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The number of conditions for a Runge–Kutta method to have effective order p

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Abstract

We count the number of conditions that a one-step numerical integrator has to satisfy to achieve a given effective order of accuracy p. Effective order refers to the order of the numerical method after the numerical solution has been enhanced by suitable pre- and post-processors. The methods considered include not only Runge–Kutta methods, but also all methods that can be represented by B-series, such as multiderivative generalizations of Runge–Kutta methods.

Keywords: Runge–Kutta method; B-series method; Order conditions; Effective order; Pre-processor; Post-processor

1. Introduction

The purpose of this paper is to count the number of conditions that a one-step numerical integrator for the problem

$$\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}x} = \boldsymbol{f}(\boldsymbol{y}), \quad \boldsymbol{y}(0) = \alpha \in \mathcal{R}^D, \tag{1}$$

has to satisfy to achieve an effective order of accuracy p. The concept of effective order goes back to [2] and refers to the order of the numerical method after the numerical solution has been enhanced by suitable pre- and post-processors.

Consider a one-step method given by a mapping $\psi_{h,\boldsymbol{f}}$ in $\mathcal{R}^D$; for instance, $\psi_{h,\boldsymbol{f}}(\boldsymbol{y}) = \boldsymbol{y} + h\boldsymbol{f}(\boldsymbol{y})$ corresponds to Euler's rule. If $\{\boldsymbol{Y}\}_{n=0}^{N}$ is a sequence obtained with the numerical method, $\boldsymbol{Y}_{n+1} = \psi_{h,\boldsymbol{f}}(\boldsymbol{Y}_n)$, $n = 0, \ldots, N-1$, then it is standard to interpret $\boldsymbol{Y}_n$ as an approximation to $\boldsymbol{y}(nh)$, where $\boldsymbol{y}(x)$ is the solution of (1). When processing is used, the vectors $\boldsymbol{Y}_n$, $n = 0, \ldots, N$, are transformed

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with the help of a suitable mapping $\pi_{h,f}$ in $\mathcal{R}^D$ and the transformed $y_n = \pi_{h,f}(Y_n)$ are seen as approximations to $y(nh)$. The mapping $\pi_{h,f}$ is close to the identity $\pi_{h,f} = \mathrm{id} + O(h)$ and has an inverse $\chi_{h,f} = \pi_{h,f}^{-1}$; to avoid a proliferation of symbols it is convenient to write $\chi_{h,f}^{-1}$ instead of $\pi_{h,f}$.

When processing is used, $y_0 = \chi_{h,f}^{-1}(Y_0)$ is seen as the approximation to $y(0) = \alpha$, and, in order to remove the initial error $y_0 - \alpha$, Y_0 should be chosen as $Y_0 = \chi_{h,f}(\alpha)$. Thus, the solution with processing of (1) involves the following stages.

(1) *Pre-processing:* Find the starting value for time-stepping $Y_0 = \chi_{h,f}(\alpha)$.
(2) *Time-stepping:* Compute $Y_{n+1} = \psi_{h,f}(Y_n)$, $n = 0, \ldots, N-1$.
(3) *Post-processing:* If output at time $t = nh$ is desired, then find $y_n = \chi_{h,f}^{-1}(Y_n)$, which provides the numerical approximation to $y(nh)$.

The preprocessor $\chi_{h,f}$ is applied only once, so that its cost may safely be ignored.

Since

$$y_{n+1} = \chi_{h,f}^{-1}(Y_{n+1}) = \chi_{h,f}^{-1}\big(\psi_{h,f}(Y_n)\big) = \chi_{h,f}^{-1}\big(\psi_{h,f}\big(\chi_{h,f}(y_n)\big)\big),$$

the processed y_n turn out to be the (unprocessed) numerical approximations corresponding to the one-step method given by the mapping

$$\widehat{\psi}_{h,f} = \chi_{h,f}^{-1} \circ \psi_{h,f} \circ \chi_{h,f}. \tag{2}$$

Processing is of interest if $\widehat{\psi}_{h,f}$ is a more accurate method than $\psi_{h,f}$ and the cost of post-processing is negligible, either because output is not frequently required or because $\chi_{h,f}^{-1}$ is cheaply evaluated. Then, processing provides the accuracy of $\widehat{\psi}_{h,f}$ at the cost of the less accurate method $\psi_{h,f}$.

The method $\psi_{h,f}$ is said to be of *effective order* p, if a processor $\chi_{h,f}$ exists for which $\widehat{\psi}_{h,f}$ is of (conventional) order p.

The preceding account has followed the approach in [8]. As mentioned before, the idea of effective order goes back to [2] (see also [4, §435] and [6, Chapter II.12]) where the processed method is implemented in a way slightly different from that described above (see Section 4 below). In the traditional setting of Runge–Kutta methods, the effective order approach has never come into practical use because of the complications associated with local error estimation and change of stepsize. Overcoming these difficulties may be possible, but no adequate solutions have yet been proposed. A revival of the idea of processing has recently taken place [7–11,13,15–17], in a context where error estimation is not considered essential.

The main result of the paper is contained in Section 3. Section 2 presents background material and the final Section 4 is devoted to some concluding remarks.

2. Order conditions for Runge–Kutta and B-series methods

It is convenient to work in a B-series context. The idea of B-series was motivated by the study of the order conditions for Runge–Kutta methods. These conditions take the form of equations that prescribe the values of the "elementary weights" associated with a particular method. A second motivation is the characterization of the composition of two methods in terms of the elementary weights of the individual methods being composed.

Let T_n denote the set of (rooted) trees with n vertices. If $\{b_i\}$ and $\{a_{ij}\}$ are the weights and coefficients of a Runge–Kutta method, then associated with each $t \in T_n$ there is an order condition of the form $\boldsymbol{c}(t) = 1/\gamma(t)$, where $\boldsymbol{c}(t)$, known as the "elementary weight", depends only on the numerical method, and $\gamma(t)$ is the "density" of t [4, §144]. For order p, these conditions must hold for each tree in $\bigcup_{n=1}^{p} T_n$. The two simplest examples of these order conditions are for the tree τ with one vertex, $\boldsymbol{c}(\tau) = \sum_i b_i = 1/\gamma(\tau) = 1$, and for the tree $[\tau]$ with two vertices, $\boldsymbol{c}([\tau]) = \sum_{i,j} b_i a_{ij} = 1/\gamma([\tau]) = 1/2$.

If a second method, with weights and coefficients $\{\bar{b}_i\}$ and $\{\bar{a}_{ij}\}$, is used for a step that follows the step performed by the previous method, then it is easy to see that the combined effect of the two methods is the same as for a method with weights $\{\widehat{b}_i\}$ and $\{\widehat{a}_{ij}\}$, given by the arrays

$$\widehat{b}^{\mathsf{T}} = [b^{\mathsf{T}}, \bar{b}^{\mathsf{T}}], \qquad \widehat{A} = \begin{bmatrix} A & 0 \\ eb^{\mathsf{T}} & \bar{A} \end{bmatrix},$$

with b^{T}, $\bar{b}^{\mathsf{T}}$, A, $\bar{A}$, the weight and coefficient arrays with elements $\{b_i\}$, $\{\bar{b}_i\}$, $\{a_{ij}\}$ and $\{\bar{a}_{ij}\}$, respectively and e a vector with each component equal to 1. If the elementary weights for the method used in the second step are $\bar{\boldsymbol{c}}(t)$ and those for the combined method are $\widehat{\boldsymbol{c}}(t)$, then it is possible to express the values of $\widehat{\boldsymbol{c}}$ in terms of the values of $\boldsymbol{c}$ and $\bar{\boldsymbol{c}}$. As we will see in the next section, the use of combinations of methods is crucial to the derivation of conditions for effective order.

The reason for the order conditions being of the form $\boldsymbol{c}(t) = 1/\gamma(t)$ is as follows. A Runge–Kutta method has the formal Taylor series

$$\psi_{h,\boldsymbol{f}}(y) = \boldsymbol{y} + \sum_{n=1}^{\infty} h^n \sum_{t \in T_n} \frac{1}{\sigma(t)} \boldsymbol{c}(t) \boldsymbol{F}(t)(\boldsymbol{y}), \tag{3}$$

where $\sigma(t)$ is the number of symmetries of t [4, §14] and $\boldsymbol{F}(t)$ denotes the "elementary differential" [4, §301] evaluated at $\boldsymbol{y}$. Furthermore, the *exact* solution, that is the flow of the differential equation system in (1), has the formal Taylor series

$$\phi_{h,\boldsymbol{f}}(y) = \boldsymbol{y} + \sum_{n=1}^{\infty} h^n \sum_{t \in T_n} \frac{1}{\sigma(t)} \frac{1}{\gamma(t)} \boldsymbol{F}(t)(\boldsymbol{y}). \tag{4}$$

The order conditions follow by comparing the series given by (3) and (4). Since, by definition, a method has (conventional) order $\geqslant p$, p a positive integer, if, for arbitrary, smooth $\boldsymbol{f}$,

$$\psi_{h,\boldsymbol{f}} = \phi_{h,\boldsymbol{f}} + \mathrm{O}\big(h^{p+1}\big), \tag{5}$$

order $\geqslant p$ is equivalent to

$$\boldsymbol{c}(t) = \frac{1}{\gamma(t)}, \quad t \in T_n,\ n = 1, 2, \ldots, p, \tag{6}$$

because the elementary differentials are independent [4, §306].

An expression like the right-hand side of (3) is known as a B-series and denoted by $B(\boldsymbol{c}, \boldsymbol{y})$ [6, Chapter II.12]. In this paper we assume that we deal with numerical methods $\psi_{h,\boldsymbol{f}}$ that are B-series

Table 1
Number ν_p of rooted trees with p vertices, number o_p of conditions for order $\geqslant p$ and number e_p of conditions for effective order $\geqslant p$

p	ν_p	o_p	e_p
1	1	1	1
2	1	2	2
3	2	4	3
4	4	8	5
5	9	17	10
6	20	37	21
7	48	85	49
8	115	200	116
9	286	486	287
10	719	1205	720

methods. This means that we assume that, for $\boldsymbol{f}$ smooth, the Taylor expansion of $\psi_{h,\boldsymbol{f}}$ in powers of h is given by a B-series

$$B(\boldsymbol{c},\boldsymbol{y}) = \boldsymbol{y} + \sum_{n=1}^{\infty} h^n \sum_{t\in T_n} \frac{1}{\sigma(t)} \boldsymbol{c}(t)\boldsymbol{F}(t)(\boldsymbol{y}).$$

The family of B-series methods includes not only Runge–Kutta methods but also Taylor series methods and multiderivative RK methods.

If ν_n denotes the number of trees in T_n, then (6) comprises $o_p = \nu_1 + \cdots + \nu_p$ conditions (see Table 1). For RK methods [4, §306], the elementary weights are independent functions of the weights $\{b_i\}$ and coefficients $\{a_{ij}\}$ and hence in (6) there are o_p independent order conditions on the tableau elements $\{b_i\}$, $\{a_{ij}\}$.

3. Conditions for effective order

According to (2) and (5), $\psi_{h,\boldsymbol{f}}$ has effective order $\geqslant p$ if a transformation $\chi_{h,\boldsymbol{f}}$ exists for which

$$\chi_{h,\boldsymbol{f}}^{-1} \circ \psi_{h,\boldsymbol{f}} \circ \chi_{h,\boldsymbol{f}} = \phi_{h,\boldsymbol{f}} + \mathrm{O}\big(h^{p+1}\big), \tag{7}$$

a requirement that is convenient to write in the form (recall that $\chi_{h,\boldsymbol{f}} = \mathrm{id} + \mathrm{O}(h)$)

$$\psi_{h,\boldsymbol{f}} \circ \chi_{h,\boldsymbol{f}} = \chi_{h,\boldsymbol{f}} \circ \phi_{h,\boldsymbol{f}} + \mathrm{O}\big(h^{p+1}\big). \tag{8}$$

It is natural to consider processors $\chi_{h,\boldsymbol{f}}$ that can be expanded in a B-series

$$B(\boldsymbol{d},\boldsymbol{y}) = \boldsymbol{y} + \sum_{n=1}^{\infty} h^n \sum_{t\in T_n} \frac{1}{\sigma(t)} \boldsymbol{d}(t)\boldsymbol{F}(t)(\boldsymbol{y}).$$

Then the left-hand side of (8) evaluated at y is $B(c, B(d, y))$, a composition of B-series that is in turn a B-series $B(cd, y)$ [6, Chapter II.12] whose coefficients $(cd)(t)$ are polynomials in the $c(t)$ and $d(t)$. For instance, for the trees with one, two or three vertices,

$$(cd)(\tau) = d(\tau) + c(\tau), \tag{9}$$

$$(cd)([\tau]) = d([\tau]) + c(\tau)d(\tau) + c([\tau]), \tag{10}$$

$$(cd)([\tau^2]) = d([\tau^2]) + c(\tau)d(\tau)^2 + 2c([\tau])d(\tau) + c([\tau^2]), \tag{11}$$

$$(cd)([[\tau]]) = d([[\tau]]) + c(\tau)d([\tau]) + c([\tau])d(\tau) + c([[\tau]]). \tag{12}$$

Here we have used the notation of [4, §143]; $[\tau^2]$ denotes the bushy tree with three vertices obtained by grafting two copies of τ to a common root and $[[\tau]]$ represents the tall tree with three vertices resulting by grafting $[\tau]$ to a new root. For a general tree t, the coefficient $(cd)(t)$ is given by [4, §146], [6, Chapter II.12] and [12]

$$(cd)(t) = d(t) + \sum_z c(z)d^{(z)}(t) + c(t), \tag{13}$$

where the summation is extended to all nonempty, proper subtrees z of t and $d^{(z)}(t)$ is a polynomial in the $d(u)$ corresponding to the trees u that arise by removing from t the vertices in z and the adjacent edges.

Similarly, the composition $\chi_{h,f} \circ \phi_{h,f}$ in (8) can be expanded in a B-series with coefficients $(de)(t)$, where e is defined by $e(t) = 1/\gamma(t)$. Hence, (8) is equivalent to

$$(cd)(t) = (de)(t), \quad t \in T_n,\ n = 1, 2, \ldots, p. \tag{14}$$

Our aim is to investigate Eq. (14). For $p = 1$ there is only the tree τ to be considered and, in view of (9), the order condition reads

$$d(\tau) + c(\tau) = \frac{1}{\gamma(\tau)} + d(\tau)$$

i.e., $c(\tau) = 1$. This is of course the condition that ensures that the method has (conventional) order $\geqslant 1$. Thus, effective order $\geqslant 1$ and conventional order $\geqslant 1$ are equivalent; an inconsistent method cannot be rendered consistent by processing.

For effective order $\geqslant 2$ we additionally consider the tree $[\tau]$ with equation (see (10))

$$d([\tau]) + c(\tau)d(\tau) + c([\tau]) = \frac{1}{\gamma([\tau])} + d(\tau)\frac{1}{\gamma(\tau)} + d([\tau]).$$

This leads to $c([\tau]) = 1/2$; effective order $\geqslant 2$ is equivalent to conventional order $\geqslant 2$.

For effective order $\geqslant 3$, we additionally consider (see (11) and (12))

$$\begin{aligned} &d([\tau^2]) + c(\tau)d(\tau)^2 + 2c([\tau])d(\tau) + c([\tau^2]) \\ &\quad = \frac{1}{\gamma([\tau^2])} + d(\tau)\frac{1}{\gamma(\tau)^2} + 2d([\tau])\frac{1}{\gamma(\tau)} + d([\tau^2]), \end{aligned} \tag{15}$$

$$\begin{aligned} &d([[\tau]]) + c(\tau)d([\tau]) + c([\tau])d(\tau) + c([[\tau]]) \\ &\quad = \frac{1}{\gamma([[\tau]])} + d(\tau)\frac{1}{\gamma([\tau])} + d([\tau])\frac{1}{\gamma(\tau)} + d([[\tau]]). \end{aligned} \tag{16}$$

Here $\boldsymbol{c}(\tau)$, $\boldsymbol{c}([\tau])$ have known values if the method has (effective) order $\geqslant 2$. Eq. (16) is then equivalent to $\boldsymbol{c}([[\tau]]) = 1/\gamma([[\tau]])$. Eq. (15) involves, after cancelling $\boldsymbol{d}([\tau^2])$, the variables $\boldsymbol{c}([\tau^2])$, $\boldsymbol{d}(\tau)$ and $\boldsymbol{d}([\tau])$; we may let $\boldsymbol{c}([\tau^2])$ and $\boldsymbol{d}(\tau)$ be free parameters. Therefore there is only one condition for a method of (effective) order $\geqslant 2$ to have effective order $\geqslant 3$; by comparison there are two conditions for a method of order $\geqslant 2$ to have order $\geqslant 3$.

Some notation will be helpful to deal with general $p \geqslant 3$. For $n \geqslant 3$, we partition the trees in T_n into two groups. The first F_n consists of the trees with n vertices that can be written as a product [4, §143] $t \cdot \tau$, where t has $n-1$ vertices, i.e., of the n-trees where the root has a child that is a terminal vertex. The second group S_n consists of the remaining n-trees. It is obvious that,

$$\#F_n = \nu_{n-1}, \quad \#S_n = \nu_n - \nu_{n-1}, \qquad n \geqslant 3. \tag{17}$$

Note that, in the case $n = 3$, F_3 consists of the tree $[\tau^2] = [\tau] \cdot \tau$ whose $\boldsymbol{c}$ was a free parameter in the discussion of (15) and (16) and S_3 consists of the tree $[[\tau]]$, whose $\boldsymbol{c}$ was determined by the order conditions. We extend our notation to the cases $n = 1, 2$ by setting $F_1 = F_2 = \emptyset$, $S_1 = T_1$, $S_2 = T_2$.

The discussion (15)–(16) can be extended to general p as follows.

Theorem 1. *For any choice of* $\boldsymbol{c}(t)$, $t \in F_n$, $n = 1, \ldots, p$ *and* $\boldsymbol{d}(\tau)$ *Eq.* (14) *uniquely determine* $\boldsymbol{c}(t)$, $t \in S_n$, $n = 1, \ldots, p$ *and* $\boldsymbol{d}(t)$, $t \in T_n$, $n = 2, \ldots, p-1$.

Proof. By induction in p. The cases $p = 1, 2, 3$ have been dealt with above. In particular, for $p = 1, 2$, the set of trees $t \in T_n$, $n = 2, \ldots, p-1$ whose coefficient $\boldsymbol{d}(t)$ is determined by the order conditions is empty.

Assume then that $p > 3$ and that the theorem holds for $p-1$. Then the coefficients $\boldsymbol{c}(t)$, $t \in S_n$, $n = 1, \ldots, p-1$ and $\boldsymbol{d}(t)$, $t \in T_n$, $n = 2, \ldots, p-2$ are known functions of the free parameters and we have to consider, as t ranges in T_p, the ν_p equations

$$(\boldsymbol{cd})(t) = (\boldsymbol{de})(t) \tag{18}$$

in the $\nu_p = (\nu_p - \nu_{p-1}) + \nu_{p-1}$ (see (17)) unknowns

$$\boldsymbol{c}(t), \quad t \in S_p, \qquad \boldsymbol{d}(\widehat{t}), \quad \widehat{t} \in T_{p-1}. \tag{19}$$

According to (13), Eq. (18) reads, after cancellation of $\boldsymbol{d}(t)$,

$$\sum_z \boldsymbol{c}(z)\boldsymbol{d}^{(z)}(t) + \boldsymbol{c}(t) = \frac{1}{\gamma(t)} + \sum_z \boldsymbol{d}(z)\varepsilon(z,t), \tag{20}$$

where the $\varepsilon(z,t)$ are rational numbers > 0.

We first consider Eq. (20) with t ranging in F_p. For these trees t, the left-hand side of (20) does not involve any of the unknowns (19). This is proved as follows. If $t \in T_p$ and z is a proper (nonempty) subtree of t, then z has at most $p-1$ vertices and $\boldsymbol{c}(z)$ does not feature in (19). Furthermore, $\boldsymbol{d}(u)$ with $u \in T_{p-1}$ can be implicitly in $\boldsymbol{d}^{(z)}(t)$, $t \in T_p$, only if z has only one vertex, i.e., is the root of t; but for $t \in F_p$ removing the root of t does not give rise to any trees u of order $p-1$. This concludes the proof that, for $t \in F_p$, the left-hand side of (20) does not involve any of the unknowns. The corresponding right-hand side involves the unknowns $\boldsymbol{d}(z)$, where z is any of the trees obtained by removing a terminal vertex of t. To sum up, as t ranges in F_p, we have ν_{p-1} linear equations (20) in the ν_{p-1} unknowns $\boldsymbol{d}(\widehat{t})$, $\widehat{t} \in T_{p-1}$. We shall show that it is possible to order the trees $\widehat{t} \in T_{p-1}$

in such a way that (20) with $t = \widehat{t} \cdot \tau \in F_p$ is a nonsingular, lower-triangular linear system in the unknowns $\boldsymbol{d}(\widehat{t})$, $\widehat{t} \in T_{p-1}$. Indeed, it is enough to consider the $\widehat{t}$'s in such a way that $\widehat{u}$ comes before $\widehat{v}$ if in $\widehat{u}$ the root has more children than in $\widehat{v}$. Eq. (20) for $t = \widehat{t} \cdot \tau$, where the root of $\widehat{t}$ has, say, k children, involves $\boldsymbol{d}(\widehat{t})$ ($\widehat{t}$ arises by removing from t a terminal vertex child of the root) and, if $k < p-2$, $\boldsymbol{d}(\widehat{u})$'s where $\widehat{u}$ is the result of removing from t a terminal vertex that is not a child of the root. Those $\widehat{u}$ have roots with $k+1$ children and precede $\widehat{t}$ and we are in fact dealing with a lower triangular system.

After having determined the $\boldsymbol{d}(\widehat{t})$, $\widehat{t} \in T_{p-1}$ by a recursive forward solve, Eq. (20) with $t \in S_p$ directly yields the value of $\boldsymbol{c}(t)$. □

In Theorem 1 we let $\boldsymbol{d}(\tau)$ be one of the free parameters. This freedom will be discussed next. We begin by noticing that $\boldsymbol{d}(\tau)$ measures the length of the interval of the independent variable x over which the mapping $\chi_{h,\boldsymbol{f}}$ advances the numerical solution. More precisely, $\chi_{h,\boldsymbol{f}}$ is a consistent approximation to (i.e., differs in $\mathrm{O}(h^2)$ terms from) the true $\boldsymbol{d}(\tau)h$-flow $\phi_{\boldsymbol{d}(\tau)h,\boldsymbol{f}}$. Now assume that (7) holds for a processor $\chi_{h,\boldsymbol{f}}$ with $\boldsymbol{d}(\tau) = 0$. Then composing (7) with $\phi_{\delta h,\boldsymbol{f}}$ and $\phi^{-1}_{\delta h,\boldsymbol{f}}$, δ an arbitrary real number, we obtain

$$(\chi_{h,\boldsymbol{f}} \circ \phi_{\delta h,\boldsymbol{f}})^{-1} \circ \psi_{h,\boldsymbol{f}} \circ (\chi_{h,\boldsymbol{f}} \circ \phi_{\delta h,\boldsymbol{f}}) = \phi_{h,\boldsymbol{f}} + \mathrm{O}\big(h^{p+1}\big),$$

and therefore the processor $\chi^*_{h,\boldsymbol{f}} = \chi_{h,\boldsymbol{f}} \circ \phi_{\delta h,\boldsymbol{f}}$ can be used instead of $\chi_{h,\boldsymbol{f}}$ to achieve effective order $\geqslant p$. Since $\chi^*_{h,\boldsymbol{f}}$ has coefficient $\boldsymbol{d}^*(\tau) = \delta$, we conclude that $\boldsymbol{d}(\tau)$ is a normalizing length, whose value does not affect the solvability of the conditions for effective order. Probably the most natural choice is $\boldsymbol{d}(\tau) = 0$, so that the processor $\chi_{h,\boldsymbol{f}}$ does not advance the independent variable x and, with the notation of the introduction, $\boldsymbol{y}_n = \boldsymbol{Y}_n + \mathrm{O}(h^2)$.

Corollary 1. *For $p > 1$, the condition that a B-series method has effective order $\geqslant p$ under B-series processing imposes $e_p = \nu_p + 1$ independent conditions on the coefficients $\mathbf{c}(t)$, $t \in T_n$, $n = 1, \ldots, p$.*

Proof. By the preceding discussion, we may assume that $\boldsymbol{d}(\tau) = 0$. Then (14) includes $o_p = \nu_1 + \cdots + \nu_p$ relations with $\nu_2 + \cdots + \nu_{p-1}$ free parameters $\boldsymbol{c}(t)$. □

For an RK method the e_p conditions on the B-series coefficients lead to as many independent equations on the tableau coefficients $\{b_i\}$, $\{a_{ij}\}$. A comparison between the number of conditions for order $\geqslant p$ and for effective order $\geqslant p$ can be made in Table 1.

4. Discussion

In the discussion of (16), we noticed that the standard order condition associated with the tall tree with three vertices $[[\tau]]$ is necessary for effective order $\geqslant 3$. In general, the standard order condition for the tall tree with p vertices,

$$\boldsymbol{c}\big([_{p-1}\tau]_{p-1}\big) = \frac{1}{\gamma([_{p-1}\tau]_{p-1})} \tag{21}$$

($[_{p-1}$ and $]_{p-1}$ respectively stand for $p-1$ copies of [and]) is necessary for effective order $\geqslant p$. A proof of this follows. Consider (8) when (1) is a linear problem, i.e., when $\boldsymbol{f}(\boldsymbol{y}) = A\boldsymbol{y}$, A a

constant $D \times D$ matrix. In this case, the B-series of the mappings $\psi_{h,\boldsymbol{f}}$, $\chi_{h,\boldsymbol{f}}$, $\phi_{h,\boldsymbol{f}}$ are linear in $\boldsymbol{y}$ with matrices that are power series in A. Then these B-series commute and (8) is equivalent to (5): for linear problems there is no distinction between order and effective order. Since it is well known that (21) is necessary for $\psi_{h,\boldsymbol{f}}$ to have order $\geqslant p$ in linear problems, we conclude that (21) is also necessary for $\psi_{h,\boldsymbol{f}}$ to have effective order $\geqslant p$ in linear problems and *a fortiori* to have effective order $\geqslant p$.

Since

$$\overbrace{\widehat{\psi}_{h,\boldsymbol{f}} \circ \cdots \circ \widehat{\psi}_{h,\boldsymbol{f}}}^{n \text{ times}} = \left(\chi_{h,\boldsymbol{f}}^{-1} \circ \psi_{h,\boldsymbol{f}}\right) \circ \overbrace{\psi_{h,\boldsymbol{f}} \circ \cdots \circ \psi_{h,\boldsymbol{f}}}^{n-2 \text{ times}} \circ (\psi_{h,\boldsymbol{f}} \circ \chi_{h,\boldsymbol{f}}),$$

n steps of the processed method can be implemented by taking $n-2$ steps of the unprocessed method, preceded by an application of the transformation $\psi_{h,\boldsymbol{f}} \circ \chi_{h,\boldsymbol{f}}$ and followed an application of the transformation $(\chi_{h,\boldsymbol{f}}^{-1} \circ \psi_{h,\boldsymbol{f}})$. For consistent $\psi_{h,\boldsymbol{f}}$ and under the condition $\boldsymbol{d}(\tau) = 0$, these starting and finishing transformations advance the variable x by h units and can be realized (or at least approximated to any desired order) by a step of length h of a suitably chosen consistent RK formula; this is the original approach in [2]. Note also that, if the transformation $\chi_{h,\boldsymbol{f}}$ is a step of a Runge–Kutta method, then it is easy to define a method corresponding to $\chi_{h,\boldsymbol{f}}^{-1}$, by simply solving for the vector input to a step in terms of the output value from the step. It turns out that if $\chi_{h,\boldsymbol{f}}$ is associated with the Runge–Kutta method characterized by $\{b_i\}$ and $\{a_{ij}\}$, then $\chi_{h,\boldsymbol{f}}^{-1}$ is associated with the method characterized by $\{-b_i\}$ and $\{a_{ij} - b_j\}$.

We have written the B-series (3) using $1/\sigma(t)$ as a normalizing factor. This convention, followed in [4] (see, e.g., formula (432a)) and in [12], is perhaps more convenient than that employed in [6], where a different normalizing factor is introduced. With our normalization, the B-series coefficients of an RK method are the elementary weights $\sum_i b_i$, $\sum_{ij} b_i a_{ij}, \ldots$.

When composing B-series we write $\boldsymbol{cd}$ if $\boldsymbol{d}$ acts first and is followed by $\boldsymbol{c}$. This differs from the original formulation of the composition operation [3] where the order of the factors is reversed. Our notation is consistent with the standard ordering used to express compositions of mappings. However, the notation in [3], also used in [4], does have one advantage. If the B-series $B(\boldsymbol{c}, \boldsymbol{y})$ is modified to the form

$$B(\boldsymbol{c}, \boldsymbol{y}) = \boldsymbol{c}(t_0)\boldsymbol{y} + \sum_{n=1}^{\infty} h^n \sum_{t \in T_n} \frac{1}{\sigma(t)} \boldsymbol{c}(t) \boldsymbol{F}(t)(\boldsymbol{y}),$$

where t_0 is an additional tree, known as the "empty tree" and represented by the symbol $\emptyset$, then $B(\boldsymbol{c}, \boldsymbol{y})$ can be used to represent a variety of quantities arising in a numerical process. This type of generalized B-series has a central role in the analysis of multivalue methods. With this change, the formula for $\boldsymbol{cd}$ is linear in $\boldsymbol{c}$ and is therefore more naturally written with the factors in the reverse order. For a novel approach to the composition of B-series and P-series see [12].

The material presented in this paper can be extended in different directions. First of all, the attention may be restricted to B-series methods that are symplectic [14]. For these, the values $\boldsymbol{c}(t)$ are constrained and the standard order conditions $\boldsymbol{c}(t) = 1/\gamma(t)$ are not independent [5]; there is only one independent order condition per nonsuperfluous free tree. It is of interest to count the number of conditions that a symplectic B-series method has to satisfy to achieve effective order $\geqslant p$ after suitably processed with a symplectic $\chi_{h,\boldsymbol{f}}$. With the techniques used in this paper it is possible to prove that for effective

order $\geqslant p$, $p > 1$, the number of conditions is one more than the number of nonsuperfluous free trees with p vertices. A second extension, that can also be undertaken with the techniques here, refers to methods, general or symplectic, whose expansions are not B-series but P-series or even NB-series [1].

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