associated with the formula (I) in GLMM, differentiate $e(x)=y(x)-H(x)$ with respect to x and divide its derivative by $r'_k(x)$. Then we have

$$\frac{e'(x_{n+s})}{r'_k(x_{n+s})}=\frac{y'(x_{n+s})}{r'_k(x_{n+s})}-\frac{H'(x_{n+s})}{r'_k(x_{n+s})}.$$

In addition, after differentiating the Hermite interpolation polynomial $H(x)$ given in (2.1) and substituting it for the equation above, we have

$$\frac{e'(x_{n+s})}{r'_k(x_{n+s})} = h\gamma y'(x_{n+s})+\sum_{i=0}^{k}\alpha_i y(x_{n+i}) +h\sum_{i=0}^{k}\beta_i y'(x_{m+i}), \qquad (2.3)$$

where the coefficients α_i, β_i, and γ are defined as, for i=0, ..., k,

$$\alpha_i(s)=-\frac{r'_i(x_{n+s})}{r'_k(x_{n+s})},\ \beta_i(s)=-\frac{1}{h}\frac{s'_i(x_{n+s})}{r'_k(x_{n+s})},$$
$$\text{and } \gamma(s)=\frac{1}{h}\frac{1}{r'_k(x_{n+s})}. \qquad (2.4)$$

By using (2.3), the associated difference operator L_k for the formula (I) can be defined as

$$L_k(y;h) = h\gamma y'(x_{n+s})+\sum_{i=0}^{k}\alpha_i y(x_{n+i}) +h\sum_{i=0}^{k}\beta_i y'(x_{m+i}).$$

From this operator, a local truncation error of the formula (I) is defined as

$$T_n(s)=\frac{e'(x_{n+s})}{r'_k(x_{n+s})}. \qquad (2.5)$$

The other difference operator $\hat{L}_n$ associated with the formula (II) can be immediately derived from $e(x)=y(x)-H(x)$. In fact, putting $x=x_{n+s}$ in the equation, we have

$$e(x_{n+s}) = y(x_{n+s})-\sum_{i=0}^{k}\hat{\alpha}_i(x_{n+s})\,y(x_{n+i}) -h\sum_{i=0}^{k}\hat{\beta}_i(x_{n+s})\,y'(x_{n+i}), \qquad (2.6)$$

where the coefficients $\hat{\alpha}_i$ and $\hat{\beta}_i$ are defined as

$$\hat{\alpha}_i(s)=r_i(x_{n+s}),\quad \hat{\beta}_i(s)=s_i(x_{n+s})/h. \qquad (2.7)$$

By using (2.6), the associated difference operator for the formula (II) can be defined as

$$\hat{L}_n(y;h) = y(x_{n+s})-\sum_{i=0}^{k}\hat{\alpha}_i(x_{n+s})\,y(x_{n+i}) -h\sum_{i=0}^{k}\hat{\beta}_i(x_{n+s})\,y'(x_{n+i}).$$

Then the local truncation error of the formula (II) becomes

$$\hat{T}_n(s)=e(x_{n+s}). \qquad (2.8)$$

It should be noted that the coefficients defined by (2.4) and (2.7) depend only on s, and art given by

$$\alpha_i(s) = \frac{\hat{r}'_i(s)}{\hat{r}'_k(s)},\quad \beta_i(s) = \frac{\hat{s}'_i(s)}{\hat{r}'_k(s)},$$
$$\hat{\alpha}_i(s) = \hat{r}_i(s),\quad \hat{\beta}_i(s) = \hat{s}_i(s),$$
$$\text{and } \gamma(s) = \frac{1}{\hat{r}'_k(s)},$$

where

$$\begin{cases} \hat{r}_i(s) = \{1-2\hat{g}_i(i)(s-i)\}\,\hat{\ell}_i(i)^2, \\ \hat{s}_i(s) = (s-i)\hat{\ell}_i(s)^2, \\ \hat{\ell}_i(s) = \prod\limits_{\substack{p=0\\p\neq i}}^{k}\dfrac{s-p}{i-p},\quad \hat{g}_i(s) = \sum\limits_{\substack{p=0\\p\neq i}}^{k}\dfrac{1}{s-p}. \end{cases}$$

The subject considered hereafter is restricted to a family of GLMMs determined by coefficients defined above. In Appendix A.1, each coefficient for $k = 1, 2,$ and 3 is shown for convenient.

2.2 Order of k-Step GLMM

The definition of order for formulas follows Henrici [6]. To investigate orders of GLMM with coefficients (2.4), we need an evaluation of the local truncation error $T_n(s)$. The following lemma is useful to evaluate the truncation error of the formula (I).

Lemma 1 If y is a sufficiently smooth function, then there exists a point $\xi_1 \in \hat{I}$ such that

$$e'(x) = \frac{2\omega(x)\omega'(x)}{(2k+2)!}y^{(2k+2)}(\xi_0) + \frac{\omega(x)^2}{(2k+3)!}y^{(2k+3)}(\xi_1). \qquad \blacksquare$$

The proof of this lemma is easy [9].

By Lemma 1, the local truncation error of the formula (I) can be evaluated as follows.

$$T_n(s) = -\frac{1}{r'_k(x_{n+s})}\left\{\frac{2\omega(x_{n+s})\omega'(x_{n+s})}{(2k+2)!}y^{(2k+2)}(\xi_0) + \frac{\omega(x_{n+s})^2}{(2k+3)!}y^{(2k+3)}(\xi_1)\right\}.$$

In addition, putting $x_{n+i}=x_n+ih$ and $x_{n+s}=x_n+sh$, we get

$$T_n(s) = -\frac{h^{2k+2}}{\hat{r}'_k(s)}\left\{\frac{2\hat{\omega}(s)\hat{\omega}'(s)}{(2k+2)!}y^{(2k+2)}(\xi_0) + h\frac{\hat{\omega}(s)^2}{(2k+3)!}\frac{d}{dx}y^{(2k+3)}(\xi_1)\right\},$$

$$\hat{\omega}(s) = \prod_{p=0}^{k}(s-p).$$

This means that the order of the formula (I) is at least $2k+1$.

On the other hand, the local truncation error of the formula (II) is

$$\hat{T}_n(s) = \frac{\omega(x_{n+s})^2}{(2k+2)!}y^{(2k+2)}(\xi_0),$$

from (2.2). By putting $x_{n+i}=x_n+ih$ and $x_{n+s}=x_n+sh$, then we get

$$\hat{T}_n(s) = h^{2k+2}\frac{\hat{\omega}(s)}{(2k+2)!}y^{(2k+2)}(\xi_0).$$

Therefore the formula (II) is of order $2k+1$.

It should be noted that both formulas, (I) and (II), generally have same order $2k+1$. However it is sufficient to have the accuracy of order $2k$ with respect to y_{n+s}, because it is used in the term $hf(x_{n+s}, y_{n+s})$. Conversely if the order of the formula (I) is just one higher than the formula (II), then the accuracy of y_{n+k} has order $2k+2$. The following theorem concerns with the order of the formula (I).

Table 1 Point s that gives maximum order.

Optimum Point s^k_{op} $(k = 1, \ldots, 7)$
$s^1_{\mathrm{op}}=\frac{1}{2}$
$s^2_{\mathrm{op}}=1+\frac{\sqrt{3}}{3}\approx 1.57735$
$s^3_{\mathrm{op}}=\frac{3+\sqrt{5}}{2}\approx 2.6803$
$s^4_{\mathrm{op}}=\frac{20+\sqrt{150+10\sqrt{145}}}{10}\approx 3.64443$
$s^5_{\mathrm{op}}=\frac{15+\sqrt{105+24\sqrt{7}}}{6}\approx 4.66345$
$s^6_{\mathrm{op}}=3+\frac{\sqrt{1395+42\cdot 7^{\frac{2}{3}}\cdot 2481997^{\frac{1}{6}}\cos\frac{\theta_6}{3}}}{21}\approx 5.67084$
$s^7_{\mathrm{op}}=\frac{7+\sqrt{21+8\cdot 7^{\frac{1}{2}}\cos\frac{\theta_7}{3}}}{2}\approx 6.68972$
Here $\left(\theta_6=\tan^{-1}\frac{54\sqrt{591}}{871}\right)$ $\left(\theta_7=\tan^{-1}\frac{3\sqrt{31}}{8}\right)$

Theorem 1 For each k, if there exists a points s^k_{op} such that $\hat{\omega}'(s^k_{\mathrm{op}})=0$, then the formula (I) of k-step GLMM at $s=s^k_{\mathrm{op}}$ has order $2k+2$. Such order is said to be optimum. $\blacksquare$

The value of s^k_{op} that gives the optimum order for each k $(1 \le k \le 7)$ is shown in **Table 1**.

3. Zero-Stability Property

The zero-stability property of k-step GLMM is determined on the basis of the associated characteristic polynomial,

$$\pi_k(\xi) = \sum_{i=0}^{k}\alpha_i\xi^i,$$

with k-th order linear difference equation obtained by vanishing the step size h in the formulas of (I) and (II). In fact, a GLMM is said to be zero-stable if the modulus of any root of $\pi_k(\xi)$ is less than or equal to 1 and the root of modulus 1 is simple [7]. Since this $\pi_k(\xi)$ is consisting of terms that not contain h in the formulas, the zero-stability is independent of the formula (II). Therefore the zero-stability of GLMM in this paper exactly agrees with the Butcher's zero-stability result [1] which had been shown in graph.

Table 2 Range of s for GLMM to be zero-stable.

Interval I_z^k (k=1, . . . , 4)
$I_z^1=[\frac{1}{2},\ \infty)$
$I_z^2=[1,\ \infty)$
$I_z^3=[\frac{1}{2}(3+\sqrt{3}),\ \frac{1}{14}(21+5\sqrt{21})]\approx(2.366, 3.136)$
$I_z^4\approx(3.527,\ 4.000)$
$I_z^5\approx(4.605,\ 4.755)$
$I_z^6\approx(5.633,\ 5.717)$
$I_z^7\approx(6.663,\ 6.693)$

If there exists an interval of s in which the method is zero-stable, then we call it zero-stable interval and denote it by I_z^k. The following theorem guarantees the existence of zero-stable interval for GLMMs of k=1 up to 3

Theorem 2 Let $1 \le k \le 3$. For each k, if s belongs to the interval I_z^k in **Table 2**, then the k-step GLMM is zero-stable. ∎

Unfortunately, any zero-stable interval for the k-step GLMM of k exceed 3 is not exactly obtained yet. Therefore the zero-stable interval of s shown in Table 2 for GLMM with $k = 4, \ldots, 7$ is approximately given.

It should be noted that Butcher[1)] numerically showed that the GLMMs for k=1 up to 7 have such zero-stable intervals of s and Suzuki[8)] also showed up to 8 for a slight modified GLMM. Under these zero-stable interval of s, the following theorem is obtained.

Theorem 3 For each k ($1\le k\le 7$), the k-step GLMM with $s=s_{\mathrm{op}}^k$ is zero-stable, and of order $2k+2$. ∎

4. Absolute stability Property

If the numerical solution obtained by applying GLMM with $h>0$ to the test problem $y'=\lambda y$, ($\lambda\in C$, $\Re\lambda<0$) with any initial value y_0 tends to zero as n tends to ∞, the method is said to be absolute stable at λh. The k-step GLMM is absolute stable if and only if the modulus of any root of the associated characteristic polynomial

$$\begin{aligned}\pi_k(\xi;z,s) &= \rho(\xi)\\ &\quad +\lambda h\Big(\sigma(\xi)+\gamma\big(\hat\rho(\xi)+\lambda h\hat\sigma(\xi)\big)\Big),\\ &= \sum_{i=0}^{k}\Big(\alpha_i+\big(\beta_i+\gamma\hat\alpha_i\big)z+\gamma\hat\beta_i z^2\Big)\xi^i\end{aligned}$$

is less than one, where $z=\lambda h$, $\alpha_k=-1$,

$$\begin{aligned}\rho(\xi) &= \sum_{i=0}^{k}\alpha_i\xi^i, \quad \sigma(\xi) = \sum_{i=0}^{k}\beta_i\xi^i,\\ \hat\rho(\xi) &= \sum_{i=0}^{k}\hat\alpha_i\xi^i, \quad \hat\sigma(\xi) = \sum_{i=0}^{k}\hat\beta_i\xi^i.\end{aligned}\tag{4.1}$$

For given GLMM, we call an absolute stability region the set of λh for which GLMM is absolute stable, and if the absolute stability region contains $C^-=\{z\in C : \Re z<0\}$, then the GLMM is said to be A-stable.

In this section, we investigate the property of absolute stability by analysing the characteristic polynomial. The characteristic polynomial for k=1 is given by

$$\begin{aligned}\pi_1(\xi;z,s) &= \Big(1-\frac{s+1}{3}z+\frac{s}{6}z^2\Big)\xi\\ &\quad -\Big(1-\frac{s-2}{3}z-\frac{s-1}{6}z^2\Big),\end{aligned}$$

and, for k=2, . . ., 5, the coefficients of characteristic polynomials are given in Appendix A.2.

4.1 A-Stable One-Step GLMMs with Order 3 and with Order 4

By computing the root of the characteristic polynomial $\pi_1(\xi;z,s)$ for the one-step GLMM, the following theorem is proved.

Theorem 4 If $s\ge 1/2$, then the one-step GLMM with any s is A-stable. In this GLMM, furthermore, the method with $s>1/2$ has order 3 and the method of $s=1/2$ has order 4. ∎

Proof The root of $\pi_1(\xi;z,s)$ with respect to z is given by

$$\xi(z;s) = \frac{1-\frac{1}{3}(s-2)z-\frac{1}{6}(s-1)z^2}{1-\frac{1}{3}(s+1)z+\frac{1}{6}sz^2},$$

and by setting $t=s-1/2$, the root can be rewritten as

$$\xi(z;t)=\frac{12-2(2t-3)z-(2t-1)z^2}{12-2(2t+3)z+(2t+1)z^2},\quad (t\ge 0).$$

In order to prove that this GLMM is A-stable for some t, it is sufficient to show that $\xi(z;t)$ satisfies $|\xi(z;t)|<1$ for any $z\in C^-$. By the Möbius transformation, $\zeta=(\xi-1)/(\xi+1)$, from ξ to ζ, we have

$$\zeta = \frac{2(3z-tz^2)(12-4t\bar z+\bar z^2)}{|12-4tz+z^2|^2}.$$

By this transformation, it is sufficient to show that ζ belongs to C^- for any $z\in C^-$. Let $t\ge 0$ and $\Gamma=(3z-tz^2)(12-4t\bar z+\bar z^2)$, then we can show that $\Re\Gamma<0$ ($z\in C^-$). In fact, the real part of Γ becomes

$$\begin{aligned}\Re\Gamma &= u\big(36+(3+4t^2)(u^2+v^2)\big)\\ &\quad -t\big(24u^2+(u^2+v^2)^2\big),\end{aligned}$$

Table 3 Functions $\varphi_k(s)$ specifying absolute stability interval.

$\varphi_2(s)=\dfrac{15(s-1)}{3s^2-6s+1}$
$\varphi_3(s)=\dfrac{35(2s^2-6s+3)}{(5s^2-15s+1)(2s-3)}$
$\varphi_4(s)=\dfrac{105(3s^3-18s^2+29s-10)}{35s^4-280s^3+685s^2-500s+12}$
$\varphi_5(s)=\dfrac{231(6s^4-60s^3+195s^2-225s+62)}{126s^5-1575s^4+6860s^3-12075s^2+7024s-60}$
$\varphi_6(s)=\dfrac{1001(s^5-15s^4+81s^3-189s^2+176s-42)}{77s^6-1386s^5+9380s^4-29400s^3+41783s^2-20874s+60}$
$\varphi_7(s)=\dfrac{143(30s^6-630s^5+5075s^4-19600s^3+36799s^2-29498s+6378)}{286s^7-7007s^6+67837s^5-328790s^4+829759s^3-1013663s^2+454938s-420}$

where $z=u+iv$ $(u, v\in R)$ since Γ can be developed as

$$\Gamma = 36z - 12t|z|^2 + 3\bar{z}|z|^2 - 12tz^2 + 4t^2z|z|^2 - t|z|^4.$$

Consequently, we have that $\Re\Gamma<0$ since $u<0$ and $t\geq 0$ by assumption . ∎

4.2 Absolute Stability Interval on Real Axis and Stiffly-Stable GLMM

Let us introduce a new concept of stability.

Definition 1 For a method having an absolute stability region $R_{\rm A}$, if there exists an interval $I_{\rm A}$ on the real axis such that $I_{\rm A}\subset\Re R_{\rm A}$ and the closure of $I_{\rm A}$ contains the origin of the complex plane C, then we call $I_{\rm A}$ a real absolute stability interval. ∎

In general, the real absolute stability interval for GLMM depends on the parameter s by which the coefficients are determined, and the interval can be represented in form $I_{\rm A}^k=(\varphi_k(s), 0)$ for k-step GLMM $(2\leq k\leq y)$ if $\varphi_k(s)<0$ for $s\in I_{\rm z}^k$, where each $\varphi_k(s)$ is given in **Table 3**.

Theorem 5 For the k-step GLMM, the following propositions are satisfied.

(i) For each k $(2\leq k\leq y)$, there exists a subinterval (of $I_{\rm z}^k$) consisting of s such that the k-step GLMM has the real absolute stability interval $I_{\rm A}^k$.

(ii) For each k $(2\leq k\leq 4)$, there exists a point $s_{\rm c}^k\in I_{\rm z}^k$ with which $I_{\rm A}^k$ becomes the left-half infinite interval $(-\infty, 0)$. Hereafter, we call a critical point such $s_{\rm c}^k$ (see **Table 4**). ∎

Assertion 1 The two-step GLMM with s is stiffly stable if the value of s is grater than the critical point $s_{\rm c}^2$, and the GLMM is of order 5 (see **Fig. 1**-(b)). ∎

Assertion 2 If the value of $s\in I_{\rm z}^3$ is grater than the value of the critical point $s_{\rm c}^3$, then the three-step GLMM with s is stiffly stable (see **Fig. 2**-(b)). Here

$$I_{\rm z}^3 = ((3+\sqrt{3})/2,\ (21+5\sqrt{21})/14).$$

It should be noted that this GLMM is of order 7. ∎

Table 4 Critical point of s in GLMM.

$s_{\rm c}^k$ $(k=2,\ldots,4)$
$s_{\rm c}^2=\dfrac{3+\sqrt{6}}{3}\approx 1.8165$
$s_{\rm c}^3=\dfrac{15+\sqrt{205}}{10}\approx 2.9318$
$s_{\rm c}^4=\dfrac{140+\sqrt{10850+70\sqrt{13945}}}{70}\approx 3.9752$

4.3 Stability Property of GLMM for System of ODEs

Applying GLMM to the system of ordinary differential equations, $\boldsymbol{y}'=A\boldsymbol{y}$, where $\boldsymbol{y}\in R^d$ and A is a $d\times d$ constant matrix whose each component may be a complex number, we can obtain the corresponding characteristic polynomial

$$\pi_k^{(d)}(\xi; hA) = \det\left[\rho(\xi)I + \{\sigma(\xi)I + \gamma hA\big(\hat{\rho}(\xi)I + hA\hat{\sigma}(\xi)\big)\}\right],$$

where I is the $d\times d$ identity matrix. By using this polynomial, therefore, the following theorem concerning to stability property of the method is obtained.

Theorem 6 Let $\lambda_1,\ldots,\lambda_d$ be eigenvalues of A and $\Re\lambda_i<0$ for $i=1,\ldots,d$, then GLMM (1.1) with an absolute stability region R_A is absolutely stable for $\boldsymbol{y}'=A\boldsymbol{y}$ if and only if it holds that $h\lambda_i\in R_{\rm A}$ for $i=1,\ldots,d$.

Proof Based on linear algebra, for the coefficient matrix A, there exists a $d\times d$ nonsingular

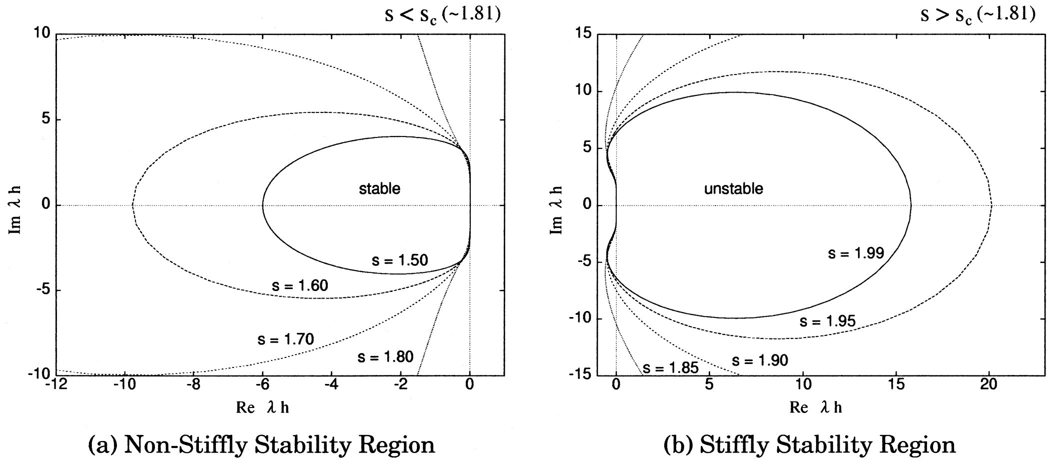

Fig. 1 Absolute stability region of two-step GLMM.

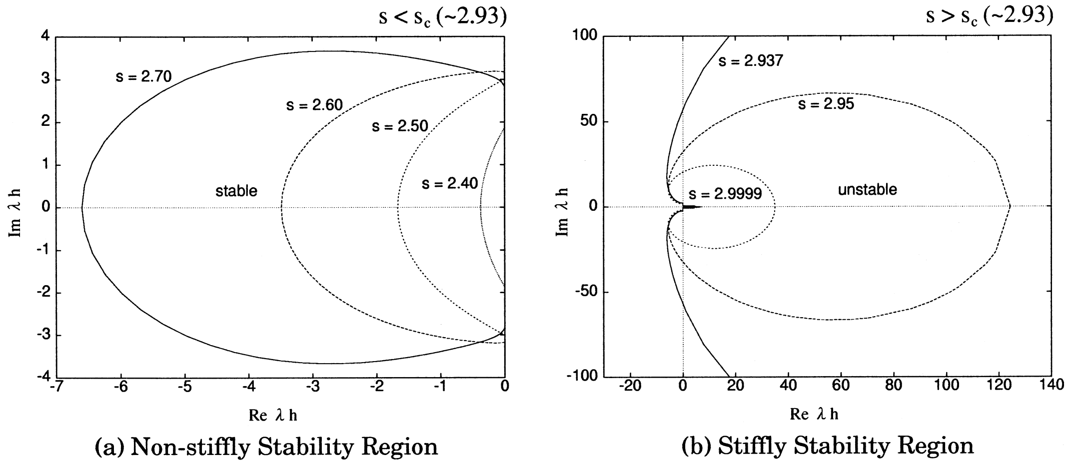

Fig. 2 Absolute stability region of three-step GLMM.

matrix B such that

$$A = B^{-1}\Lambda B, \quad \Lambda = \begin{pmatrix} \lambda_1 & & * \\ & \ddots & \\ \mathbf{0} & & \lambda_d \end{pmatrix},$$

where Λ is an appropriate upper-triangular matrix whose diagonal elements are the eigenvalues of A. By using this representation for A, the characteristic polynomial can be rewritten as

$$\pi_k^{(d)}(\xi; hA) = \prod_{p=1}^{d}\Big(\rho(\xi) + \big(\sigma(\xi)+\gamma(\hat\rho(\xi)+\hat\sigma(\xi)(h\lambda_p))\big)(h\lambda_p)\Big) = \prod_{p=1}^{d}\pi_k(\xi; h\lambda_p, s).$$

Therefore, if ξ is a root of $\pi_k^{(d)}(\xi; hA)$, then $\pi_k(\xi; h\lambda_p, s)=0$ for some p. This means that $|\xi|<1$ since $h\lambda_p \in R_{\mathrm{A}}$ for every p $(1\le p\le d)$. ∎

5. Numerical Example

The one-step GLMM of order 4 with $s = 0.5$ and two-step GLMM of order 5 with $s=0.85$ are applied to following problem

$$\begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = -\frac{1}{2}\begin{pmatrix} \lambda+1 & \lambda-1 \\ \lambda-1 & \lambda+1 \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix},$$

$$\begin{pmatrix} y_{1,0} \\ y_{2,0} \end{pmatrix} = \begin{pmatrix} 100 \\ 100 \end{pmatrix}.$$

The property of accuracy and stability for numerical solution is verified. This equation is make-up so that stiffness ratio just becomes λ. The exact solution is given as

Table 5 Relative (Absolute) errors evaluated at $x = 50$.

Stiffness Rate λ	GLMM k-Step / Order	Stepsize h 1.00	0.50	0.10	0.05	0.01
50	1-Step/4-Order	2.656e+00 (3.62e-20)	4.370e-03	6.935e-06	4.337e-07	6.943e-10
	2-Step/5-Order	2.567e-02	8.119e-04	2.557e-07	7.971e-09	2.183e-12
500	1-Step/4-Order	2.920e+04 (2.98e-16)	8.144e+03 (1.11e-16)	6.935e-06	4.337e-07	6.952e-10
	2-Step/5-Order	7.397e-01	8.122e-04	2.557e-07	7.970e-09	3.342e-12
5000	1-Step/4-Order	2.291e+05 (3.12e-15)	2.584e+04 (3.52e-16)	4.544e+01 (6.12e-19)	4.336e-07	7.100e-10
	2-Step/5-Order	3.270e-01	8.460e-04	2.558e-07	7.974e-09	3.363e-12
50000	1-Step/4-Order	1.057e+05 (1.44e-15)	1.914e+06 (2.61e-14)	4.544e+01 (4.48e-14)	4.336e-07 (7.43e-17)	7.100e-10
	2-Step/5-Order	1.034e+00	1.134e-04	2.558e-07	8.028e-09	3.410e-12

$$\begin{pmatrix} y_1'(x) \\ y_2'(x) \end{pmatrix} = \begin{pmatrix} y_{1,0}\exp(-\lambda x) - y_{2,0}\exp(-x) \\ y_{1,0}\exp(-\lambda x) + y_{2,0}\exp(-x) \end{pmatrix}.$$

The results of numerical experiment done under the following conditions are shown in **Table 5**.

(i) Stepsize of Integration: 1, 0.5, 0.05, 0.01
(ii) Length of Integration: 50
(iii) Stiffness Ratio: 50, 500 5000, 50000
(iv) GLMM is solved by the Gauss elimination method.

From this result, it seems that our method is useful for very strong stiffness problems. It should be noted that the classical Runge-Kutta method is unstable for $\lambda h > 2.8$.

6. Concluding Remarks

In this paper, it is proved that there exists a family of A-stable one-step GLMMs with order 3 and, furthermore, there uniquely exists the A-stable one-step GLMM of order 4. It is also shown that there exists a family of stiffly stable two-step GLMMs with order 5 and a family of stiffly stable three-step GLMMs with order 7.

References

1) Butcher, J.C.: A Modified Multistep Method for the Numerical Integration of Ordinary Differential Equations, *J. ACM*, Vol.12, pp.124–135 (1965).
2) Butcher, J.C.: Multistep Generalization of Runge-Kutta Methods with Four or Five Stages, *J.ACM*, Vol.14, pp.84–99 (1967).
3) Dahlquist, G.: Convergence and Stability in The Numerical Integration of Ordinary Differential Equations, *Math. Scand.*, Vol.4, pp.33–53 (1956).
4) Dahlquist, G.: A Special Stability Problem for Linear Multistep Methods, *BIT*, Vol.8, pp.27–43 (1963).
5) Gragg, W.B. and Stetter, H.J.: Generalized Multistep Predictor-Corrector Methods, *J. ACM*, Vol.11, pp.188–209 (1964).
6) Henrici, P.: *Discrete Variable Methods in Ordinary Differential Equations*, John Wiley & Sons (1962).
7) Lambert, J.D.: *Numerical Methods for Ordinary Differential Systems*, John Wiley & Sons (1991).
8) Suzuki, C.: Off-Grid Type Numerical Integration Methods in Orbit Computation, *Fujitsu Sci. Tech. J.*, Vol.10, pp.53–82 (1974).
9) Suzuki, C.: Introduction to Numerical Functional Analysis (in Japanese), Morikita Shuppan (2001).

Appendix

A.1 Coefficients of k-Step GLMM

Coefficients of formula (I) for k=1 :

$$\begin{cases} \alpha_0 = 1 \\ \alpha_1 = -1 \\ \beta_0 = (3s-1)/(6s) \\ \beta_1 = (3s-2)/(6s-6) \\ \gamma \ = 1/(6s-6s^2) \end{cases}$$

Coefficients of formula (II) for k=1 :

$$\begin{cases} \hat{\alpha}_0 = (s-1)^2(2s+1) \\ \hat{\alpha}_1 = s^2(3-2s) \\ \hat{\beta}_0 = s(s-1)^2 \\ \hat{\beta}_1 = s^2(s-1) \end{cases}$$

Coefficients of formula (I) for k=2 :

$$\begin{cases} \alpha_0 = (15s-23)/t \\ \alpha_1 = 16/t \\ \alpha_2 = -1 \\ \beta_0 = (u+s-1)/(st) \\ \beta_1 = 4(u+1)/((s-1)t) \\ \beta_2 = (u-s+1)/((s-2)t) \\ \gamma\ = -4/(s(s-1)(s-2)t) \end{cases}$$

Here t=15s−7, u=5s^2−10s+3.

Coefficients of formula (II) for k=2 :

$$\begin{cases} \hat{\alpha}_0 = (s-1)^2(s-2)^2(3s+1)/4 \\ \hat{\alpha}_1 = s^2(s-2)^2 \\ \hat{\alpha}_2 = s^2(s-1)^2(7-3s)/4 \\ \hat{\beta}_0 = s(s-1)^2(s-2)^2/4 \\ \hat{\beta}_1 = s^2(s-1)(s-2)^2 \\ \hat{\beta}_2 = s^2(s-1)^2(s-2)/4 \end{cases}$$

Coefficients of formula (I) for k=3 :

$$\begin{cases} \alpha_0=(77s^2-312s+291)/t \\ \alpha_1=27(7s-18)s/t \\ \alpha_2=-27(s-3)(7s-3)/t \\ \alpha_3=-1 \\ \beta_0=3(7s^3-30s^2+33s-6)/(st) \\ \beta_1=27(7s^3-31s^2+38s-12)/((s-1)t) \\ \beta_2=27(7s^3-32s^2+41s-12)/((s-2)t) \\ \beta_3=3(7s^3-33s^2+42s-12)/((s-3)t) \\ \gamma\ = -108/(s(s-1)(s-2)(s-3)t) \end{cases}$$

Here t=77s^2−150s+48.

Coefficients of formula (II) for k=3 :

$$\begin{cases} \hat{\alpha}_0=(11s+3)(s-1)^2(s-2)^2(s-3)^2/108 \\ \hat{\alpha}_1=s^3(s-2)^2(s-3)^2/4 \\ \hat{\alpha}_2=-s^2(s-1)^2(s-3)^3/4 \\ \hat{\alpha}_3=s^2(s-1)^2(s-2)^2(36-11s)/108 \\ \hat{\beta}_0=s(s-1)^2(s-2)^2(s-3)^2/36 \\ \hat{\beta}_1=s^2(s-1)(s-2)^2(s-3)^2/4 \\ \hat{\beta}_2=s^2(s-1)^2(s-2)(s-3)^2/4 \\ \hat{\beta}_3=s^2(s-1)^2(s-2)^2(s-3)/36 \end{cases}$$

A.2 Characteristic Polynomial for k-Step GLMM

Let

$$\pi_k(\xi; z, s) = \sum_{i=0}^{k} c_i \xi^i,$$

where $c_i=\alpha_i+(\beta_i+\gamma\hat{\alpha}_i)z+\gamma\hat{\beta}_i z^2$.

For k=2:

$$\begin{cases} c_2 = -\{(15s-7)-(s+1)(3s-2)z \\ \qquad -s(s-1)z^2\}/t \\ c_1 = 4\{4+4(s-1)z-s(s-2)z^2\}/t \\ c_0 = \{(15s-23)-(s-3)(3s-4)z \\ \qquad -(s-1)(s-2)z^2\}/t \end{cases}$$

Here t=15s−7.

For k=3:

$$\begin{cases} c_3=\{(3s^3-9s^2+6s)z^2 \\ \qquad +(-11s^3+15s^2+14s-12)z \\ \qquad\quad +(77s^2-150s+48)\}/t \\ c_2=\{(27s^3-108s^2+81s)z^2 \\ \qquad +(-27s^2-54s^2+351s-162)z \\ \qquad\quad +(189s^2-648s+243)\}/t \\ c_1=\{(27s^3-135s^2+162s)z^2 \\ \qquad +(27s^3-297s^2+702s-324)z \\ \qquad\quad +(-189s^2+486s)\}/t \\ c_0=\{(3s^3-18s^2+33s-18)z^2 \\ \qquad +(11s^3-84s^2+193s-132)z \\ \qquad\quad +(-77s^2+312s-291)\}/t \end{cases}$$

Here t=−77s^2+150s−48.

For k=4:

$$\begin{cases} c_4=\{-318+1199s-998s^2+225s^3 \\ \quad +(72-114s-59s^2+102s^3-25s^4)z \\ \quad\quad -6(6s-11s^2+6s^3-s^4)z^2\}/t \\ c_3=32\{-96+344s-254s^2+45s^3 \\ \quad +(48-128s+56s^2+11s^3-5s^4)z \\ \quad\quad -3(8s-14s^2+7s^3-s^4)z^2\}/t \\ c_2=216\{-12+32s-8s^2 \\ \quad +(24-76s+48s^2-8s^3)z \\ \quad\quad -(12s-19s^2+8s^3-s^4)z^2\}/t \\ c_1=32\{96-472s+286s^2-45s^3 \\ \quad +(144-432s+292s^2-69s^3+5s^4)z \\ \quad\quad -(72s-78s^2+27s^3-3s^4)z^2\}/t \\ c_0=\{2910-4015s+1702s^2-225s^3 \\ \quad +(1200-2090s+1235s^2-298s^3+25s^4)z \\ \quad\quad +(144-300s+210s^2-60s^3+6s^4)z^2\}/t \end{cases}$$

Here $t=318-1199s+998s^2-225s^3$.

For k=5:

$$\begin{cases} c_5=\{6864-29200+31040s^2-11945s^3+1507s^4 \\ \quad -(1440-2712s-550s^2+2395s^3-1070s^4 \\ \quad\quad +137s^5)z+30(24s-50s^2+35s^3 \\ \quad\quad\quad -10s^4+s^5)z^2\}/t \\ c_4=125\{870-3613s+3655s^2-1295s^3+143s^4 \\ \quad -(360-1074s+683s^2+5s^3-83s^4+13s^5)z \\ \quad +6(30s-61s^2+41s^3-11s^4+s^5)z^2\}/t \\ c_3=1000\{240-936s+830s^2-240s^3+22s^4 \\ \quad -2(120-428s+363s^2-95s^3+3s^4+s^5)z \\ \quad\quad +3(40s-78s^2+49s^3-12s^4+s^5)z^2\}/t \\ c_2=1000\{-60+364s-530s^2+200s^3-22s^4 \\ \quad -2(180-702s+638s^2-215s^3+28s^4-s^5)z \\ \quad\quad +3(60s-107s^2+59s^3-13s^4+s^5)z^2\}/t \\ c_1=125\{-1680+7312s-5680s^2+1565s^3-143s^4 \\ \quad -(1440-5256s+4558s^2-1595s^3+242s^4 \\ \quad\quad -13s^5)z+6(120s-154s^2+71s^3-14s^4 \\ \quad\quad\quad +s^5)z^2\}/t \\ c_0 = \{-85614+138825s-77915s^2+18195s^3 \\ \quad -1507s^4-(32880-64538s+46125s^2 \\ \quad\quad -15245s^3+2355s^4-137s^5)z \\ \quad\quad\quad -(3600-8220s+6750s^2-2550s^3 \\ \quad\quad\quad\quad +450s^4-30s^5)z^2\}/t \end{cases}$$

Here $t=-6864+29200s-31040s^2+11945s^3-1507s^4$.

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