Applied Numerical Mathematics 120 (2017) 165–175

Contents lists available at ScienceDirect

Applied Numerical Mathematics

www.elsevier.com/locate/apnum

Starting procedures for general linear methods

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ARTICLE INFO

Article history:
Received 16 March 2017
Accepted 17 May 2017

Keywords:
General linear methods
Order conditions
Starting procedures
Generalized Runge–Kutta methods

ABSTRACT

We present a systematic approach to the construction of starting procedures for general linear methods (GLMs) of order p and stage order $q = p$. Order conditions for starting procedures based on the generalized Runge–Kutta (RK) are derived using the theory of rooted trees, elementary differentials, and elementary weights, and examples of generalized RK formulas are given up to the order $p = 4$.

1. Introduction

Consider the initial-value problem for systems of ordinary differential equations (ODEs)

$$\begin{cases} y'(t) = f\big(y(t)\big), & t \in [t_0, T], \\ y(t_0) = y_0 \in \mathbb{R}^m, \end{cases} \tag{1.1}$$

where the function $f : \mathbb{R}^m \to \mathbb{R}^m$ is sufficiently smooth. For the numerical solution of this problem we consider a large class of GLMs introduced by Burrage and Butcher [1] and further investigated in [2–5,12,13,6–10,16,20,21]. On the uniform grid $\{t_n\}_{n=0}^N$,

$$t_n = t_0 + nh, \quad n = 0, 1, \ldots, N, \quad Nh = T - t_0,$$

these methods are defined by

$$\begin{cases} Y_i^{[n]} = h \displaystyle\sum_{j=1}^{s} a_{ij} f\big(Y_j^{[n]}\big) + \sum_{j=1}^{r} u_{ij} y_j^{[n-1]}, & i = 1, 2, \ldots, s, \\ y_i^{[n]} = h \displaystyle\sum_{j=1}^{s} b_{ij} f\big(Y_j^{[n]}\big) + \sum_{j=1}^{r} v_{ij} y_j^{[n-1]}, & i = 1, 2, \ldots, r, \end{cases} \tag{1.2}$$

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[1] The work of this author was supported by grant from University of Salerno.
[2] The work of this author was partially supported by INdAM-GNCS.

http://dx.doi.org/10.1016/j.apnum.2017.05.009

$n = 1, 2, \dots, N$. Here, the internal approximations or stages $Y_i^{[n]}$ satisfy

$$Y_i^{[n]} = y(t_{n-1} + c_i h) + O(h^{q+1}), \quad i = 1, 2, \dots, s, \tag{1.3}$$

and the external approximations $y_i^{[n]}$, which propagate from step to step, satisfy

$$y_i^{[n]} = \sum_{k=0}^{p} q_{ik} h^k y^{(k)}(t_n) + O(h^{p+1}), \quad i = 1, 2, \dots, r, \tag{1.4}$$

for some real parameters q_{ik}, $i = 1, 2, \dots, r$, $k = 0, 1, \dots, p$. Put

$$\mathbf{q}_k = \begin{bmatrix} q_{1,k} & q_{2,k} & \cdots & q_{r,k} \end{bmatrix}^T \in \mathbb{R}^r, \quad k = 0, 1, \dots, p.$$

The GLMs (1.2) are characterized by the abscissa vector $\mathbf{c} = [c_1, \dots, c_s]^T \in \mathbb{R}^s$, the coefficient matrices

$$\mathbf{A} = [a_{ij}] \in \mathbb{R}^{s\times s}, \quad \mathbf{U} = [u_{ij}] \in \mathbb{R}^{s\times r}, \quad \mathbf{B} = [b_{ij}] \in \mathbb{R}^{r\times s}, \quad \mathbf{V} = [v_{ij}] \in \mathbb{R}^{r\times r},$$

the vectors $\mathbf{q}_k$, $k = 0, 1, \dots, p$, appearing in (1.4), and four integers: the order of the method p, the stage order q, the number of external approximations r, and the number of internal approximations or stages s.

Introducing the notation

$$Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix}, \quad f\left(Y^{[n]}\right) = \begin{bmatrix} f\left(Y_1^{[n]}\right) \\ \vdots \\ f\left(Y_s^{[n]}\right) \end{bmatrix}, \quad y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix},$$

the GLM (1.2) can be written in a more compact vector form

$$\begin{cases} Y^{[n]} = h(\mathbf{A} \otimes \mathbf{I}) f\left(Y^{[n]}\right) + (\mathbf{U} \otimes \mathbf{I}) y^{[n-1]}, \\ y^{[n]} = h(\mathbf{B} \otimes \mathbf{I}) f\left(Y^{[n]}\right) + (\mathbf{V} \otimes \mathbf{I}) y^{[n-1]}, \end{cases} \tag{1.5}$$

$n = 1, 2, \dots, N$, where $\mathbf{I}$ is the identity matrix of dimension m, and the relations (1.3) and (1.4) can be rewritten as

$$Y^{[n]} = y(t_{n-1} + \mathbf{c}h) + O(h^{q+1}), \tag{1.6}$$

$$y^{[n]} = \sum_{k=0}^{p} (\mathbf{q}_k \otimes \mathbf{I}) h^k y^{(k)}(t_n) + O(h^{p+1}). \tag{1.7}$$

Here, $y(t_{n-1} + \mathbf{c}h)$ is defined by

$$y(t_{n-1} + \mathbf{c}h) = \begin{bmatrix} y(t_{n-1} + c_1 h) \\ \vdots \\ y(t_{n-1} + c_s h) \end{bmatrix} \in \mathbb{R}^{sm}.$$

In what follows we will be interested in GLMs (1.5) which have order p and stage order $q = p$ with respect to the starting procedure

$$y^{[0]} = \sum_{k=0}^{p} (\mathbf{q}_k \otimes \mathbf{I}) h^k y^{(k)}(t_0) + O(h^{p+1}). \tag{1.8}$$

It was proved by Butcher [3] (see also [21]) that this is a case if and only if

$$e^{\mathbf{c}z} = z\mathbf{A}e^{\mathbf{c}z} + \mathbf{U}\mathbf{w}(z) + O(z^{p+1}), \tag{1.9}$$

and

$$e^{z}\mathbf{w}(z) = z\mathbf{B}e^{\mathbf{c}z} + \mathbf{V}\mathbf{w}(z) + O(z^{p+1}), \tag{1.10}$$

where

$$\mathbf{w}(z) := s\sum_{k=0}^{p} \mathbf{q}_k z^k, \quad e^{\mathbf{c}z} := \begin{bmatrix} e^{c_1 z} & e^{c_2 z} & \dots & e^{c_s z} \end{bmatrix}^T.$$