ORDER CONDITIONS FOR GENERAL TWO-STEP RUNGE-KUTTA METHODS

ERNST HAIRER† AND GERHARD WANNER†

Abstract. The use of B-series for the derivation of order conditions for general two-step Runge-Kutta methods is illustrated.

Key words. two-step Runge-Kutta methods, general linear methods, order conditions, B-series

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1. Introduction. Recently, Jackiewicz and Tracogna [3] introduced the interesting class of two-step Runge-Kutta methods

$$
\begin{aligned}
y_{n+1} &= \theta y_{n-1} + (1-\theta) y_n + h \sum_{i=1}^{s} \Big(v_i f(Y_{n-1}^i) + w_i f(Y_n^i) \Big) \\
Y_n^i &= \alpha_i y_{n-1} + (1-\alpha_i) y_n + h \sum_{j=1}^{s} \Big(a_{ij} f(Y_{n-1}^j) + b_{ij} f(Y_n^j) \Big)
\end{aligned} \tag{1}
$$

for the numerical solution of $y' = f(y)$. After experiencing difficulties applying the approaches of [1] and [2], they turned to an approach due to Albrecht to derive order conditions for the method. In this note we show how to apply the theory of B-series (see [1], Sect. 432, or [2], Sects. II.11 and III.8) to obtain a much shorter derivation of the equations of condition. The approach also makes clear how the starting values must be determined. Although we consider here only the case of constant step size, it is straightforward to deal with nonuniform meshes.

2. Formulation as General Linear Method. In addition to an initial value y_0, approximations y_1 and $Y_0^1, \ldots, Y_0^s$ are needed to start the integration. Introducing the vector $u_n := (y_{n+1}, y_n, Y_n^1, \ldots, Y_n^s)^T$, the method can be written in the form

$$
\begin{aligned}
u_0 &= \varphi(h) \\
u_{n+1} &= S u_n + h \Phi(u_n, h).
\end{aligned} \tag{2}
$$

Here $\varphi(h)$ specifies the "starting procedure", the matrix S is given by

$$
S = \begin{pmatrix} 1-\theta & \theta & 0 \\ 1 & 0 & 0 \\ \mathbb{1} - a & a & 0 \end{pmatrix}, \qquad \mathbb{1} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}, \qquad a = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_s \end{pmatrix}, \tag{3}
$$

and the increment function $\Phi(u, h)$ is implicitly defined by (1). We further consider the "correct value function"

$$
z(x,h) = \Big(y(x+h), y(x), B\big(\Phi_1, y(x)\big), \ldots, B\big(\Phi_s, y(x)\big) \Big)^T, \tag{4}
$$

† Dept. de mathématiques, Université de Genève, CH-1211 Genève 24, Switzerland (Ernst.Hairer@math.unige.ch, Gerhard.Wanner@math.unige.ch)

which specifies the quantities which the vector u should approximate, as an arbitrary B-series

$$B(\Phi_i, y) = y + h\Phi_i(\bullet)f(y) + \frac{h^2}{2!}\Phi_i([\bullet])f'(y)f(y) + \dots\ .$$

Using this formulation, the results of [2], Sect. III.8, can be applied directly.

The method (2) is *stable* (Def. III.8.8 of [2]) if $-1 < \theta \le 1$. This will be assumed throughout this note.

For the study of the order conditions, the matrix

$$E = (1+\theta)^{-1}\begin{pmatrix}1\\1\\\mathbb{1}\end{pmatrix}\bigl(1, \theta, 0, \dots, 0\bigr), \tag{5}$$

which for $|\theta| < 1$ is equal to $\lim_{n\to\infty} S^n$, plays an important role.

3. Order Conditions. With $z_n := z(x_n, h)$ the *local error* of the method (2) is defined by $d_0 := z_0 - \varphi(h)$ and

$$d_{n+1} = z_{n+1} - Sz_n - h\Phi(z_n, h).$$

The method is of order p (see Def. III.8.10 and Lemma III.8.11 of [2]) if

$$d_n = \mathcal{O}(h^p) \qquad \text{and} \qquad Ed_{n+1} = \mathcal{O}(h^{p+1}) \tag{6}$$

for all $n \ge 0$ satisfying $nh \le Const.$ This condition can be checked by investigating the defect of (1) when the quantities $y_{n+1}, y_n, y_{n-1}, Y_n^i, Y_{n-1}^i$ are replaced by $y(x+h), y(x), y(x-h), B\bigl(\Phi_i, y(x)\bigr), B\bigl(\Phi_i, y(x-h)\bigr)$, respectively. Observe that

$$y(x+h) = B\bigl(e, y(x)\bigr), \qquad y(x-h) = B\bigl(e^{-1}, y(x)\bigr)$$

are B-series with $e(t) = 1$ and $e^{-1}(t) = (-1)^{\rho(t)}$ for all $t \in T$ and that the composition of B-series is again a B-series (see Sect. II.11 of [2]; Sect. II.12 of the second edition)

$$B\bigl(\Phi_i, y(x-h)\bigr) = B\bigl(\Phi_i, B\bigl(e^{-1}, y(x)\bigr)\bigr) = B\bigl(e^{-1}\Phi_i, y(x)\bigr).$$

The expression $(e^{-1}\Phi_i)(t)$ is given by (c.f. Def. II.11.4 and Formula (III.8.30) of [2])

$$(e^{-1}\Phi_i)(t) = \sum_{j=0}^{\rho(t)} \binom{\rho(t)}{j} \frac{(-1)^{\rho(t)-j}}{\alpha(t)} \sum_{all\ labellings} \Phi_i\bigl(s_j(t)\bigr).$$

THEOREM 3.1. *If the starting procedure satisfies $\varphi(h) - z(x_0, h) = \mathcal{O}(h^p)$, the method (1) is convergent of order p if, and only if,*

$$1 \;=\; \theta(-1)^{\rho(t)} + \sum_{i=1}^{s}\Bigl(v_i(e^{-1}\Phi_i)'(t) + w_i\Phi_i'(t)\Bigr) \qquad \textit{for}\ \ \rho(t) \le p \tag{7}$$

$$\Phi_i(t) \;=\; \alpha_i(-1)^{\rho(t)} + \sum_{j=1}^{s}\Bigl(a_{ij}(e^{-1}\Phi_j)'(t) + b_{ij}\Phi_j'(t)\Bigr) \qquad \textit{for}\ \ \rho(t) \le p-1 \tag{8}$$

(for the definition of $\Phi_i'(t)$ and $(e^{-1}\Phi_i)'(t)$ see Corollary II.11.7 of [2]).

Proof. Conditions (7) and (8) are equivalent to the fact that the defects of the first and second relations of (1) are of size $\mathcal{O}(h^{p+1})$ and $\mathcal{O}(h^p)$, respectively. This proves (6) by use of the Implicit Function Theorem. The statement then follows from Lemma III.8.11 and Theorem III.8.13 of [2]. □

The relations (8) can be considered as a definition of $\Phi_i(t)$ for $t \in T$, whereas the equations (7) constitute the *order conditions* for the method (1). They are equivalent to those obtained in [3].

Because the starting values Y_0^i have to be $\mathcal{O}(h^p)$ approximations to $B(\Phi_i, y_0)$ for the method to be of order p, they must be computed by some numerical method, e.g., a Runge-Kutta method, which realizes the corresponding B-series $B(\Phi_i, y_0)$ up to this order.

4. Order Conditions for a Special Situation. Both the starting procedures and the order conditions simplify considerably when

$$\Phi_i(t) = c_i^{\rho(t)} \qquad \text{for} \quad \rho(t) \le p-1, \tag{9}$$

Such a method has stage order $p-1$, meaning that $B\big(\Phi_i, y(x)\big) = y(x+c_ih) + \mathcal{O}(h^p)$. It follows from (9) and $B\big(e^{-1}\Phi_i, y(x)\big) = B\big(\Phi_i, y(x-h)\big) = y\big(x+(c_i-1)h\big) + \mathcal{O}(h^p)$ that

$$(e^{-1}\Phi_i)(t) = (c_i-1)^{\rho(t)} \qquad \text{for} \quad \rho(t) \le p-1$$

and $\Phi_i'(t) = \rho(t)c_i^{\rho(t)-1}$, so that the relations (8) become

$$c_i^q = \alpha_i(-1)^q + q\sum_{j=1}^{s}\Big(a_{ij}(c_j-1)^{q-1} + b_{ij}c_j^{q-1}\Big) \qquad \text{for} \quad q = 1,\ldots,p-1.$$

These are linear equations for a_{ij}, b_{ij} that have to be satisfied by the coefficients of the method. If these relations are fulfilled, the order conditions (7) become simply

$$1 = \theta(-1)^q + q\sum_{i=1}^{s}\Big(v_i(c_i-1)^{q-1} + w_ic_i^{q-1}\Big) \qquad \text{for} \quad q = 1,\ldots,p.$$

These conditions are linear in v_i and w_i. We remark that all the methods constructed in [3] satisfy (9).

REFERENCES

[1] J. C. Butcher, *The Numerical Analysis of Ordinary Differential Equations*, John Wiley & Sons, 1987.

[2] E. Hairer, S. P. Nørsett, and G. Wanner, *Solving Ordinary Differential Equations I. Nonstiff Problems*, Springer Series in Computational Mathematics 8, Springer-Verlag, 1987, *Second Revised Edition*, 1993.

[3] Z. Jackiewicz and S. Tracogna, *A general class of two-step Runge-Kutta methods for ordinary differential equations*, SIAM J. Numer. Anal., 32 (1995), pp. 1390–1427.