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Runge–Kutta–Collocation methods for systems of functional-differential and functional equations

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Abstract Systems of functional-differential and functional equations occur in many biological, control and physics problems. They also include functional differential equations of neutral type as special cases. In this paper we present a numerical method that is based on the continuous extension of the Runge–Kutta method (for ordinary differential equations) and the collocation method (for functional equations). Order of approximation and stability of this Runge–Kutta-Collocation method are discussed.

1 Introduction

In this paper we study the numerical solution of the system of functional-differential and functional equations

$$\begin{cases} y'(t) = f(t, y(t), y(\phi(t)), z(\phi(t))), \\ z(t) = g(t, y(t), y(\phi(t)), z(\phi(t))), \end{cases} \qquad t \geq t_0, \tag{1.1}$$

with the initial conditions

$$y(t) = Y(t), \quad z(t) = Z(t), \qquad t \leq t_0, \tag{1.2}$$

where y and z are unknown vectors of complex functions, f and g are given vectors of complex functions with appropriate domains of definition, ϕ is the (time) delay function which satisfies $\phi(t) \leq t$ for $t \geq t_0 \in \mathbb{R}$, and Y, Z are given vectors of complex functions that satisfy the consistent condition

$$Z(t_0) = g(t_0, Y(t_0), Y(\phi(t_0)), Z(\phi(t_0))).$$

The following system of functional-differential and functional equations

$$\begin{cases} y'(t) = f(t, y(t), y(\phi(t)), z(t), z(\phi(t))), \\ z(t) = g(t, y(t), y(\phi(t)), z(\phi(t))), \end{cases} \qquad t \geq t_0 \tag{1.3}$$

can be transformed into (1.1) by a simple substitution.

Systems of the form (1.1) is sometimes called hybrid systems [16]. Special cases of (1.1) and (1.3) have occured in many biological, control and physics problems [1, 3, 4, 6, 11, 13]. Furthermore, functional differential equations of neutral type can be transformed into (1.1). The (explicit) neutral equation

$$y'(t) = f(t, y(t), y(\phi(t)), y'(\phi(t))) \tag{1.4}$$

is equivalent to

$$\begin{cases} y'(t) = f(t, y(t), y(\phi(t)), z(\phi(t))), \\ z(t) = f(t, y(t), y(\phi(t)), z(\phi(t))), \end{cases} \tag{1.5}$$

while the (implicit) neutral equation

$$[z(t) - g(t, z(\phi(t)))]' = f(t, z(t), z(\phi(t))) \tag{1.6}$$

is equivalent to

$$\begin{cases} y'(t) = f(t, y(t) + g(t, z(\phi(t))), z(\phi(t))), \\ z(t) = y(t) + g(t, z(\phi(t))). \end{cases} \tag{1.7}$$

Numerical solution of (1.4) has been studied extensively in recent years. Typical numerical methods for (1.4) include various continuous extentions of the Runge–Kutta methods. There seems to be little point in transforming (1.4) into (1.5) and solving (1.5) numerically. However, the situation with the implicit neutral equation (1.6) is very different. Even in the case where (1.6) can be transformed into the form of (1.4), there are certain advantages in solving it by formulating numerical schemes based on its equivalent form (1.7). This has been discussed in Liu [19].

The purpose of this paper is to present a systematic study of the numerical solution of the initial value problem (1.1,1.2). In the next section we formulate a class of Runge–Kutta-Collocation (RKC) methods by applying the continuous Runge–Kutta method and the collocation method, respectively, to the first and the second equations of (1.1). The order of approximation of this RKC method is analysed in Section 3. In particular, we show that on the so called constraint grid optimal order of approximation on the grid points can be achieved for a large class of RKC methods. In Section 4 we investigate the linear stability of the some RKC methods and prove that the long time dynamical behaviour of the exact solution of the test problem can be preserved by the numerical solutions.

The second equation in (1.1) becomes an algebraic one at vanishing-delay points (i.e., fixed points of ϕ, if exist). However, we do not dicuss this case in this paper even though our numerical methods to be formulated in the next section remain valid. Some numerical aspects of the so called delay differential algebraic equations are discussed in Hauber [10] and Zhu and Petzold [25].

2 Numerical methods

Let $t_0 < t_1 < t_2 < \ldots$ be a subdivision of the integration interval $[t_0, T]$ for some $T > 0$, and let $h = \max h_n$, where $h_n = t_{n+1} - t_n$, $n = 0, 1, \ldots$, are the stepsizes.

Before formulating numerical methods for solving the initial value problem (1.1,1.2) we describe briefly the continuous extension of the Runge–Kutta method for ordinary differential equations and the collocation method for functional equations.

2.1 Ordinary differential equations

For the initial value problem

$$y'(t) = f(t, y(t)), \quad t > t_0, \qquad y(t_0) = y_0, \tag{2.1}$$

the s-stage Runge–Kutta method defined by the Butcher tableau

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} \tag{2.2}$$

can be written as

$$y_{n+1} = y_n + h_n \sum_{i=1}^{s} b_i K_i,$$

where K_i, $i = 1, \ldots, s$, are determined by the system of algebraic equations

$$K_i = f\left(t_n + c_i h_n, y_n + h_n \sum_{j=1}^{s} a_{ij} K_j\right), \qquad i = 1, \ldots, s.$$

A continuous extension of the Runge–Kutta method gives a continuous numerical solution of the form

$$y^h(t_n + \tau h_n) = y_n + h_n \sum_{i=1}^{s} b_i(\tau) K_i, \qquad \tau \in [0, 1], \tag{2.3}$$

where $b_i(\tau)$, $i = 1, \ldots, s$, are polynomials that obey

$$b_i(0) = 0, \quad b_i(1) = b_i, \qquad i = 1, 2, \ldots, s.$$

A typical example of a continuous Runge–Kutta method is the collocation Runge–Kutta method [7, p. 211]. Other continuous Runge–Kutta methods can be found in Zennaro [23], Hairer, Nørsett and Wanner [7] and Owren and Zennaro [20]. Of particular interest is the linear θ-method defined by the Butcher tableau

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1-\theta & \theta \\ \hline & 1-\theta & \theta \end{array}$$

where $\theta \in [0, 1]$ is a parameter. The linear θ-method for the initial value problem (2.1) can be conveniently written as

$$y_{n+1} = y_n + h_n \left[(1-\theta) f(t_n, y_n) + \theta f(t_{n+1}, y_{n+1})\right], \qquad n = 0, 1, \ldots. \tag{2.4}$$

Its continuous extension can be obtained by letting

$$y^h(t_n + \tau h_n) = (1-\tau)y_n + \tau y_{n+1}, \qquad \tau \in [0,1]. \tag{2.5}$$

There are other ways of generating continuous numerical solutions, for instance, the Hermite interpolation [21] and the boot-strapping process [5].

2.2 Functional equations

Consider the initial value problem

$$z(t) = g(t, z(\phi(t))), \quad t > t_0, \qquad z(t) = Z(t), \quad t \le t_0, \tag{2.6}$$

where ϕ is a given function that satisfies $\phi(t) \le t$ for $t \ge t_0 \in \mathbb{R}$, and Z is a given initial function that satisfies the consistent condition

$$Z(t_0) = g(t_0, Z(\phi(t_0))).$$

Let $z^h(t) = Z(t)$ for $t \le t_0$. The collocation method with the collocation points $t_n + c_i^* h_n$, $i = 1, \dots, s^*$, $n = 0, 1, \dots$, gives the continuous numerical solution

$$z^h(t_n + \tau h_n) = \sum_{i=1}^{s^*} B_i(\tau) M_{n,i}, \qquad \tau \in (0,1] \tag{2.7}$$

where c_i^*, $i = 1, 2, \dots, s^*$, are distinct points in $[0,1]$,

$$B_i(\tau) = \prod_{j=1, j\ne i}^{s^*} \frac{\tau - c_j^*}{c_i^* - c_j^*}, \qquad i = 1, \dots, s^*,$$

and $M_{n,i}$, $i = 1, \dots, s^*$, are determined by the system of algebraic equations

$$M_{n,i} = g(t_n + c_i^* h_n, z^h(\phi(t_n + c_i^* h_n))), \qquad i = 1, \dots, s^*. \tag{2.8}$$

It is clear that $M_{n,i}$ is our approximation to the unknown function $z(t)$ at $t_n + c_i h_n$, $z^h(t)$ is simply the Lagrange interpolation of $(t_n + c_i^* h_n, M_{n,i})$, $i = 1, \dots, s^*$, and the first equation of (2.6) is satisfied by z^h at the collocation points.

An alternative but straightforward way of solving (2.6) is to use the recurrence relation

$$z(\phi^m(t_n)) = g(\phi^m(t), z(\phi^{m+1}(t_n))), \qquad m = 0, 1, \dots, m_0 - 1,$$

where

$$\phi^0(t_n) = t_n, \qquad \phi^{m+1}(t_n) = \phi(\phi^m(t_n)), \qquad m = 0, 1, \dots$$

and $m_0 \in \mathbb{N}$ such that

$$\phi^{m_0}(t_n) \le t_0$$

or

$$\phi^{m_0}(t_n) = t^*,$$

where t^* is a fixed point of ϕ. However, this is a very expansive method as the computation cost for generating $z(t_k)$, $k = 1, \dots, n$, is $\mathcal{O}(n^2)$, unless $\phi(t) \not\equiv t$. By contrast, the cost of the collocation method (2.7,2.8) is $\mathcal{O}(n)$ only.

2.3 Hybrid systems

Denote by $(y^h(t), z^h(t))$ our approximation to the exact solution $(y(t), z(t))$ of the initial value problem (1.1,1.2) and let

$$y^h(t) = Y(t), \quad z^h(t) = Z(t), \qquad t \leq t_0.$$

Suppose that the numerical solution $(y^h(t), z^h(t))$ for $t \leq t_n$ is known for some $n \geq 0$. Then the solution in the interval $(t_n, t_{n+1}]$ can be obtained by letting

$$\begin{cases} y^h(t_n + \tau h_n) = y_n + h_n \sum_{i=1}^{s} b_i(\tau) K_{n,i}, \\ z^h(t_n + \tau h_n) = \sum_{i=1}^{s^*} B_i(\tau) M_{n,i}, \end{cases} \qquad 0 < \tau \leq 1, \tag{2.9}$$

where $\{K_{n,i}\}_{i=1}^{s}$ and $\{M_{n,i}\}_{i=1}^{s^*}$ are determined by the system of algebraic equations

$$\begin{cases} K_{n,i} = f(t_n + c_i h_n, y_n + h_n \sum_{j=1}^{s} a_{ij} K_{n,j}, \\ \qquad\qquad y^h(\phi(t_n + c_i h_n)), z^h(\phi(t_n + c_i h_n))), \qquad i = 1, 2, \ldots, s, \\ M_{n,i} = g(t_n + c_i^* h_n, y^h(t_n + c_i^* h_n), \\ \qquad\qquad y^h(\phi(t_n + c_i^* h_n)), z^h(\phi(t_n + c_i^* h_n))), \qquad i = 1, 2, \ldots, s^*. \end{cases} \tag{2.10}$$

In the sequel, we refer to it as a RKC method.

Corresponding to the linear θ-method (2.4,2.5), we have

$$\begin{cases} y^h(t_n + \tau h_n) = (1 - \tau) y_n + \tau y_{n+1}, \\ z^h(t_n + \tau h_n) = (1 - \tau) z_n + \tau z_{n+1}, \end{cases} \qquad 0 < \tau \leq 1, \tag{2.11}$$

where $(y_0, z_0) = (Y(t_0), Z(t_0))$, and (y_n, z_n), $n = 1, 2, \ldots$, are given by the recurrence relation

$$\begin{cases} y_{n+1} = y_n + h_n[(1 - \theta) f(t_n, y_n, y^h(\phi(t_n)), z^h(\phi(t_n))) \\ \qquad\qquad + \theta f(t_{n+1}, y_{n+1}, y^h(\phi(t_{n+1})), z^h(\phi(t_{n+1})))], \\ z_{n+1} = g(t_{n+1}, y_{n+1}, y^h(\phi(t_{n+1})), z^h(\phi(t_{n+1}))), \end{cases} \qquad n = 0, 1, \ldots. \tag{2.12}$$

We call (2.11,2.12) the linear θ-method for the initial value problem (1.1,1.2).

3 Order of convergence

In this section we assume

(S_1) There is no vanishing delay in (1.1), namely, $\phi(t) < t$ for every $t \geq t_0$;

(S_2) The functions f, g and ϕ are sufficiently smooth;

(S_3) The exact solution (y, z) of (1.1,1.2) is sufficiently smooth except possibly at some grid points;

The first assumption implies that one can choose h_n small enough such that

$$\phi(t) \leq t_n - \frac{1}{2} \max_{t\in[t_0,T]} [t - \phi(t)], \qquad t \in (t_n, t_{n+1}].$$

Hence, the usual existence and uniqueness theory of the Runge–Kutta method for ordinary differential equations applies to the RKC method (2.9,2.10). For instance, if f is assumed to be Lipschitz continuous with respect to its second argument then (2.10) has a unique solution if h_n is sufficiently small.

A positive integer q is said to be the *uniform order* of the RKC method (2.9,2.10) if

$$|y^h(t) - y(t)| + |z^h(t) - z(t)| = \mathcal{O}(h^q), \qquad t \in [t_0, T],$$

where (y, z) is the solution of (1.1,1.2) and (y^h, z^h) is the corresponding numerical solution. We recall that the *uniform order* of the continuous Runge–Kutta method defined by (2.2,2.3) is $m \in \mathbb{N}$ if

$$y^h(t) - y(t) = \mathcal{O}(h_0^{m+1}), \qquad t \in [t_0, t_1],$$

where y is the solution of (2.1), y^h is the corresponding numerical solution.

Theorem 1 *If the uniform order of the continuous Runge–Kutta method defined by (2.2,2.3) is p^* then the uniform order of the RKC method (2.9,2.10) is* $\min\{p^*, s^*\}$.

Proof. We use the so called method-of-steps. Let $\xi_0 = t_0$ and define recursively

$$\xi_m = \max\{t_n \mid \phi(t) \leq \xi_{m-1} \text{ for every } t \leq t_n \leq T\}, \qquad m = 1, 2, \ldots.$$

The assumption (S_1) implies that there exists $M \in \mathbb{N}$ such that $\xi_M = T$. Assume that

$$|y^h(t) - y(t)| + |z^h(t) - z(t)| = \mathcal{O}\left(h^{\min\{p^*,s^*\}}\right), \qquad t \in [t_0, \xi_m]$$

for some $m < M$. Since the uniform order of the corresponding Runge-Kutta method is p^*, it is true that

$$|y^h(t) - y(t)| = \mathcal{O}\left(h^{\min\{p^*,s^*\}}\right), \qquad t \in [\xi_m, \xi_{m+1}].$$

Therefore,

$$|z(t_n + c_i^* h_n) - M_{n,i}| = \mathcal{O}\left(h^{\min\{p^*,s^*\}}\right), \qquad i = 1, \ldots, s^*, \quad t_n \in [\xi_m, \xi_{m+1}).$$

From the preceding estimate, we get

$$\begin{aligned} |z(t) - z^h(t)| &\leq \left| z(t) - \sum_{i=1}^{s^*} B_i((t - t_n)/h_n) z(t_n + c_i^* h_n) \right| \\ &\qquad + \sum_{i=1}^{s^*} |B_i((t - t_n)/h_n)| |z(t_n + c_i^* h_n) - M_{n,i}| \\ &= \mathcal{O}\left(h^{\min\{p^*,s^*\}}\right), \qquad t \in [t_n, t_{n+1}] \subset [\xi_m, \xi_{m+1}]. \end{aligned}$$

By induction, we conclude that the uniform order of the RKC method (2.9,2.10) is $\min\{p^*, s^*\}$. □

In the rest of this section we assume, in addition to (S_1)–(S_3), the following two assumptions:

(S_4) The delay function ϕ is strictly increasing and its inverse ψ is sufficiently smooth; and

(S_5) Each grid point is mapped into another one by the function ϕ.

A grid with the property (S_5) is called a constraint grid. In practice, it is impossible to use a constraint grid since the stepsizes are usually determined by various error control strategy. The purpose of using a constraint grid is to show that with some additional assumptions, order of approximation at grid points can be higher than the uniform order of approximation. To start, we recall that the continuous extension (2.3) is said to be a *NCE* of order p and degree d if the polynomials b_i, $i = 1, 2, \ldots, s$, are of degree $\leq d$ such that

$$\max_{t\in[t_0,t_1]} |y'(t) - (y^h)'(t)| = \mathcal{O}\big(h^d\big)\,, \tag{3.1}$$

$$\int_{t_0}^{t_1} G(t)\left[y'(t) - (y^h)'(t)\right]\,\mathrm{d}t = \mathcal{O}\Big(h_0^{p+1}\Big) \tag{3.2}$$

for every sufficiently smooth matrix function $G(t)$, where $p \in \mathbb{Z}^+$ is the order of the Runge–Kutta method. Some properties of a NCE method proved by Zennaro [23] include

$$\max_{t\in[t_0,t_1]} |y^{(k)}(t) - (y^h)^{(k)}(t)| = \mathcal{O}\big(h_0^{d+1-k}\big)\,, \tag{3.3}$$

$$\int_{t_0}^{t_1} G(t)\left[y(t) - y^h(t)\right]\,\mathrm{d}t = \mathcal{O}\Big(h_0^{p+1}\Big)\,, \tag{3.4}$$

$$[(p+1)/2] \leq d \leq \min\{\nu^*, p\}, \tag{3.5}$$

where $[(p+1)/2]$ denotes the integer part of $(p+1)/2$ and ν^* is the number of distinct values of c_i, $i = 1, 2, \ldots, s$. As a preliminary to our next result on the order of approximation of the RKC method at grid points we consider the following two initial value problems:

$$\begin{cases} u'(t) = f(t, u(t), y(\phi(t)), z(\phi(t))), \\ v(t) = g(t, u(t), y(\phi(t)), z(\phi(t))), \end{cases} \qquad t \in [t_n, t_{n+1}] \tag{3.6}$$

with the initial value condition

$$u(t_n) = u_n \tag{3.7}$$

and

$$\begin{cases} w'(t) = f(t, w(t), y^h(\phi(t)), z^h(\phi(t))), \\ x(t) = g(t, w(t), y^h(\phi(t)), z^h(\phi(t))), \end{cases} \qquad t \in [t_n, t_{n+1}] \tag{3.8}$$

with the initial value condition

$$w(t_n) = u_n, \tag{3.9}$$

where $n \in \mathbb{N}$ such that $\phi(t_n) = t_0$ and $\phi(t_{n+1}) = t_1$, y^h is an approximation to the function y with the properties (3.1–3.5), and z^h is the Lagrange interpolation of the function z:

$$z^h(t_0 + \tau h_0) = \sum_{i=1}^{s^*} B_i(\tau) z(t_0 + c_i^* h_0), \qquad \tau \in (0, 1].$$

In the sequel we assume that

$$\int_0^1 t^k \prod_{i=1}^{s^*} (t - c_i^*)\, \mathrm{d}t = 0, \qquad k = 0, 1, \ldots, k^* - 1 \tag{3.10}$$

for some $k^* \in \mathbb{Z}^+$.

Lemma 2 *Suppose that $s^* \geq d$. If (u, v) and (w, x) are smooth solutions of (3.6,3.7) and (3.8,3.9), respectively, then*

$$\max_{t \in [t_0, t_1]} |u^{(k)}(t) - w^{(k)}(t)| = \mathcal{O}\left(h_0^{\min\{d+1, s^*\} - k}\right) \tag{3.11}$$

$$\max_{t \in [t_0, t_1]} |v^{(k)}(t) - x^{(k)}(t)| = \mathcal{O}\left(h_0^{\min\{d+1, s^*\} - k}\right) \tag{3.12}$$

for $k = 0, 1, \ldots, d$ with all the higher derivatives of w and x remain uniformly bounded as $h_0 \to 0$, and

$$|u(t_{n+1}) - w(t_{n+1})| = \mathcal{O}\left(h_0^{\min\{p, s^* + k^*\} + 1}\right) \tag{3.13}$$

$$\int_{t_0}^{t_1} G(t) \left[u^{(k)}(t) - w^{(k)}(t)\right] \mathrm{d}t = \mathcal{O}\left(h_0^{\min\{p, s^* + k^*\} + 1}\right), \quad k = 0, 1 \tag{3.14}$$

$$\int_{t_0}^{t_1} G(t) \left[v(t) - x(t)\right] \mathrm{d}t = \mathcal{O}\left(h_0^{\min\{p, s^* + k^*\} + 1}\right) \tag{3.15}$$

for every sufficiently smooth matrix function $G(t)$. Moreover, if $1 \in \{c_i^*\}_{i=1}^{s^*}$ then

$$|v(t_{n+1}) - x(t_{n+1})| = \mathcal{O}\left(h_0^{\min\{p, s^* + k^*\} + 1}\right). \tag{3.16}$$

Proof. The estimates (3.11) and (3.14) can be proved in the same way as that of Theorem 10 of Zennaro [23]. The estimates (3.12) and (3.16) are obvious. To prove (3.15), we note that (3.10) implies that

$$\int_{t_0}^{t_1} G(t)[z(t) - z^h(t)]\, \mathrm{d}t = \mathcal{O}\left(h_0^{s^* + k^* + 1}\right)$$

for every sufficiently smooth matrix function $G(t)$. Therefore,

$$\begin{aligned} &\int_{t_n}^{t_{n+1}} G(t)[v(t) - x(t)]\, \mathrm{d}t \\ = &\int_{t_n}^{t_{n+1}} G(t) g_2(t, u(t), y(\phi(t)), z(\phi(t)))[u(t) - w(t)]\, \mathrm{d}t \end{aligned}$$

$$
\begin{aligned}
&+\int_{t_0}^{t_1} G(\psi(t))g_3(\psi(t),u(\psi(t)),y(t),z(t))\psi'(t)[y(t)-y^h(t)]\,\mathrm{d}t\\
&+\int_{t_0}^{t_1} G(\psi(t))g_4(\psi(t),u(\psi(t)),y(t),z(t))\psi'(t)[z(t)-z^h(t)]\,\mathrm{d}t\\
&+\mathcal{O}\left(h_0^{2\min\{d+1,s^*\}+1}\right),
\end{aligned}
$$

where g_2, g_3 and g_4 are derivatives of g with respect to its second, third and fourth arguments. Since $2d \geq p$ and $s^* \geq k^*$, the above estimate yields (3.15). □

Using Lemma 2 and by induction we obtain the following result:

Theorem 3 *Suppose that the continuous Runge–Kutta method in the RKC method (2.9,2.10) is a NCE of order* p *and degree* d*. If* $s^* \geq d$ *then*

$$|y_n - y(t_n)| = \mathcal{O}\left(h^{\min\{p,s^*+k^*\}}\right), \qquad t_n \in [t_0, T].$$

Moreover, if $1 \in \{c_i^*\}_{i=1}^{s^*}$ *then*

$$|z^h(t_n) - z(t_n)| = \mathcal{O}\left(h^{\min\{p,s^*+k^*\}}\right), \qquad t_n \in [t_0, T]. \tag{3.17}$$

If $1 \notin \{c_i^*\}_{i=1}^{s^*}$ then we can not expect to have the error estimate (3.17), due to the nature of the Lagrange interpolation (2.7). However, using the recurrence relation

$$z_n = g(t_n, y_n, y_m, z_m), \qquad n = 1, 2, \ldots,$$

where m depends on n in such a way that $\phi(t_n) = t_m$, we have the following analogue of (3.17):

$$|z_n - z(t_n)| = \mathcal{O}\left(h^{\min\{p,s^*+k^*\}}\right), \qquad t_n \in [t_0, T].$$

Therefore, the optimal order of approximation at grid points can still be achieved.

If the Runge–Kutta method defined by the Butcher tableau (2.2) is *non-confluent*, namely, $c_i \neq c_j$ if $i \neq j$, then a necessary condition for it to have an order $p \geq s$ is that

$$\int_0^1 t^k \prod_{i=1}^{s}(t - c_i)\,\mathrm{d}t = 0, \qquad k = 0, 1, \ldots, p - s - 1. \tag{3.18}$$

Comparing (3.10) with (3.18), a sensible choice of $\{c_i^*\}_{i=1}^{s^*}$ would be $\{c_i\}_{i=1}^{s}$.

4 Stability analysis

To study the stability of the RKC method (2.9,2.10) we use the following test model

$$\begin{cases} y'(t) + A_1 y(t) + A_2 y(t-r) + B_1 z(t-r) = 0, \\ z(t) + A_3 y(t) + A_4 y(t-r) + B_2 z(t-r) = 0, \end{cases} \qquad t \geq 0, \tag{4.1}$$

where $r > 0$, and the coefficient matrices $A_1, A_2 \in \mathbb{C}^{d_1 \times d_1}$, $A_3, A_4 \in \mathbb{C}^{d_2 \times d_1}$, $B_1 \in \mathbb{C}^{d_2 \times d_1}$, $B_2 \in \mathbb{C}^{d_2 \times d_2}$ are such that (4.1) is *stable globally* in the sense that the zero solution of (4.1) is asymptotically stable for every $r > 0$. Since (4.1) is a linear system with constant coefficients, the asymptotic stability of its zero solution is equivalent to that every solution of (4.1) tends to zero as $t \to \infty$.

In the sequel, $\sigma[C]$, $\rho(C)$ and $\alpha[C]$ for a matrix C designate the spectrum, spectral radius and maximal real parts of the eigenvalues of C, respectively. Other notation include

$$\mathbb{C}^+ = \{z \in \mathbb{C} \mid \operatorname{Re} z > 0\},\ \ \mathbb{C}^0 = \{z \in \mathbb{C} \mid \operatorname{Re} z = 0\},\ \ \mathbb{C}^- = \{z \in \mathbb{C} \mid \operatorname{Re} z < 0\},$$
$$D = \{z \in \mathbb{C} \mid |z| < 1\}, \quad \Gamma = \{z \in \mathbb{C} \mid |z| = 1\}.$$

The characteristic function of (4.1) is $P(z, \mathrm{e}^{-rz})$ with the function P defined by

$$P(z,\xi) = \begin{vmatrix} zI_{d_1} + A_1 + A_2\xi & B_1\xi \\ A_3 + A_4\xi & I_{d_2} + B_2\xi \end{vmatrix}.$$

Since (4.1) is stable globally, it can be shown that the following (sufficient and necessary) conditions hold:

(H_1) $\rho(B_2) < 1$,

(H_2) $P(z,\xi) \neq 0$ for all $z \in \mathbb{C}^0\backslash\{0\}$ and $\xi \in \Gamma$,

(H_3) $\alpha(B_1(I_{d_2} + B_2)^{-1}(A_3 + A_4) - A_1 - A_2) < 0$.

Moreover, the following are also true:

(H_4) $\alpha[A_1] < 0$,

(H_5) $P(z,\xi) \neq 0$ for all $z \in \mathbb{C}^0$ and $\xi \in D$,

(H_6) $P(z,\xi) \neq 0$ for all $z \in \mathbb{C}^+$ and $\xi \in D \cup \Gamma$.

To prove the above statement we note that the characteristic function of the system of neutral functional differential equations

$$\begin{cases} y'(t) + A_1 y(t) + A_2 y(t-r) + B_1 z(t-r) = 0, \\ z'(t) + A_3 y'(t) + A_4 y'(t-r) + B_2 z'(t-r) = 0, \end{cases} \qquad t \geq 0 \tag{4.2}$$

is $zP(z, \mathrm{e}^{-rz})$. Therefore, the general theory of Hale, Infante and Tsen [9] can be applied to (4.2) to obtain (H_1)–(H_5). To prove (H_6) by contradiction. we assume that there exist $z_0 \in \mathbb{C}^+$ and $\xi_0 \in D \cup \Gamma$ such that $P(z_0, \xi_0) = 0$. Let

$$\omega(t) = \max\{\operatorname{Re} z \mid P(z, t\xi_0) = 0\}.$$

We have $\omega(0) = \alpha[A_0] < 0$ and $\omega(1) \geq \operatorname{Re} z_0 > 0$. Hence, there exists $t_0 \in (0,1)$ such that $\omega(t_0) = 0$, which contradicts (H_5).

Having specified the test equation we now describe the RKC method whose stability we intend to analyse:

1. The s-stage Runge–Kutta method defined by the Butcher tableau (2.2) is nonconfluent and its continuous extension (2.3) is *natural* in the sense that

$$b_i(c_j) = a_{ji}, \qquad i, j = 1, 2, \dots, s; \tag{4.3}$$

and

2. The set of collocation points of the collocation method for (2.6) in the interval $[t_n, t_{n+1}]$ include $\{t_n + c_i h, i = 1, \dots, s\}$ as a subset and may also include t_n and/or t_{n+1}, but no other points.

The following result provides a criterion on whether a Runge–Kutta method can have a continuous extension that is natural.

Proposition 4 *The Runge–Kutta method defined by (2.2) has a continuous extension that is natural if and only if*

$$c_k = c_l, \;\; 0 \le k, l \le s+1 \Longrightarrow a_{kj} = a_{lj}, j = 1, 2, \dots, s, \tag{4.4}$$

where $c_0 = 0$, $c_{s+1} = 1$, $a_{0,j} = 0$, *and* $a_{s+1,i} = b_i$ *for* $i = 1, 2, \dots$.

Under the condition (4.4), one can easily construct a continuous extension that is natural by choosing b_i as a polynomial interpolation of

$$(c_j, a_{ji}), \qquad j = 0, 1, \dots, s+1.$$

For instance, if $c_i \neq c_j$ for every $i \neq j$ then one can choose

$$b_i(\tau) = \sum_{j=0}^{s+1} \left(\prod_{k=0, k\neq j}^{s+1} \frac{\tau - c_l}{c_j - c_k} \right) a_{ji}.$$

Besides the collocation method [7, p. 211], Heun method [7, p. 135], SDIRK (of order 3) [7, p. 207] and SDIRK (of order 4) [8, p. 106] have natural continuous extensions as well.

In Zennaro [24], the continuous extension (2.3) of the Runge–Kutta method defined by (2.2) is called natural if it is a NCE and satisfies (4.3). An interested result in [24] is that if the Runge–Kutta defined by (2.2) is nonconfluent and it has a natural continuous extension (in Zennaro's definition) then it is equivalent to a projection method in some polynomial space.

4.1 Stability on a constraint uniform grid

The subdivision $0 = t_0 < t_1 < t_2 < \dots$ of $[0, \infty)$ is said to be a constraint uniform grid if $t_n = nh$ for $n \ge 0$, where $h = r/k$ for some positive integer k is the stepsize. Without lose of generality, we assume that $c_i^* = c_i$ for $i = 1, \dots, s$. The RKC method (2.9,2.10), upon applying to (4.1), gives the continuous numerical solution

$$\begin{cases} y^h(t_n + \tau h) = y_n + h_n \sum_{i=1}^{s} b_i(\tau) K_{n,i}, \\ z^h(t_n + \tau h) = \sum_{i=1}^{s^*} B_i(\tau) M_{n,i}, \end{cases} \qquad 0 < \tau \le 1, \; n = 0, 1, \dots, \tag{4.5}$$

where $(K_{n,i}, M_{n,i})$, $i = 1, \ldots, s$, are defined by the recurrence relations

$$\begin{cases} K_{n,i} + A_1(y_n + h\sum_{j=1}^{s} a_{ij}K_{n,j}) + A_2(y_{n-k} + h\sum_{j=1}^{s} a_{ij}m_{n-k,j}) \\ \qquad\qquad\qquad\qquad\qquad\qquad +B_1M_{n-k,i} = 0, \\ M_{n,i} + A_3(y_n + h\sum_{j=1}^{s} a_{ij}K_{n,j}) + A_4(y_{n-k} + h\sum_{j=1}^{s} a_{ij}K_{n-k,j}) \\ \qquad\qquad\qquad\qquad\qquad\qquad +B_2M_{n-k,i} = 0, \end{cases}$$
$$i = 1, 2, \ldots, s.$$

In the case $s^* > s$,

$$K_{n,i} = \begin{cases} z_n, & \text{if } c_i^* = 0, \\ z_{n+1}, & \text{if } c_i^* = 1, \end{cases} \qquad i = s+1, \ldots, s^*,$$

where $z_0 = z(t_0)$, z_n is our approximation to $z(t_n)$, $n = 1, \ldots$, and it satisfies the recurrence relation

$$z_n = -\left(A_3y_n + A_4y_{n-k} + B_2z_{n-k}\right), \qquad n = 1, 2, \ldots. \tag{4.6}$$

Theorem 5 *If the corresponding Runge–Kutta method is A-stable then the numerical solution (4.5) tends to zero uniformly in τ as $n \to \infty$ whenever $k \geq 1$.*

Proof. Let

$$X_n = (y_{n+1}^{\mathrm{T}}, K_{n,1}^{\mathrm{T}}, \ldots, K_{n,s}^{\mathrm{T}}, M_{n,1}^{\mathrm{T}}, \ldots, M_{n,s}^{\mathrm{T}})^{\mathrm{T}}.$$

Then X_n, $n = 0, 1, \ldots$, satisfy the following system of difference equations

$$L_0X_n + L_1X_{n-1} + L_2X_{n-k} + L_3X_{n-1-k} = 0, \qquad n = 0, 1, \ldots, \tag{4.7}$$

where

$$L_0 = \begin{pmatrix} I_{d_1} & -hb^T \otimes I_{d_1} & 0 \\ 0 & I_{sd_1} + hA \otimes A_1 & 0 \\ 0 & hA \otimes A_3 & I_{sd_2} \end{pmatrix}, \qquad L_1 = \begin{pmatrix} -I_{d_1} & 0 & 0 \\ e_{d_1} \otimes A_1 & 0 & 0 \\ e_{d_2} \otimes A_3 & 0 & 0 \end{pmatrix},$$

$$L_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & hA \otimes A_2 & I_s \otimes B_1 \\ 0 & hA \otimes A_4 & I_s \otimes B_2 \end{pmatrix}, \qquad L_3 = \begin{pmatrix} 0 & 0 & 0 \\ e_{d_1} \otimes A_2 & 0 & 0 \\ e_{d_2} \otimes A_4 & 0 & 0 \end{pmatrix},$$

where the symbols $\otimes$ denotes the Kronecker product, I_d is the $d \times d$ identity matrix, and $e_d = (1, 1, \ldots, 1)^T$.

We recall that the Runge–Kutta method defined by (2.2) is A-stable if and only if

$$|R(z)| < 1, \qquad \mathrm{Re}\, z > 0,$$

where

$$R(z) = 1 - zb^T(I_s + zA)^{-1}e_s.$$

Clearly, A-stability implies that $\alpha(A) \geq 0$. It follows from the (H_4) that the matrix $I_{sd_1} + hA \otimes A_1$ is nonsingular since

$$|I_{sd_1} + hA \otimes A_1| = \prod_{\mu \in \sigma[A]} |1 + \mu hA_1|.$$

Therefore, given the initial data $X_{-1}, X_{-2}, \ldots, X_{-k-1}$, the system (4.7) has a unique solution.

The characteristic polynomial of (4.7) is

$$|z^{k+1}L_0 + z^k L_1 + zL_2 + L_3| = z^{kd_1+(k+1)(d_1+d_2)s}P^*(z),$$

where

$$P^*(z) = \begin{vmatrix} (z-1)I_{d_1} & -hb^T \otimes I_{d_1} & 0 \\ e_{d_1} \otimes (A_1 + z^{-k}A_2) & I_{sd_1} + hA \otimes (A_1 + z^{-k}A_2) & z^{-k}I_s \otimes B_1 \\ e_{d_1} \otimes (A_3 + z^{-k}A_4) & hA \otimes (A_3 + z^{-k}A_4) & I_{sd_2} + z^{-k}I_s \otimes B_2 \end{vmatrix}.$$

First, we prove by contradiction that the characteristic equation $P^*(z) = 0$ has no solution outside the open unit disc D. Suppose that there exists λ such that $P^*(\lambda) = 0$ and $|\lambda| \geq 1$. Let

$$D_1 = A_1 + \lambda^{-k}A_2, \quad D_2 = \lambda^{-k}B_1, \quad D_3 = A_3 + \lambda^{-k}A_4, \quad D_4 = \lambda^{-k}B_2$$

and

$$W = \begin{pmatrix} I_{sd_1} + hA \otimes D_1 & I_s \otimes D_2 \\ hA \otimes D_3 & I_{sd_2} + I_s \otimes D_4 \end{pmatrix}.$$

Since

$$|W| = \prod_{\mu \in \sigma[A]} \begin{vmatrix} I_{d_1} + \mu hD_1 & D_2 \\ \mu hD_3 & I_{d_2} + D_4 \end{vmatrix},$$

the condition (H_6) implies that the matrix W is nonsingular. Let

$$D_5 = D_1 - D_2(I_{d_2} + D_4)^{-1}D_3.$$

Since

$$\begin{aligned}
& P^*(\lambda) \\
= \;& |W| \cdot \left| (\lambda - 1)I_{d_1} - h(b^T \otimes I_{d_1}, 0)W^{-1} \begin{pmatrix} e_{d_1} \otimes D_1 \\ e_{d_2} \otimes D_3 \end{pmatrix} \right| \\
= \;& |W| \cdot |(\lambda - 1)I_{d_1} - h(b^T \otimes I_{d_1})(I_{sd_1} + hA \otimes D_1 - h(I_s \otimes D_2)(I_{sd_2} + I_s \otimes D_4)^{-1} \\
& \cdot (A \otimes D_3))^{-1}(e_{d_1} \otimes D_1 - (I_s \otimes D_2)(I_{sd_2} + I_s \otimes D_4)^{-1}(e_{d_2} \otimes D_3))| \\
= \;& |W| \cdot |\lambda I_{d_1} - I_{d_1} - h(b^T \otimes I_{d_1})(I_{sd_1} + hA \otimes D_5)^{-1}(e_{d_1} \otimes D_5)| \\
= \;& |W| \prod_{\mu \in \sigma[D_5]} (\lambda - R(h\mu)) \\
= \;& 0,
\end{aligned}$$

there exists at least one $\mu_0 \in \sigma[D_5]$ such that $\lambda = R(h\mu_0)$. Since

$$P(-\mu_0, \lambda^{-k}) = |I_{d_2} + D_4| \cdot | - \mu_0 I_{d_1} + D_5| = 0,$$

it follows from (H_6) that either $\operatorname{Re}\mu_0 > 0$ or $\operatorname{Re}\mu_0 = 0$. If $\operatorname{Re}\mu_0 > 0$ we have $|\lambda| = |R(h\mu_0)| < 1$ which contradicts our assumption that $|\lambda| \geq 1$. If $\operatorname{Re}\mu_0 = 0$ then $|\lambda| = |R(h\mu_0)| = 1$. According to (H_2), it must be $\mu_0 = 0$. Therefore, $\lambda = R(h\mu_0) = 1$. Since $\lambda = 1$ implies that $D_5 = A_1 + A_2 - B_1(I_{d_2} + B_2)^{-1}(A_3 + A_4)$, therefore, $\mu_0 = 0 \in \sigma[D_5]$ contradicts (H_3).

The fact that the characteristic polynomial of (4.7) has no solution outside the open unit disc implies that the solution X_n of (4.7) tends to zero as n tends to infinity. If $s^* = s$ then it is obvious that Theorem 5 holds. If $s^* > s$, it follows from (4.6) that $K_{n,i}$ tends to zero as n tends to infinity for every $i > s$, because of the condition (H_1). Hence, Theorem 5 still holds. $\square$

4.2 Stability on a uniform grid

In this subsection we consider the stability of the linear θ-method (2.11,2.12) on a uniform grid, i.e., $t_n = nh$, $n = 0, 1, \ldots$, for some $h > 0$. Let $k := \lceil r/h \rceil \geq 1$ and $\delta = k - r/h \in [0, 1)$. The linear θ-method, upon applying to (4.1), gives the continuous numerical solution

$$\begin{cases} y^h(t_n + \tau h) = (1-\tau)y_n + \tau y_{n+1}, \\ z^h(t_n + \tau h) = (1-\tau)z_n + \tau z_{n+1}, \end{cases} \qquad \tau \in [0,1],\ n = 0, 1, \ldots, \tag{4.8}$$

where (y_n, z_n), $n = 0, 1, \ldots$, satisfy the recurrence relations

$$\begin{aligned} y_{n+1} - y_n + h\{&(1-\theta)(A_1 y_n + A_2((1-\delta)y_{n-k} + \delta y_{n-k+1}) \\ &+ B_1((1-\delta)z_{n-k} + \delta z_{n-k+1})) \\ &+ \theta(A_1 y_{n+1} + A_2((1-\delta)y_{n-k+1} + \delta y_{n-k+2}) \\ &+ B_1((1-\delta)z_{n-k+1} + \delta z_{n-k+2}))\} = 0, \end{aligned} \tag{4.9}$$

$$\begin{aligned} z_n + A_3 y_n + A_4(&(1-\delta)y_{n-k} + \delta y_{n-k+1}) \\ &+ B_2((1-\delta)z_{n-k} + \delta z_{n-k+1}) = 0. \end{aligned} \tag{4.10}$$

The linear θ-method (2.4,2.5) for the initial value problem (2.1) is A-stable if and only if $\theta \geq 1/2$. Correspondingly, we have the following result.

Theorem 6 *If $\theta \geq 1/2$ then the numerical solution (4.8) tends to zero uniformly in τ as $n \to \infty$ whenever $h > 0$.*

Proof. Let $X_n = (y_n, z_n)^T$. Then (4.9,4.10) can be written as

$$L_0 X_{n+1} + L_1 X_n + L_2 X_{n-k+2} + L_3 X_{n-k-1} + L_4 X_{n-k} = 0, \qquad n = 0, 1, \ldots, \tag{4.11}$$

where

$$L_0 = \begin{pmatrix} I_{d_1} + \theta h A_1 & 0 \\ A_3 & I_{d_2} \end{pmatrix}, \qquad L_1 = \begin{pmatrix} -I_{d_1} + (1-\theta)hA_1 & 0 \\ 0 & 0 \end{pmatrix},$$

$$L_2 = \begin{pmatrix} \theta\delta h A_2 & \theta\delta h B_1 \\ \delta A_4 & \delta B_2 \end{pmatrix},$$

$$L_3 = \begin{pmatrix} ((1-\theta)\delta + \theta(1-\delta)hA_2 & ((1-\theta)\delta + \theta(1-\delta)hb_1 \\ (1-\delta)A_4 & (1-\delta)B_2 \end{pmatrix},$$

$$L_4 = \begin{pmatrix} (1-\theta)(1-\delta)hA_2 & (1-\theta)(1-\delta)hB_1 \\ 0 & 0 \end{pmatrix}.$$

Because of (H_4) the system (4.11) has a unique solution. The characteristic polynomial of (4.11) is

$$|z^{k+1}L_0 + z^k L_1 + z^2 L_2 + zL_3 + L_4| = z^{(k+1)(d_1+d_2)s} P^*(z),$$

where

$$P^*(z) = \begin{vmatrix} (1-z^{-1})I_{d_1} + p(z)hA_1 + p(z)q(z)hA_2 & p(z)q(z)hB_1 \\ A_3 + q(z)A_4 & I_{d_2} + q(z)B_2 \end{vmatrix}$$

with

$$p(z) = \theta + (1-\theta)z^{-1}, \qquad q(z) = (\delta + (1-\delta)z^{-1})z^{-k+1}.$$

Hence, we need only to prove that the characteristic equation $P^*(z) = 0$ has no solution outside the open unit disc. This can be proved by contradiction. Suppose that there exists a solution λ such that $P^*(\lambda) = 0$ and $|\lambda| \geq 1$. We claim that $p(\lambda) \neq 0$. Otherwise, $P^*(\lambda) = 0$ implies that $\lambda = 1$ which in turn implies that $p(\lambda) = 1$. Therefore, $p(\lambda) \neq 0$ and

$$\begin{aligned} P^*(\lambda) &= (p(\lambda)h)^{d_1} |I_{d_2} + B_2 q(\lambda)| \\ &\quad \cdot \left| \frac{1-\lambda^{-1}}{p(\lambda)h} I_{d_1} + A_1 + A_2 q(\lambda)(I_{d_2} + B_2 q(\lambda))^{-1}(A_3 + A_4 q(\lambda)) \right| = 0. \end{aligned}$$

We note that either $|q(\lambda)| = 1$ or $|q(\lambda)| < 1$. If $|q(\lambda)| = 1$ then $\delta = 0$. This is the case we have considered in Theorem 5. If $|q(\lambda)| < 1$ then we can see from (H_5) and (H_6) that either $\lambda = 1$ or $\mathrm{Re}\,((1-\lambda^{-1})/p(\lambda)) < 0$. If $\lambda = 1$ then $P^*(1) = 0$ which contradicts (H_3). If $\lambda \neq 1$ then $\mathrm{Re}\,((1-\lambda^{-1})/p(\lambda)) < 0$ which contradicts our assumptions that $|\lambda| \geq 1$ and $\theta \geq 1/2$. Hence, Theorem 6 holds. □

It should be noted that Theorem 5 does not hold in the case of uniform mesh if the corresponding Runge–Kutta method is nonconfluent, $c_i < 1$ for $i = 1, \ldots, s$, and

$$b_i(\tau) = \int_0^\tau \prod_{k=1,k\neq i}^{s} \frac{t - c_k}{c_i - c_k}\, \mathrm{d}t, \qquad i = 1, \ldots, s.$$

This is essentially a direct consequence of a result of in't Hout [14] where the test equation is a linear functional differential equation of retarded type.

There are many practical issues we have not addressed in this paper, in particular, how to choose the collocation points c_i^*, $i = 1, \ldots, s^*$. Because of Theorem 3, a sensible choice of $\{c_i^*\}_{i=1}^{s^*}$ would be $\{c_i\}_{i=1}^{s}$, provided that the corresponding Runge–Kutta method is nonconfluent. However, if the corresponding Runge–Kutta method is confluent, are extra collocation points needed in order to have a reasonably high order of uniform approximation? Theorem 1 may have provided a good indication as to the appropriate number of collocation points. Another question is whether $\{0,1\}$ should be included in the set $\{c_i^*\}_{i=1}^{s^*}$ or not. In other words, how necessary is it to have the continuity of $z^h(t)$ at the grid points? As to system (1.3), we know that it can be reduced to the form (1.1). However, it may be better to solve (1.3) directly. This is also relevant to functional-differential equations of neutral type since the implicit neutral equation (1.6) is equivalent to

$$\begin{cases} y'(t) = f(t, z(t), z(\phi(t))) \\ z(t) = y(t) + g(t, z(\phi(t))) \end{cases}$$

which is a special case of (1.3). We hope to answer these questions with numerical examples in a forthcoming paper.

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