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A STUDY ON NUMERICAL METHODS FOR ORDINARY DIFFERENTIAL EQUATIONS

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0. Introduction

In order to obtain numerical solutions of initial value problem for stable system with large Lipschitz constants, Lawson [4] consider a function

$$x(t) = \exp(-tA)y(t),$$

where A is a real square matrix and it is appropriately extracted from the Jacobian matrix of the system.

In this paper, we consider an exponentially dominant order α of a problem, and the matrix A is replaced by this number α in the above function. In Section 1, the Runge-Kutta method and the multistep methods generalized by this function. When the exponentially dominant order is positive, its numerical solutions can be accurately computed by these generalized methods. In Section 2, A- and B-stability of the generalized Runge-Kutta methods are tested. Finally, in Section 3, a concept of AB-stability is introduced. And we study some sufficient conditions under which the generalized Runge-Kutta methods are AB-stable.

1. Generalized Formulas

In the following, we deal with the initial value problem

$$(1.1) \qquad y'(t) = f(t, y(t)), \quad f: \mathbb{R}^{m+1} \to \mathbb{R}^m, \quad t \geq 0, \; y(0) = y_0,$$

where $f = (f^1, f^2, \cdots, f^m)$ is possibly nonlinear in the the dependent and independent variables.

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Let us denote the exact solution of the initial value problem (1.1) as $y(t) = (y^1(t), y^2(t), \cdots, y^m(t))$, where $y^j : \mathbb{R}^1 \to \mathbb{R}^1$. We assume that each component $y^j(t)$ is exponentilly dominated by the term $c_j(t)$ $\exp((\alpha_j + i\beta_j)t)$ as $t \to \infty$.

$$\lim_{t\to\infty} |y^j(t) - c_j(t)\exp((\alpha_j + i\beta_j)t)| = 0, \quad i = 1, 2, \dots, m.$$

Here c_j is a polynomial of t, and α_j and β_j are suitable constants. Then there is a real number α such that

$$\alpha = \max\{\alpha_1, \alpha_2, \cdots, \alpha_m\}.$$

This real number α is called an *exponentially dominant order* of the initial value problem (1.1). Throughout this paper we shall consider only such exponentially dominent problems.

Let us consider the function $z^i(t) = c_i \exp(\alpha_i t)$ and its tangent line at $(t_n, z^i(t_n))$:

$$z^i(t) = z^i(t_n) + \alpha_i z^i(t_n)(t - t_n),$$

then α_i can be obtained as follows:

$$\alpha_i = \frac{z^i(t_{n+1}) - z^i(t_n)}{hz^i(t_n)}, \quad h = t_{n+1} - t_n, \ i = 1, 2, \dots, m.$$

Similarly, if the problem (1.1) has the exponentially dominant order, we have

(1.2)
$$\alpha_i = \lim_{n\to\infty} \frac{y^i(t_{n+1}) - y^i(t_n)}{hy^i(t_n)} = \lim_{n\to\infty} \frac{f^i(t_n, y^i(t_n))}{y^i(t_n)}, \quad i = 1, 2, \dots, m,$$

where

$$y^i(t_{n+1}) = y^i(t_n) + hf^i(t_n, y^i(t_n)).$$

Let us now apply the function

$$x(t) = \exp(-\alpha t)y(t)$$

to the initial value problem (1.1). Then we have a transformed initial problem for $x(t)$:

$$x'(t) = \exp(-\alpha t)\, g(t, \exp(\alpha t)x(t)), \quad t \geq 0,\ x(0) = y_0, \tag{1.3}$$

where

$$g(t, z) = f(t, z) - \alpha z, \quad g : \mathbb{R}^{m+1} \to \mathbb{R}^m. \tag{1.4}$$

In order to obtain a numerical approximation of the transformed problem (1.3), we intend to use the s-stage Runge-Kutta methods given by

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & b_1 & b_2 & \cdots & b_s \end{array} \quad = \quad \begin{array}{c|c} c & A \\ \hline & b^T \end{array} \tag{1.5}$$

where $c_i = \sum_{i=1}^{s} a_{ij}$, $A = [a_{ij}]$, $b^T = [b_1, b_2, \cdots, b_s]$ and $c^T = [c_1, c_2, \cdots, c_s]$. Then we have

$$x_{n+1} = x_n + h \sum_{i=1}^{s} b_i \tilde{k}_i, \quad n = 0, 1, 2, \ldots, \tag{1.6}$$

where

$$\tilde{k}_i = \exp(-\alpha t_{n,i})\, g(t_{n,i}, \exp(\alpha t_{n,i}) x_{n,i}),$$

$$x_{n,i} = x_n + h \sum_{j=1}^{s} a_{ij} \tilde{k}_j, \quad i = 1, 2, \ldots, s.$$

In this case $h = t_{n+1} - t_n$, $t_{n,i} = t_n + c_i h$, and x_n and $x_{n,i}$ represent the approximations to $x(t_n)$ and $x(t_{n,i})$, respectively.

We observe, however, that the product of the form $\exp(\alpha t_{n,i}) x_{n,i}$ in the equation (1.6) approximates to the solution $y(t_{n,i})$ of the original problem (1.1). So we can replace x_n, $x_{n,i}$ and $\tilde{k}_i$ by $\exp(-\alpha t_n) y_n$,

$\exp(-\alpha t_{n,i})y_{n,i}$ and $\exp(-\alpha t_{n,i})g(t_{n,i}, y_{n,i})$, respectively. Then we have the *generalized Runge-Kutta* (GRK) methods with the exponentially dominant order α :

$$y_{n+1} = \exp(\alpha h)y_n + h\sum_{i=1}^{s} b_i \exp((1-c_i)\alpha h)k_i, \tag{1.7}$$

where

$$k_i = g(t_{n,i}, y_{n,i}), \quad i = 1, 2, \ldots, s,$$
$$y_{n,i} = \exp(c_i\alpha h)y_n + h\sum_{j=1}^{s} a_{ij}\exp((c_i - c_j)\alpha h)k_j.$$

REMARK. If we apply the linear multistep methods

$$\sum_{i=0}^{k} a_i y_{n+1-i} = h\sum_{i=0}^{k} b_i f(t_{n+1-i}, y_{n+1-i})$$

to obtain a numerical approximation of the transformed problem (1.3), the *generlized linear multistep* (GLM) methods with the exponentially dominant order α is similarly derived as follows:

$$\sum_{i=0}^{k} a_i \exp(i\alpha h)y_{n+1-i} = h\sum_{i=0}^{k} b_i \exp(i\alpha h)g(t_{n+1-i}, y_{n+1-i}).$$

2. Stability Properties

Let us consider the scalar test equation

$$y'(t) = \lambda y(t), \quad t \geq 0, \; y(0) = y_0, \tag{2.1}$$

where λ is a complex number and $\mathrm{Re}(\lambda)$ is nonpositive. By applying the GRK methods (1.7) to the equation (2.1), we have obtained

$$y_{n+1} = \exp(\alpha h)R(h\bar{\lambda})y_n, \tag{2.2}$$

where $\bar{\lambda} = \lambda - \alpha$, and R is the stability function of the original Runge-Kutta methods (1.5)

$$R(\theta) = \frac{\det(I - \theta A + \theta e b^T)}{\det(I - \theta A)} \text{ or } R(\theta) = 1 + \theta b^T (I - \theta a)^{-1} e \text{ (see [3] \& [5])}.$$

In this case A and b are the coefficients of the original Rung-Kutta methods (1.5) and $e = [1, 1, \ldots, 1]^T$.

Using the formula (1.2), we know that the exponentially dominant order of the test problem (2.1) is λ. Hence $\bar{\lambda} = 0$, $R(h\bar{\lambda}) = 1$ and

$$y_{n+1} = \exp(\lambda h) y_n.$$

Therefore we have the following result.

PROPOSITION 2.1. *The GRK methods (1.7) is A-stable in the sense of Dahlquist* [2].

Let us replace the test equation (2.1) by the nonautonomous scalar equation

$$y'(t) = \lambda(t) y(t), \quad t \geq 0, \ y(0) = y_0, \tag{2.3}$$

where $\lambda : \mathbb{R} \to \mathbb{C}$ is continuous and $\mathrm{Re}(\lambda(t))$ is nonpositive. And applying the GRK methods (1.7) to the equation (2.3), we have

$$y_{n+1} = \exp(\alpha h)\, K(\Lambda)\, y_n,$$

where

$$\Lambda = \mathrm{diag}[h\{\lambda(t_n + c_1 h) - \alpha\}, h\{\lambda(t_n + c_2 h) - \alpha\}, \cdots, h\{\lambda(t_n + c_s h) - \alpha\}] \tag{2.4}$$

and

$$K(\Lambda) = \frac{\det(I - A\Lambda + e b^T \Lambda)}{\det(I - A\Lambda)} \text{ or } K(\Lambda) = 1 + b^T \Lambda (I - A\Lambda)^{-1} e.$$

Then we have the following result.

PROPOSITION 2.2. *The GRK methods (1.7) is AN-stable in the sense of Burrage and Butcher* [1], *if the stability function K satisfies*

$$|K(\Lambda)| < \exp(-\alpha h),$$

where Λ is the diagonal matrix given by (2.4).

We now consider the nonlinear test system

$$y'(t) = f(t, y(t)), \quad f : \mathbb{R}^{m+1} \to \mathbb{R}^m, \ t \geq 0, \ y(0) = y_0, \tag{2.5}$$

such that

$$\langle f(t,y) - f(t,z), y - z\rangle \leq \nu \|y - z\|^2, \quad \nu \leq 0, \tag{2.6}$$

for all y, $z \in \mathbb{R}^m$ and $t \in \mathbb{R}$. Here,$\langle .,.\rangle$ is an inner product on $\mathbb{R}^m$ with the corresponding norm, $\|.\|$. Then the following inequality follows the equation (1.4) and the inequality (2.6).

$$\langle g(t,y) - g(t,z), \ y - z\rangle \leq \bar{\nu}\|y - z\|^2, \quad \bar{\nu} = \nu - \alpha. \tag{2.7}$$

Let y_n, y_{n+1} and $y_{n,i}$ be numerical solutions of the test system (2.5) defined by the GRK methods (1.7), and suppose that z_n, z_{n+1} and $z_{n,i}$ are solutions obtained by perturbations or different starting values of the test system (2.5), which satisfy

$$\begin{aligned} z_{n+1} &= \exp(\alpha h) z_n + h \sum_{i=1}^{s} b_i \exp((1 - c_i)\alpha h) g(t_{n,i}, z_{n,i}), \\ z_{n,i} &= \exp(c_i \alpha h) z_n + h \sum_{j=1}^{s} a_{ij} \exp((c_i - c_j)\alpha h) g(t_{n,j}, z_{n,j}). \end{aligned}$$

If we use the algebraic stability in the sense of Burrage and Butcher [1], then we have the following theorem.

THEOREM 2.3. *The GRK methods (1.7) is BN-stable in the sense of Burrage and Butcher* [1], *if the following conditions are satisfied:*

1. *the original Runge-Kutta methods (1.5) is algebraiclly stable,*
2. $\nu \leq \alpha \leq 0$.

Proof. We define $u = y_n - z_n$, $w = y_{n+1} - z_{n+1}$, $v_i = y_{n,i} - z_{n,i}$ and $\phi_i = h\exp(-c_i\alpha h)\{g(t_{n,i}, y_{n,i}) - g(t_{n,i}, z_{n,i})\}$. Then the following relation can be deduced from v_i :

$$u = \exp(-c_i\alpha h)v_i - \sum_{j=1}^{s} a_{ij}\phi_j.$$

By substituting the above expression into the squared norm of w, we obtain

$$\begin{aligned}
\|w\|^2 &= \exp(2\alpha h)\left\|u + \sum_{i=1}^{s} b_i\phi_i\right\|^2 \\
&= \exp(2\alpha h)\{\|u\|^2 + 2\sum_{i=1}^{s} b_i\langle u, \phi_i\rangle + \sum_{i,j=1}^{s} b_ib_j\langle \phi_i, \phi_j\rangle\} \\
&= \exp(2\alpha h)\{\|u\|^2 + 2\sum_{i=1}^{s} b_i \exp(-c_i\alpha h)\langle v_i, \phi_i\rangle - \sum_{i,j=1}^{s} m_{ij}\langle \phi_i, \phi_j\rangle\}
\end{aligned}$$

where $m_{ij} = b_ia_{ij} + b_ja_{ji} - b_ib_j$.

Since the original Runge-Kutta methods are algebraically stable, the matrix $M = [m_{ij}]$ is nonnegative definite. Thus, the last term on the right hand side of the above equation is nonpositive. From the inequality (2.7) and the fact of $\nu \le \alpha \le 0$, we have $\langle v_i, \phi_i\rangle \le 0$. Hence we have $\|w\| \le \|u\|$, which means the BN-stability.

Since BN-stability implies B-stability, we have

COROLLARY 2.4. *Under the assumption of theorem 2.3, the GRK methods (1.7) is B-stable.*

Let us now denote the matrices P_i as follows:

$$P_i = [P_{ijk}], \quad i = 1, 2, \dots, s,$$

where

$$p_{ijk} = a_{ij}a_{jk} + a_{ik}a_{kj} - a_{ij}a_{ik}, \quad i, j, k = 1, 2, \dots, s.$$

Then we can similarly verify the following corollary.

COROLLARY 2.5. *Suppose the following conditions hold:*

1. $a_{jk} \geq 0, \quad j,k = 1,2,\ldots,s,$
2. $b_i \geq 0, \quad i = 1,2,\ldots,s,$
3. *the matrices* P_i *are nonnegative definite,* $\quad i = 1,2,\ldots,s,$
4. $\nu \leq \alpha \leq 0,$

then

$$\|y_{n,i} - z_{n,i}\| \leq \|y_n - z_n\|, \quad i = 1,2,\ldots,s.$$

3. Error Analysis

We consider again the transformed initial value problem (1.3). It can be written in an integral form

$$x(t) = x(0) + \int_0^t \exp(-\alpha\tau) g(\tau, \exp(\alpha\tau)x(\tau))\, d\tau.$$

Replacing $\exp(\alpha t)x(t)$ by $y(t)$, we have a vector integral equation for $y(t)$

$$y(t) = \exp(\alpha t)y(0) + \int_0^t \exp(\alpha(t-\tau)) g(\tau, y(\tau))\, d\tau. \tag{3.1}$$

The following relation can be deduced from the equation (3.1):

$$y(t_{n+1}) = \exp(\alpha h)y(t_n) + \int_0^h \exp(\alpha(h-\tau)) g(t_n+\tau, y(t_n+\tau))\, d\tau. \tag{3.2}$$

Comparing (3.2) and (1.7), we have the *increment function* of the GRK methods (1.7) as follows:

$$\psi(t_n, y_n) = \sum_{i=1}^{s} b_i \exp((1-c_i)\alpha h) g(t_{n,i}, y_{n,i}). \tag{3.3}$$

And we suppose that the function $g(t,y)$ satisfies the Lipschitz condition with a small Lipschitz constant $\overline{L}$:

$$\|g(t,y) - g(t,z)\| \leq \overline{L}\|y - z\|. \tag{3.4}$$

Then we have the following lemma.

LEMMA 3.1. *Suppose the following conditions hold:*

1. $a_{ij} \geq 0, \quad i, j = 1, 2, \ldots, s,$
2. $b_i \geq 0, \quad i = 1, 2, \ldots, s,$
3. *the matrix* $M = [m_{ij}]$ $(i, j = 1, 2, \ldots, s)$ *is nonnegative definite,*
4. *the matrices* $P_i = [p_{ijk}]$ $(i, j, k = 1, 2, \ldots, s)$ *are nonnegative definite,*
5. $\nu \leq \alpha \leq 0,$

Then the increment function (3.3) satisfies a Lipschitz condition

$$\|\psi(t_n, y_n) - \psi(t_n, z_n)\| \leq \delta \|y_n - z_n\|,$$

where

$$\delta = \overline{L} \left\{ \sum_{i=1}^{s} b_i \exp((1 - c_i)\alpha h) \right\}.$$

Proof. From (3.3) and (3.4), we have

$$\begin{aligned} \|\psi(t_n, y_n) - \psi(t_n, z_n)\| &= \left\| \sum_{i=1}^{s} b_i((1 - c_i)\alpha h)\{g(t_{n,i}, y_{n,i}) - g(t_{n,i}, z_{n,i})\} \right\| \\ &\leq \sum_{i=1}^{s} \{b_i \exp((1 - c_i)\alpha h)\overline{L}\|y_{n,i} - z_{n,i}\|\} \end{aligned}$$

By Theorem 2.3 and Corollarly 2.5, we have the result.

From the integral equation (3.2) and the increment function (3.3), the *residual error* of the GRK methods (1.7) can be defined as follows:

$$r_n = \int_0^h \exp(\alpha(h - \tau))\, g(t_n + \tau, y(t_n + \tau))\, d\tau - h\psi(t_n, y(t_n)). \tag{3.5}$$

Now we consider an asymptotically stable system

$$y'(t) = f(t, y(t)), \quad f : \mathbb{R}^{m+1} \to \mathbb{R}^m, \ t \geq 0, \tag{3.6}$$

such that

(i) the system has an asymtotically stable zero solution,
(ii) $\langle f(t, y) - f(t, z),\ y - z \rangle \leq \nu \|y - z\|^2, \quad \nu \leq 0.$

Then, using (3.5), the following lemmas can be easily proved and we omit the proof.

LEMMA 3.2. *If the GRK methods (1.7) is applied to the asymptotically stable system (3.6), then the residual error r_n tends to zero as $n \to \infty$.*

LEMMA 3.3. *If $0 < \theta < 1$ and $\lim_{n\to\infty} \delta_n = 0$, then*

$$\lim_{n\to\infty} \{\theta^n \delta_0 + \theta^{n-1}\delta_1 + \cdots + \theta\delta_{n-1} + \delta_n\} = 0.$$

We now introduce a concept of *AB-stability*, which stands for a numerical method is A-stable and B-stable.

DEFINITION. The GRK methods (1.7) is called *AB-stable* if its global truncation error, $E_n = y(t_n) - y_n$, for the system (3.6) tends to zero as $n \to \infty$.

THEOREM 3.4. *If the following conditions are all satisfied:*

1. $a_{ij} \geq 0, \quad i,j = 1,2,\ldots,s,$
2. $b_i \geq 0, \quad i = 1,2,\ldots,s,$
3. *the matrix $M = [m_{ij}]$ is nonnegative definite,*
4. *the matrices $P_i = [p_{ijk}]$ $(i = 1,2,\ldots,s)$ are nonnegative definite,*
5. $\nu \leq \alpha \leq 0,$
6. $\theta = \exp(\alpha h) + h\overline{L}\{\sum_{i=1}^{s} b_i \exp((1-c_i)\alpha h)\}, \quad 0 < \theta < 1.$

Then the GRK methods (1.7) is AB-stable.

Proof. By applying the GRK methods (1.7) to the test problem (3.6), its global truncation error is given by

$$E_{n+1} = \exp(\alpha h)E_n + h\{\psi(t_n, y(t_n)) - \psi(t_n, y_n)\} + r_n.$$

Hence we have

$$\|E_{n+1}\| \leq \exp(\alpha h)\|E_n\| + h\|\psi(t_n, y(t_n)) - \psi(t_n, y_n)\| + \|r_n\|.$$

By Lemma 3.1, we have

$$\|E_{n+1}\| \leq \theta\|E_n\| + \|r_n\|.$$

The error E_{n+1} after n recurrence steps satisfies

$$\|E_{n+1}\| \leq \theta^{n+1}\|E_0\| + \theta^n\|r_0\| + \theta^{n-1}\|r_1\| + \cdots + \theta\|r_{n-1}\| + \|r_n\|.$$

By Lemma 3.2 and Lemma 3.3, we have the result.

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