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MOL approximations for delay differential equations
遅延微分方程式に対するMOL近似解法

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1 Introduction

Let us consider initial value problems for delay differential equations (DDEs) of the form

$$\frac{dx}{dt} = f(t, x(t), x(t-\tau)), \quad t \geq 0, \tag{1.1}$$

$$x(t) = \varphi(t), \quad -\tau \leq t \leq 0, \tag{1.2}$$

where $\tau > 0$ is a constant delay, $x(t) \in \mathbb{R}^d$, and $\varphi \in C([-\tau, 0], \mathbb{R}^d)$. For simplicity, we assume that f is a continuous function defined on the whole space $[0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d$ and satisfies a global Lipschitz condition, i.e. there is a constant γ such that

$$| f(t, x, y) - f(t, \hat{x}, \hat{y}) | \leq \gamma(| x - \hat{x} | + | y - \hat{y} |) \tag{1.3}$$

for all $t \geq 0$ and $x, y, \hat{x}, \hat{y} \in \mathbb{R}^d$. Here, $| \cdot |$ denotes the Euclidean norm on $\mathbb{R}^d$. Under this assumption, the problem (1.1)-(1.2) has a unique solution $x(t)$ which is defined for all $t \geq -\tau$. Moreover, if $\varphi(t) \in C^1([-\tau, 0], \mathbb{R}^d)$ and

$$\varphi'(0) = f(0, \varphi(0), \varphi(-\tau)), \tag{1.4}$$

the solution $x(t)$ belongs to $C^1([-\tau, \infty), \mathbb{R}^d)$.

When $x(t) \in C^1([-\tau, \infty), \mathbb{R}^d)$, the function $u(t, \theta)$ given by

$$u(t, \theta) = x(t + \theta), \quad t \geq 0, \quad -\tau \leq \theta \leq 0, \tag{1.5}$$

satisfies the initial-boundary value problem for the convection equation

$$\frac{\partial u}{\partial t} = \frac{\partial u}{\partial \theta}, \quad t \geq 0, \quad -\tau \leq \theta \leq 0, \tag{1.6}$$

$$u(0, \theta) = \varphi(\theta), \quad -\tau \leq \theta \leq 0, \tag{1.7}$$

$$\frac{\partial u}{\partial t}(t, 0) = f(t, u(t, 0), u(t, -\tau)), \quad t \geq 0. \tag{1.8}$$

Moreover, since every C^1-function which satisfies (1.6) is represented in the form (1.5), the function $u(t, \theta)$ defined by (1.5) with the solution to (1.1)-(1.2) gives a unique solution to (1.6)-(1.8). Therefore, for an initial function which satisfies (1.4), we can obtain an approximate solution to the problem (1.1)-(1.2) by solving the initial-boundary value problem (1.6)-(1.8) with a suitable numerical method.

Such approach for solving DDEs, called semigroup method in some literatures, has been studied by many authors [1, 2, 3, 4, 5, 13, 20, 21], especially with the intension of constructing numerical methods which preserve some mathematical structures of DDEs. For example, in a series of papers, Guglielmi and Hairer [9, 10], Guglielmi [8] (see also [22]) have clarified that an asymptotic property of DDEs is not preserved by the usual methods. To overcome the defect, Bellen and Maset [3, 20, 21] have introduced a semigroup method and shown some results which suggest the efficiency of the method in this direction.

In this paper, we try to make a framework for advancing their approach. Specifically, we consider a family of method of lines (MOL) approximations to the problem (1.6)–(1.8), which is derived from RK methods, and study their convergence as solutions to DDEs.

We may regard (1.6) as an ordinary differential equation (ODE) with the independent variable θ on a function space. Hence, applying an RK method to (1.6) with respect to θ, we can get an MOL approximation of arbitrary high order in the sence of consistency. However, as is suggested by the Trotter-Kato theorem [25, 15, 16](see, also [14, 26]), a kind of stability condition is needed for convergence of the MOL approximation. The main purpose of this paper is to show that A-stability of RK methods plays such a role, that is, A-stability guarantees convergence of the MOL approximation.

2 Method of lines approximations

2.1 Space discretization by RK methods

We denote the parameters of an s-stage RK method by

$$A = [\,a_{ij}\,]_{1\le i,j\le s}, \quad b = [b_1,\ b_2,\ \dots\ ,\ b_s]^T,$$

and assume that $0 \le c_i \le 1$, $i = 1,\ 2,\ \dots\ , s$, for $c_i = \sum_{j=1}^{s} a_{ij}$. Moreover, let us consider a mesh of the form

$$-\tau = \theta_N < \ \cdots\ < \theta_n < \ \cdots\ < \theta_1 < \theta_0 = 0, \quad \theta_n = -nh, \quad h = \tau/N.$$

Applying the RK method to (1.6) with respect to θ, we obtain a system of ODEs,

$$U_{n+1}(t) = \mathbf{1} \otimes u_n(t) - h(A \otimes I_d)\frac{dU_{n+1}}{dt}\,, \tag{2.1}$$

$$u_{n+1}(t) = u_n(t) - h(b^T \otimes I_d)\frac{dU_{n+1}}{dt}\,, \tag{2.2}$$

for $n = 0,\ 1,\ \dots\ , N-1$. Here, $u_n(t)$ is an approximate value of $u(t, \theta_n)$,

$$U_n(t) = [U_{n,1}(t)^T,\ U_{n,2}(t)^T,\ \dots\ ,\ U_{n,s}(t)^T]^T \in (I\!R^d)^s$$

are intermediate variables, $\mathbf{1} = [1,\ 1,\ \dots\ ,\ 1]^T \in I\!R^s$, and $\otimes$ denotes the Kronecker product. Note that $u_n(t)$, $n = 0,\ 1,\ \dots\ ,\ N$, are aligned in the minus direction with respect to θ. This order is, in a sense, natural since the convection equation (1.6) represents a movement in the direction. We also replace the boundary condition (1.8) with

$$\frac{du_0}{dt} = f(t, u_0(t), u_N(t)). \tag{2.3}$$

In general, the total system (2.1)–(2.3) becomes a differential-algebraic equation (a singular system of ODEs), which causes some difficulty in the analysis of the MOL approximations. We assume the following conditions (C_1) and (C_2), or (C_1) and ($\hat{C}_2$) to consider cases where the system (2.1)–(2.3) contains no algebraic canstraint.

(C_1) $a_{sj} = b_j$, for $j = 1, 2, \dots, s$.

(C_2) The matrix A is invertible.

($\hat{C}_2$) $a_{1j} = 0$, for $j = 1, 2, \dots, s$, and the matrix $\hat{A} = [\, a_{ij} \,]_{2\le i,j\le s}$ is invertible.

The condition (C_1) implies that $u_n(t) = U_{n,s}(t)$ for $n = 1, 2, \dots, N$, and the last row of (2.1) coincides with (2.2). We put $U_{0,s}(t) = u_0(t)$ for consistency.

In the case of (C_2), the system (2.1)–(2.3) is rewritten as

$$\frac{du_0}{dt} = f(t, u_0(t), U_{N,s}(t)), \tag{2.4}$$

$$\frac{dU_{n+1}}{dt} = \frac{1}{h}(A^{-1} \otimes I_d)[\mathbf{1} \otimes U_{n,s}(t) - U_{n+1}(t)]. \tag{2.5}$$

In the case of ($\hat{C}_2$), it follows from $a_{1j} = 0$ that $U_{n+1,1}(t) = u_n(t)$, and hence $U_{n+1,1}(t) = U_{n,s}(t)$. The equation (2.1) is rewritten in the form

$$\frac{d\hat{U}_{n+1}}{dt} = \frac{1}{h}(\hat{A}^{-1} \otimes I_d)\Big[\hat{\mathbf{1}} \otimes U_{n,s}(t) - \hat{U}_{n+1}(t) - h(\boldsymbol{a} \otimes I_d)\frac{dU_{n,s}}{dt}\Big],$$

where

$$\hat{U}_{n+1}(t) = [U_{n+1,2}(t)^T, U_{n+1,3}(t)^T, \dots, U_{n+1,s}(t)^T]^T \in (I\!R^d)^{s-1},$$
$$\hat{\mathbf{1}} = [1, 1, \dots, 1]^T \in I\!R^{s-1}, \quad \boldsymbol{a} = [a_{21}, a_{31}, \dots, a_{s1}]^T \in I\!R^{s-1}.$$

Hence, each $d\hat{U}_n/dt$ is represented by a function of $u_0(t)$, $\hat{U}_1(t)$, ..., $\hat{U}_n(t)$ and $U_{N,s}(t)$.

In both cases, a vector-valued function

$$\boldsymbol{u}_N = [u_0^T, U_1^T, U_2^T, \dots, U_N^T]^T \; : \; [0,\infty) \to \boldsymbol{X}_N,$$
$$\boldsymbol{X}_N = I\!R^d \times \prod_{n=1}^{N} X_n, \quad X_n \simeq (I\!R^d)^s,$$

is determined from a given initial condition corresponding to (1.7), for example,

$$u_0(0) = \varphi(0), \quad U_{n,i}(0) = \varphi(\theta_n - c_i h). \tag{2.6}$$

2.2 Convergence

Some numerical experiments suggest a kind of stability condition is necessary for convergece of the MOL approximations (Sect. 3). We consider the following assumption for the RK method.

(C_3) There exists a symmetric matrix $Q \geq 0$ such that

$$\mathcal{M} \stackrel{\text{def}}{=} QA + A^TQ - bb^T \geq 0, \quad Q\mathbf{1} = b.$$

Here, the symbol "≥ 0" denotes that a symmetric matrix is nonnegative definite. We also use "> 0" to indicate that a symmetric matrix is positive definite.

This condition is known as an algebraic characterization of A-stability. An algebraically stable method (see, e.g. [11]) satisfies (C_3) with $Q = \text{diag}[b_1, b_2, \ldots, b_s]$. By the same computation as is used for proving algebraic stability implies B-stability, it is verified that (C_3) is sufficient for the method to be A-stable, i.e. the stability function

$$r(z) = 1 + zb^T(I_s - zA)^{-1}\mathbf{1} \tag{2.7}$$

satisfies

$$| r(z) | \leq 1 \quad \text{for } \operatorname{Re} z \leq 0. \tag{2.8}$$

Moreover, Scherer and Müller [23] has proved that in a wide class of RK methods the condition (C_3) is also necessary for A-stability (see also [17] on examples of Q). For example, under the assumption that $\det[A] \neq 0$ and the numerator $\det[I_s - zA + z\mathbf{1}b^T]$ and the denominator $\det[I_s - zA]$ of $r(z)$ have no common zero, (C_3) is a necessary and sufficient condition for A-stability. The Radau IIA and Lobatto IIIC methods satisfy (C_1), (C_2), (C_3). The Lobatto IIIA methods satisfy (C_1), ($\widehat{C}_2$), (C_3) (see [24] on the condition (C_3) for the methods).

Using the matrix Q in the condition (C_3), we define a symmetric (nonnegative definite) bilinear form on $\boldsymbol{X}_N$ by

$$\langle \boldsymbol{u}_N, \boldsymbol{v}_N \rangle_N = u_0^T v_0 + h \sum_{n=1}^{N} U_n^T (Q \otimes I_d) V_n, \quad \boldsymbol{u}_N, \boldsymbol{v}_N \in \boldsymbol{X}_N. \tag{2.9}$$

We also write the corresponding seminorm as $\| \boldsymbol{u}_N \|_N = \sqrt{\langle \boldsymbol{u}_N, \boldsymbol{u}_N \rangle_N}$. Recall that the Cauchy-Schwarz inequality is still valid for a nonnegative definite bilinear form.

Let p be the order of consistency of the RK method, and assume that

$$\sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{c_i^k}{k}, \quad k \leq q, \tag{2.10}$$

i.e. the stage order is q. In the remainder of this section, we assume that the exact solution $x(t)$ to the problem (1.1)-(1.2) belongs to $C^{p+1}([-\tau, T], \mathbb{R}^d)$ for some constant $T > 0$. If $\varphi \in C([-\tau, 0], \mathbb{R}^d)$ and f is sufficiently smooth, the solution $x(t)$ is C^{k+1} on $t \geq k\tau$. Hence, the assumption is not necessarily impractical, for example, in the case where the study of the asymptotic behavior of the solution is the main purpose of the numerical computation.

Put

$$\alpha_i^{(k)} = \frac{1}{(k-1)!} \Big(\sum_{j=1}^{s} a_{ij} c_j^{k-1} - \frac{c_i^k}{k} \Big), \quad 1 \leq i \leq s, \quad q+1 \leq k \leq p, \tag{2.11}$$

and define $\beta_i^{(k)}$, $1 \le i \le s$, inductively by

$$\beta_i^{(q+1)} = \alpha_i^{(q+1)}, \quad \beta_i^{(k)} = \alpha_i^{(k)} + \sum_{j=1}^{s} a_{ij}\beta_j^{(k-1)}, \quad q+2 \le k \le p. \tag{2.12}$$

Using these $\beta_i^{(k)}$ we define the function $\xi_{n+1}(t)$ by

$$\xi_{n+1,i}(t) = x(t+\theta_n - c_i h) + \sum_{k=q+1}^{p} \beta_i^{(k)} x^{(k)}(t+\theta_n)(-h)^k, \tag{2.13}$$

$$\xi_{n+1}(t) = [\xi_{n+1,1}(t)^T, \ \xi_{n+1,2}(t)^T, \ \ldots, \xi_{n+1,s}(t)^T\,]^T, \tag{2.14}$$

and put

$$e_n(t) = x(t+\theta_n) - u_n(t), \quad E_n(t) = \xi_n(t) - U_n(t),$$
$$\mathbf{e}_N(t) = [e_0(t)^T, \ E_1(t)^T, \ E_2(t)^T, \ \ldots, \ E_N(t)^T\,]^T.$$

Under the notation above we have the following theorem [18]. For the initial condition (2.6), the MOL approximation converges at a rate of $O(h^{\min\{q+1,p\}})$. By replacing the second condition of (2.6) with

$$U_{n,i}(0) = \varphi(\theta_n - c_i h) + \sum_{k=q+1}^{p_*} \beta_i^{(k)} \varphi^{(k)}(\theta_n)(-h)^k, \quad q+1 \le p_* \le p, \tag{2.15}$$

the rate is raised up to $O(h^{\min\{p_*+1,p\}})$.

Theorem 2.1 *Assume that* (C_1), (C_2), (C_3), *or* (C_1), ($\hat{C}_2$), (C_3) *are satisfied. In addition, assume that the exact solution* $x(t)$ *belongs to* $C^{p+1}([-\tau,T],\mathbb{R}^d)$ *for* $T > 0$. *Then, there is a constant* C *depending on* T *such that*

$$\max_{0\le t\le T} \| \mathbf{e}_N(t) \|_N \le C\Big(\| \mathbf{e}_N(0) \|_N + h^p\Big) \tag{2.16}$$

holds for any $N \ge 1$.

3 Numerical examples

We present numerical results which confirm the results of Sect. 2. All experiments were carried out by an 80-bit long double floating-point arithmetic (the number of bits in the mantissa is 64). We used the (4-stage 4th-order) classical RK method with a constant stepsize for time integration of the MOL approximations, which seem stiff ODE systems. In fact, rather small stepsizes, determined experimentally, are used to avoid numerical instability with respect to the time integration. Since the aim of this experiment was to test the MOL approximations, we used the classical RK method which is easy to implement. For practical applications, however, the use of a suitable integrator for stiff equations should be investigated.

We first show numerical results which suggest necessity of A-stability for convergence of the MOL approximations.

The 2-stage method

(3.1)
$$\begin{array}{c|cc} 0 & -1/2 & 1/2 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array}$$

is of order 2 and has the stability function

(3.2)
$$r(z) = \frac{1+z}{1-z^2/2}.$$

The method is I-stable but not A-stable; $r(z)$ has a pole at $z = -\sqrt{2}$.

The 3-stage method

(3.3)
$$\begin{array}{c|ccc} 0 & 1/6 & -4/3 & 7/6 \\ 1/2 & 1/6 & 2/3 & -1/3 \\ 1 & 1/6 & 2/3 & 1/6 \\ \hline & 1/6 & 2/3 & 1/6 \end{array}$$

is the adjoint method of the well-known third-order method

(3.4)
$$\begin{array}{c|ccc} 0 & & & \\ 1/2 & 1/2 & & \\ 1 & -1 & 2 & \\ \hline & 1/6 & 2/3 & 1/6 \end{array}$$

by W. Kutta. The stability function is

(3.5)
$$r(z) = \frac{1}{1 - z + z^2/2 - z^3/6},$$

which has no pole in $\mathbb{C}_-$, but the method is not I-stable; $| r(iy) | > 1$ holds for $0 < | y | < \sqrt{3}$.

We consider MOL appoximations by these methods to the following problem, whose exact solution is given by $x(t) = \cos[(\pi/2)t]$.

Problem 1 : $\dfrac{dx}{dt} = -\left(\dfrac{\pi}{2}\right) x(t-1), \quad t \geq 0, \quad x(t) = \cos\left(\dfrac{\pi}{2} t\right), \quad -1 \leq t \leq 0.$

Fig. 1 shows the functions

(3.6)
$$\log_2 |u_0(t) - x(t)|$$

in the case of the 2-stage method (3.1), which were obtained by solving the ODE system (2.4), (2.5) with the initial condition (2.6) and the stepsize $\Delta t = 10^{-3}$. The approximate solution $u_0(t)$ rapidly apparts from the exact solution.

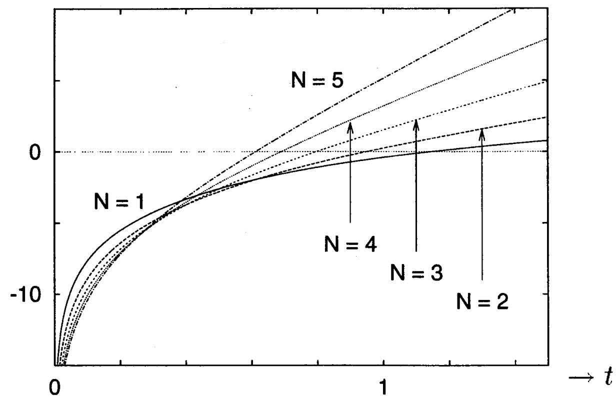

Fig. 1. Errors in the case of the 2-stage method (3.1)

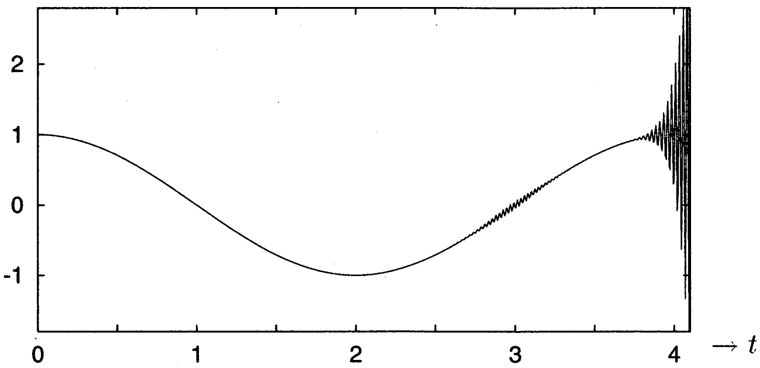

Fig. 2. Approximate solution in the case of the 3-stage method (3.3) for $N = 200$

Fig. 2 shows the approximate solution $u_0(t)$ in the case of the 3-stage method (3.3) for $N = 200$. Similar high-frequency oscillations appear for larger N, and $u_0(t)$ does not approach $x(t)$ even if a lager N is taken.

Put

$$\varphi(t) = \exp[2 + \cos^2(t)], \tag{3.7}$$

and consider a problem whose exact solution is $x(t) = \varphi(t)$.

Problem 2 : $$\frac{dx}{dt} = -x(t-1)[1 + x(t)^2] + \varphi(t-1)[1 + \varphi(t)^2] + \varphi'(t), \quad 0 \le t \le 2,$$

$$x(t) = \varphi(t), \quad -1 \le t \le 0.$$

Tables 1, 2, 3 list observed accuracy of various methods for Problem 2. Each number in a column for "dig." denotes the value

$$-\log_2 \left(\max_{0 \le t \le 2} |u_0(t) - \varphi(t)| \right), \tag{3.8}$$

the number of correct bits of the approximate solution $u_0(t)$ for the partition numeber N, and "diff." stands for the difference between the bit number for N and that for $N/2$. We used the initial condition (2.6) and the stepsize $\Delta t = 10^{-5}$.

Convergence rates of $O(h^{\min\{q+1,p\}})$ are observed for the 1-stage and 2-stage Radau IIA methods, the 2-stage Lobatto IIIC method, and the 2-stage and 3-stage Lobatto IIIA methods. For the other methods the rates seem a little higher.

Table 1. Numerical results by the Radau IIA methods

	$s=1$		$s=2$		$s=3$	
N	dig.	diff.	dig.	diff.	dig.	diff.
2	−0.45	–	2.96	–	6.80	–
4	0.24	0.70	5.68	2.72	10.78	3.98
8	1.03	0.79	8.60	2.92	15.00	4.22
16	1.86	0.83	11.56	2.95	19.24	4.23
32	2.66	0.81	14.54	2.98	23.50	4.26
64	3.56	0.90	17.52	2.98	27.87	4.37
128	4.51	0.95	20.51	2.99	32.40	4.53

Table 2. Numerical results by the Lobatto IIIC methods

	$s=2$		$s=3$		$s=4$	
N	dig.	diff.	dig.	diff.	dig.	diff.
2	0.33	–	4.82	–	6.79	–
4	1.74	1.41	8.19	3.38	11.00	4.21
8	3.69	1.96	11.97	3.78	15.32	4.31
16	5.53	1.83	15.80	3.83	19.64	4.33
32	7.46	1.93	19.12	3.32	24.05	4.41
64	9.43	1.97	22.45	3.34	28.74	4.69
128	11.42	1.99	25.89	3.44	33.49	4.75

Table 3. Numerical results by the Lobatto IIIA methods

	$s=2$		$s=3$		$s=4$	
N	dig.	diff.	dig.	diff.	dig.	diff.
2	0.73	–	4.81	–	8.61	–
4	2.88	2.15	8.65	3.83	13.24	4.63
8	4.90	2.02	12.71	4.07	18.28	5.04
16	6.89	2.00	16.68	3.97	23.32	5.04
32	8.89	1.99	20.70	4.03	28.23	4.91
64	10.89	2.00	24.70	4.00	33.65	5.42
128	12.89	2.00	28.71	4.01	39.34	5.68

Table 4 shows results by the 4-stage Lobatto IIIC method, obtained by replacing the second condition of (2.6) with

$$U_{n,i}(0) = \varphi(\theta_n - c_i h) + \sum_{k=4}^{p_*} \beta_i^{(k)} \varphi^{(k)}(\theta_n)(-h)^k. \tag{3.9}$$

The use of these initial conditions indeed reduces the error in the MOL approximation.

Table 4. Numerical results by the 4-stage Lobatto IIIC method.

	$p_* = 4$		$p_* = 5$		$p_* = 6$	
N	dig.	diff.	dig.	diff.	dig.	diff.
2	8.05	–	6.73	–	8.79	–
4	12.66	4.61	13.70	6.98	14.37	5.58
8	17.30	4.63	20.04	6.34	20.21	5.84
16	22.27	4.97	25.94	5.90	26.09	5.88
32	27.57	5.30	31.90	5.96	32.03	5.94
64	33.18	5.61	37.88	5.98	38.01	5.97
128	39.04	5.86	43.87	5.99	43.99	5.99

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