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B-series and order conditions for exponential integrators

by

Håvard Berland, Brynjulf Owren and Bård Skaflestad

PREPRINT
NUMERICS NO. 5/2004

NORWEGIAN UNIVERSITY OF SCIENCE AND
TECHNOLOGY
TRONDHEIM, NORWAY

This report has URL `http://www.math.ntnu.no/preprint/numerics/2004/N5-2004.ps`
Address: Department of Mathematical Sciences, Norwegian University of Science and Technology,
N-7491 Trondheim, Norway.

Abstract

We introduce a general format of numerical ODE-solvers which include many of the recently proposed exponential integrators. We derive a general order theory for these schemes in terms of B-series and bicoloured rooted trees. To ease the construction of specific schemes we generalise an idea of Zennaro and define Natural Continuous Extensions in the context of exponential integrators. This leads to a relatively easy derivation of some of the most popular recently proposed schemes. The general format of schemes considered here makes use of coefficient functions which will usually be selected from some finite dimensional function spaces. We will derive lower bounds for the dimension of these spaces in terms of the order of the resulting schemes. Finally we illustrate the presented ideas by giving examples of new exponential integrators of orders 4 and 5.

1 Introduction

Numerical integration schemes which use the matrix exponential go back all the way to Certaine [3], but there are also early papers by Lawson [10], Nørsett [15] and many others. Recently there has been a revived interest in these schemes, in particular for the solution of nonlinear partial differential equations, see for instance [7, 12, 4, 2, 9, 8, 11] and the references therein. The integrators found in these papers are derived in rather different ways, and they are formulated for different types of systems of differential equations. In this note, we consider the autonomous nonlinear system of ordinary differential equations

$$\dot{u} = Lu + N(u), \qquad u(0) = u_0. \tag{1}$$

Here L is a matrix and $N(u)$ a nonlinear mapping. The order theory we consider is valid for a large class of exponential integrators, including the Runge–Kutta–Munthe-Kaas (RKMK) schemes [12], the commutator-free Lie group integrators [2], and those schemes of Cox and Matthews [4] as well as Krogstad [9] which reduce to classical Runge–Kutta schemes when $L = 0$.

We present the general format for integrators of (1) as

$$N_r = N\Big(\exp(c_r hL)\, u_0 + h\sum_{j=1}^{s} a_r^j(hL)\, N_j\Big), \quad r = 1, \dots, s \tag{2}$$

$$u_1 = \exp(hL)\, u_0 + h\sum_{r=1}^{s} b^r(hL)\, N_r. \tag{3}$$

Here we assume that the functions $a_r^j(z)$, $b^r(z)$ are at least p times continuously differentiable at $z = 0$ for integration schemes of order p.

Table 1 gives the coefficient functions $a_r^j(z)$ and $b^r(z)$ for the fourth order RKMK scheme introduced in [13] in this general format when applied to the problem (1) with an affine Lie group action, and the commutator-free scheme of order 4 from [2]. In both tables $\phi_0(z) = (\mathrm{e}^z - 1)/z$.

For deriving order conditions, we expand the coefficient functions in powers of z,

$$a_r^j(z) = \sum_{k\geq 0} \alpha_r^{j,k} z^k \quad \text{and} \quad b^r(z) = \sum_{k\geq 0} \beta^{r,k} z^k$$

where the sum may terminate with a remainder term. For the schemes we consider here, these functions are in fact all entire. If $N(u) = 0$ in (1), then any scheme in the above

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\phi_0(z/2) & & & \\
\frac{1}{2} & \frac{z}{8}\phi_0(z/2) & \frac{1}{2}(1-\frac{z}{4})\phi_0(z/2) & & \\
1 & & & \phi_0(z) & \\
\hline
 & \frac{1}{6}\phi_0(z)(1+\frac{z}{2}) & \frac{1}{3}\phi_0(z) & \frac{1}{3}\phi_0(z) & \frac{1}{6}\phi_0(z)(1-\frac{z}{2})
\end{array}
$$

(a) RKMK, order 4

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\phi_0(z/2) & & & \\
\frac{1}{2} & & \frac{1}{2}\phi_0(z/2) & & \\
1 & \frac{z}{4}\phi_0(z/2)^2 & & \phi_0(z/2) & \\
\hline
 & \frac{1}{2}\phi_0(z) - \frac{1}{3}\phi_0(z/2) & \frac{1}{3}\phi_0(z) & \frac{1}{3}\phi_0(z) & -\frac{1}{6}\phi_0(z) + \frac{1}{3}\phi_0(z/2)
\end{array}
$$

(b) Commutator-free, order 4

Table 1: Examples of schemes in general format for exponential integrators

class will reproduce the exact solution in every step. Whereas if $L = 0$, the scheme (2)–(3) reduces to a classical Runge–Kutta method with coefficients $a_r^j = \alpha_r^{j,0}, b^r = \beta^{r,0}$. This scheme is henceforth called *the underlying Runge–Kutta scheme*. We will always assume that $c_r = \sum_j \alpha_r^{j,0},\ 1 \le r \le s$.

In this note, we will derive conditions on the coefficients $\alpha_r^{j,k}$ and $\beta^{r,k}$ under which the scheme (2)–(3) has order of consistency p for problems of the type (1). We will use the well known approach involving rooted trees, see for instance [6, 1]. The conditions we derive will only depend on the first $\alpha_r^{j,k},\ k \le p-2$ and on $\beta^{j,k},\ k \le p-1$, in this note we will not address issues related to the behaviour of the coefficient functions $a_r^j(z), b^r(z)$ for large values of z.

2 B-series and order conditions

Repeated differentiation of (1) with respect to time yields

$$\begin{aligned}
\frac{\mathrm{d}^2u}{\mathrm{d}t^2} &= L\dot{u} + N'(\dot{u}) \\
&= L^2u + LN + N'(Lu) + N'(N) \\
\frac{\mathrm{d}^3u}{\mathrm{d}t^3} &= L^3u + L^2N + LN'(Lu) + LN'(N) \\
&\quad + N''(Lu, Lu) + 2N''(Lu, N) + N'(L^2u) \\
&\quad + N'(LN) + N''(N, N) + N'N'(Lu) + N'N'(N)
\end{aligned}$$

etc. The exact solution of (1) has a formal expansion

$$u(h) = \sum_{q=0}^{\infty} \frac{h^q}{q!} \left.\frac{\mathrm{d}^q}{\mathrm{d}h^q}\right|_{h=0} u(h)$$

where each term in the qth derivative corresponds in an obvious way to a rooted bicoloured tree. Let for instance $\bullet \sim F(\bullet) = N(u)$ and $\circ \sim F(\circ) = Lu$ be the two trees with one node. Next define B_+ as the operation which takes a finite set of trees $\{\tau_1, \dots, \tau_\mu\}$ and connects their roots to a new common black root. Similarly, $\tau = W_+(\tau')$ connects the root of τ' to a new white root resulting in the tree τ associated to $F(\tau) = L \cdot F(\tau')$. It suffices here to allow W_+ to act on a single tree and not on a set of trees. To each tree τ with q nodes formed this way, there exists precisely one term, $F(\tau)$ called an elementary differential, in the qth derivative of the solution of (1). For $q > 1$, it is defined recursively as

$$F(B_+(\tau_1, \dots, \tau_\mu))(u) = N^{(\mu)}(F(\tau_1), \dots, F(\tau_\mu))(u) \tag{4}$$
$$F(W_+(\tau'))(u) = LF(\tau')(u) \tag{5}$$

We may denote by T the set of all bicoloured trees such that each white node has at most one child, and set $T = T_b \cup T_w$ the union of trees with black and white roots respectively. Introducing the empty set $\emptyset$, and using the convention $B_+(\emptyset) = \bullet$, $W_+(\emptyset) = \circ$, we may write

$$T \cup \emptyset = \bigcup_{m \geq 0} W_+^m(T_b \cup \emptyset), \quad T_w = \bigcup_{m \geq 1} W_+^m(T_b \cup \emptyset) \tag{6}$$

Following for instance the text by Hairer, Lubich and Wanner [5], we may work with formal B-series. For an arbitrary map $\boldsymbol{c} : T \cup \emptyset \to \mathbf{R}$, we let the formal series

$$B(\boldsymbol{c}, u) = \boldsymbol{c}(\emptyset)\, u + \sum_{\tau \in T} \frac{h^{|\tau|}}{\sigma(\tau)} \boldsymbol{c}(\tau) F(\tau)(u)$$

be a B-series, where $\sigma(\tau)$ is the symmetry coefficient defined as $\sigma(\bullet) = \sigma(\circ) = 1$, and for $\tau = B_+(\tau_1, \dots, \tau_\mu)$,

$$\sigma(\tau) = \sigma(\tau_1) \cdots \sigma(\tau_\mu)\, m_1! \cdot m_2! \cdots$$

where the m_i's count the number of equal trees among $\tau_1, \dots, \tau_\mu$.

We may present an analogue of Lemma 1.9 in [5] as follows

Lemma 2.1. *Let $\boldsymbol{c} : T \cup \emptyset \to \mathbf{R}$ satisfy $\boldsymbol{c}(\emptyset) = 1$. Then*

$$hN(B(\boldsymbol{c}, u)) = B(\boldsymbol{c}', u)$$

is again a B-series where $\boldsymbol{c}'(\emptyset) = 0$, $\boldsymbol{c}'(\bullet) = 1$, $\boldsymbol{c}'(B_+(\tau_1, \dots, \tau_\mu)) = \boldsymbol{c}(\tau_1) \cdots \boldsymbol{c}(\tau_\mu)$ and for $\tau \in T_w$ one has $\boldsymbol{c}'(\tau) = 0$.

The proof is a straightforward generalisation of the one in [5] and is therefore omitted.

If we now assume that the exact solution has a formal B-series $u(h) = B(\boldsymbol{e}, u_0)$, it follows by termwise differentiation and use of Lemma 2.1 that

$$\boldsymbol{e}(\emptyset) = 1, \quad \boldsymbol{e}(\bullet) = \boldsymbol{e}(\circ) = 1, \quad \boldsymbol{e}(\tau) = \frac{1}{|\tau|} \boldsymbol{e}(\tau_1) \cdots \boldsymbol{e}(\tau_\mu).$$

The last formula holds in either of the cases $\tau = B_+(\tau_1, \dots, \tau_\mu)$ or $\tau = W_+(\tau_1)$. It is customary to define the *density* $\gamma(\tau)$ of a tree τ recursively by setting $\gamma(\bullet) = \gamma(\circ) = 1$, and in terms of subtrees, $\gamma(\tau) = |\tau|\, \gamma(\tau_1) \cdots \gamma(\tau_\mu)$ independently of the colouring of the nodes. We then immediately see that $\boldsymbol{e}(\tau) = 1/\gamma(\tau)$ for all $\tau \in T$.

The stages (2) of the numerical scheme can be written out as

$$U_r = \mathrm{e}^{c_r hL}\, u_0 + \sum_{j=1}^{s} a_r^j(hL) hN_j, \tag{7}$$

$$N_r = N(U_r). \tag{8}$$

We now assume that U_r and hN_j both have B-series denoted $B(\boldsymbol{U}_r, u_0)$ and $B(\boldsymbol{N}_j, u_0)$ respectively. From (7) we insert $a_r^j(hL) = \sum_{m \ge 0} \alpha_r^{j,m} (hL)^m$ and calculate each side of the expression

$$u_0 + \sum_{\tau \in T} \frac{h^{|\tau|}}{\sigma(\tau)} \boldsymbol{U}_r(\tau) F(\tau)(u_0) = u_0 + \sum_{m \ge 1} \frac{c_r^m h^m}{m!} F(W_+^m(\emptyset))(u_0)$$
$$+ \sum_{m \ge 0} \sum_{\tau \in T_b} \sum_{j=1}^{s} \alpha_r^{j,m} \frac{h^{|\tau|+m}}{\sigma(\tau)} \boldsymbol{N}_j(\tau) F(W_+^m(\tau))(u_0) \tag{9}$$

We note that the first sum on the right hand side consists precisely of the (tall) trees with only white nodes, that we denote by T_0. In view of (6), one can replace $\sum_{m \ge 0} \sum_{\tau \in T_b}$ by $\sum_{\tau \in T \setminus T_0}$.

Next we notice

1. $\sigma(\tau) = \sigma(W_+^m(\tau))$ for any positive integer m and for any $\tau \in T$. $\sigma(\tau) = 1$ for $\tau \in T_0$.
2. For any $\tau \in T$ there is a unique non-negative integer m such that $\tau = W_+^m(\tau')$ with $\tau' \in T_b \cup \emptyset$.

Using these two facts and omitting u_0, we can now rewrite (9) in the form

$$\sum_{\tau \in T} \frac{h^{|\tau|}}{\sigma(\tau)} \boldsymbol{U}_r(\tau) F(\tau) = \sum_{\tau \in T_0} \frac{c_r^{|\tau|} h^{|\tau|}}{|\tau|!} F(\tau) + \sum_{\tau \in T \setminus T_0} \sum_{j=1}^{s} \alpha_r^{j,m(\tau)} \frac{h^{|\tau|}}{\sigma(\tau)} \boldsymbol{N}_j(W_+^{-m}(\tau)) F(\tau).$$

We immediately conclude that

$$\boldsymbol{U}_r(\tau) = \frac{c_r^{|\tau|}}{|\tau|!}, \quad \tau \in T_0$$

whereas

$$\boldsymbol{U}_r(\tau) = \sum_{j=1}^{s} \alpha_r^{j,m} \boldsymbol{N}_j(W_+^{-m}(\tau)), \quad \tau \in T\backslash T_0$$

or equivalently: For any non-negative integer m and $\tau \in T_b$

$$\boldsymbol{U}_r(W_+^m(\tau)) = \sum_{j=1}^{s} \alpha_r^{j,m} \boldsymbol{N}_j(\tau).$$

In view of Lemma 2.1 we have for trees $\tau = B_+(\tau_1, \dots, \tau_\mu) \in T_b$

$$\boldsymbol{U}_r(W_+^m(\tau)) = \sum_{j=1}^{s} \alpha_r^{j,m} \boldsymbol{U}_j(\tau_1) \cdots \boldsymbol{U}_j(\tau_\mu).$$

We proceed to the quantity u_1 with B-series $B(\boldsymbol{u}_1, u_0)$ to find that

$$u_0 + \sum_{\tau \in T} \frac{h^{|\tau|}}{\sigma(\tau)} \boldsymbol{u}_1(\tau) F(\tau)(u_0) =$$

$$u_0 + \sum_{\tau \in T_0} \frac{h^{|\tau|}}{|\tau|!} F(\tau)(u_0) + \sum_{m \geq 0} \sum_{\tau \in T_b} \sum_{r=1}^{s} \beta^{r,m} \frac{h^{|\tau|+m}}{\sigma(\tau)} \boldsymbol{N}_r(\tau) F(W_+^m(\tau))(u_0)$$

so as before, we conclude that

$$\boldsymbol{u}_1(\tau) = \frac{1}{|\tau|!}, \quad \tau \in T_0.$$

Certainly, $\boldsymbol{u}_1(\emptyset) = 1$ so for every $\tau = B_+(\tau_1, \dots, \tau_\mu) \in T_b$ and non-negative integer m we have

$$\boldsymbol{u}_1(W_+^m(\tau)) = \sum_{r=1}^{s} \beta^{r,m} \boldsymbol{U}_r(\tau_1) \cdots \boldsymbol{U}_r(\tau_\mu).$$

The order conditions are obtained by matching the coefficients of the exact and numerical solution, setting

$$\boldsymbol{u}_1(\tau) = \boldsymbol{e}(\tau) = 1/\gamma(\tau), \quad \text{for all } \tau \in T \text{ such that } |\tau| \leq p.$$

Note that $\gamma(W_+^m(\emptyset)) = \gamma(B_+^m(\emptyset)) = m!$ for any non-negative integer m so the order conditions are automatically satisfied for all trees $\tau \in T_0$ of arbitrary order. In other words, it suffices to consider trees in $T\backslash T_0$.

But there is more. Suppose that a tree in $T\backslash T_0$ has a white leaf. This leaf is attached to a subtree $\tau = W_+^m B_+(\tau_1, \ldots, \tau_\mu, \omega)$, $\omega \in T_0$, for some $m \geq 0$. We compute

$$\begin{aligned}
\boldsymbol{U}_r(\tau) &= \sum_{j=1}^{s} \alpha_r^{j,m} \boldsymbol{U}_j(\tau_1) \cdots \boldsymbol{U}_j(\tau_\mu) \cdot \boldsymbol{U}_j(\omega) \\
&= \sum_{j=1}^{s} \alpha_r^{j,m} \boldsymbol{U}_j(\tau_1) \cdots \boldsymbol{U}_j(\tau_\mu) \cdot c_j^{|\omega|}/|\omega|! \\
&= \frac{1}{|\omega|!} \sum_{j=1}^{s} \alpha_r^{j,m} \boldsymbol{U}_j(\tau_1) \cdots \boldsymbol{U}_j(\tau_\mu) \cdot \underbrace{\boldsymbol{U}_j(\bullet) \cdots \boldsymbol{U}_j(\bullet)}_{|\omega|} \\
&= \frac{1}{|\omega|!} \boldsymbol{U}_r(W_+^m B_+(\tau_1, \ldots, \tau_\mu, \bullet, \ldots, \bullet)) := \frac{1}{|\omega|!} \boldsymbol{U}_r(\bar{\tau})
\end{aligned}$$

A similar argument holds for $\boldsymbol{u}_1(\tau)$. Note also that $\gamma(\tau) = |\omega|!\gamma(\bar{\tau})$ which implies that the the order condition for a tree τ containing a leaf or string $\omega \in T_0$ is equivalent to the order condition for the tree $\bar{\tau}$. By repeating this argument we may conclude that it suffices to consider the order conditions of trees which have only black leaves, or equivalently, the set of all bicoloured rooted trees where every white node has precisely one child. We have arrived at the main result

Theorem 2.2. *Let $T' \subset T$ be the set of bicoloured rooted trees such that every white node has precisely one child. An exponential integrator defined by* (2)–(3) *has order of consistency p if*

$$\boldsymbol{u}_1(\tau) = \frac{1}{\gamma(\tau)}, \quad \textit{for all } \tau \in T' \textit{ such that } |\tau| \leq p,$$

where

$$\begin{aligned}
\boldsymbol{u}_1(\emptyset) = \boldsymbol{U}_r(\emptyset) &= 1, \quad 1 \leq r \leq s, \\
\boldsymbol{u}_1(W_+^m B_+(\tau_1, \ldots, \tau_\mu)) &= \sum_r \beta^{r,m} \boldsymbol{U}_r(\tau_1) \cdots \boldsymbol{U}_r(\tau_\mu) \\
\boldsymbol{U}_r(W_+^m B_+(\tau_1, \ldots, \tau_\mu)) &= \sum_j \alpha_r^{j,m} \boldsymbol{U}_j(\tau_1) \cdots \boldsymbol{U}_j(\tau_\mu)
\end{aligned}$$

There is an interesting connection between the set of trees T' and the trees used to develop the order theory for composition methods in [14]. White nodes appear as connected strings of nodes which, except from the root, have exactly one parent and one child, and always terminating in a black node. Therefore one can remove all white nodes and assign to the terminating black node the number of removed nodes plus one. Black nodes not connected to a white node is assigned the number one. These multilabelled trees are precisely those appearing in [14], they can also be identified as the set of rooted trees of nonempty sets. The generating function for these trees is well-known,

$$M(x) = \frac{x}{1-x} \exp\left(M(x) + \frac{M(x^2)}{2} + \frac{M(x^3)}{3} + \cdots\right).$$

The number of order conditions for each order 1 to 9 is 1, 2, 5, 13, 37, 108, 332, 1042, 3360.

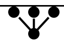
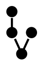
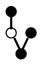
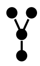
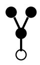
	$\lvert\tau\rvert$	Tree	$F(\tau)$	$\gamma(\tau)$	$\boldsymbol{u}_1(\tau)$	$\sigma(\tau)$
1	1		N	1	$\sum_r \beta^{r,0}$	1
2	2		$N'N$	2	$\sum_r \beta^{r,0} c_r$	1
3	2		LN	2	$\sum_r \beta^{r,1}$	1
4	3		$N''(N,N)$	3	$\sum_r \beta^{r,0} c_r^2$	2
5	3		$N'N'N$	6	$\sum_{r,j} \beta^{r,0} \alpha_r^{j,0} c_j$	1
6	3		$N'(LN)$	6	$\sum_{r,j} \beta^{r,0} \alpha_r^{j,1}$	1
7	3		$LN'N$	6	$\sum_r \beta^{r,1} c_r$	1
8	3		L^2N	6	$\sum_r \beta^{r,2}$	1
9	4		$N'''(N,N,N)$	4	$\sum_r \beta^{r,0} c_r^3$	6
10	4		$N''(N'N,N)$	8	$\sum_{r,j} \beta^{r,0} \alpha_r^{j,0} c_j c_r$	1
11	4		$N''(LN,N)$	8	$\sum_{r,j} \beta^{r,0} \alpha_r^{j,1} c_r$	1
12	4		$N'N''(N,N)$	12	$\sum_{r,j} \beta^{r,0} \alpha_r^{j,0} c_j^2$	2
13	4		$N'N'N'N$	24	$\sum_{r,j,k} \beta^{r,0} \alpha_r^{j,0} \alpha_j^{k,0} c_k$	1
14	4		$N'N'(LN)$	24	$\sum_{r,j,k} \beta^{r,0} \alpha_r^{j,0} \alpha_j^{k,1}$	1
15	4		$N'(LN'N)$	24	$\sum_{r,j} \beta^{r,0} \alpha_r^{j,1} c_j$	1
16	4		$N'(L^2N)$	24	$\sum_{r,j} \beta^{r,0} \alpha_r^{j,2}$	1
17	4		$LN''(N,N)$	12	$\sum_r \beta^{r,1} c_r^2$	2
18	4		$LN'N'N$	24	$\sum_{r,j} \beta^{r,1} \alpha_r^{j,0} c_j$	1
19	4		$LN'(LN)$	24	$\sum_{r,j} \beta^{r,1} \alpha_r^{j,1}$	1
20	4		$L^2N'N$	24	$\sum_r \beta^{r,2} c_r$	1
21	4		L^3N	24	$\sum_r \beta^{r,3}$	1

Table 2: Trees, elementary differentials and coefficients for $\tau \in T'$ with $\lvert\tau\rvert \leq 4$

3 Construction of exponential integrators

The schemes of Lawson [10] are exponential integrators derived simply by introducing a change of variable, $w(t) = \mathrm{e}^{-tL}\, u(t)$ in (1), and by applying a standard Runge–Kutta scheme to the resulting ODE. This approach results in a formula for w_1 in terms of w_0 By setting $u_n = \mathrm{e}^{tL}\, w_n$ one gets a scheme of the form (2)–(3) in which

$$a_r^j(z) = \alpha_r^{j,0}\, \mathrm{e}^{(c_r - c_j)z} \quad \text{and} \quad b^r(z) = \beta^{r,0}\, \mathrm{e}^{(1-c_r)z}.$$

This scheme has order p if the underlying scheme determined by $\alpha_r^{j,0}$ and $\beta^{r,0}$ is of order p. This gives us a very useful tool for constructing exponential integrators with given underlying Runge–Kutta schemes. We express this in a proposition

Proposition 3.1. Suppose that the coefficients $\alpha_r^{j,0}$ and $\beta^{r,0}$, $1 \le r, j \le s$ define a Runge–Kutta scheme of order p. Then, any exponential integrator of the form (2)–(3) satisfying

$$\alpha_r^{j,m} = \frac{1}{m!}(a_r^j)^{(m)}(0) = \frac{1}{m!}\alpha_r^{j,0}(c_r - c_j)^m, \quad 0 \le m \le p-2, \tag{10}$$

$$\beta^{r,m} = \frac{1}{m!}(b_r^j)^{(m)}(0) = \frac{1}{m!}\beta^{r,0}(1 - c_r)^m, \quad 0 \le m \le p-1, \tag{11}$$

is of order p. In the above expression we use $0^0 := 1$.

Proof. Order conditions for exponential integrators of order p involve $\alpha_r^{j,m}$, $0 \le m \le p-2$ and $\beta^{r,m}$, $0 \le m \le p-1$. On the other hand, the Lawson schemes must satisfy the order conditions for exponential integrators, and their values for these coefficients a precisely those specified in the proposition. $\square$

It is convenient to introduce finite dimensional function spaces V_a and V_b to which the respective coefficient functions $a_r^j(z)$ and $b^r(z)$ will belong. For the purpose of calculations, it is also useful to work with basis functions ψ_k for these spaces,

$$a_r^j(z) = \sum_{k=0}^{K_a-1} A_r^{j,k}\psi_k(z) \quad \text{and} \quad b^r(z) = \sum_{k=0}^{K_b-1} B^{r,k}\psi_k(z) \tag{12}$$

where $K_a = \dim(V_a)$ and $K_b = \dim(V_b)$. There is a technical assumption that we will adopt to the end of this note.

Assumption 3.2. Any finite dimensional function space V of dimension K used for coefficient functions $a_r^j(z)$ or $b^r(z)$ has the property that the map from V to $\mathbf{R}^K$ defined by

$$f \in V \;\mapsto\; (f(0), f'(0), \ldots, f^{(K-1)}(0))^T$$

is injective. Equivalently, any function in V is uniquely determined by its first K Taylor coefficients.

3.1 Deriving schemes with Natural Continuous Extensions

The approach of Krogstad in [9] is to approximate the nonlinear function $N(u(t_0 + \theta h))$, $0 < \theta < 1$ with a polynomial in θ. Assuming that the functions $a_r^j(z)$ for the internal stages are given, one lets $N(u(t_n + \theta h))$ be approximated by

$$\bar{N}(t_0 + \theta h) = \sum_{r=1}^{s} w_r'(\theta) N_r. \tag{13}$$

where $N_r = N(U_r)$ are the stage derivatives and $w_r(\theta)$ are polynomials of degree d, with $w(0) = 0$, such that $\bar{N}(t_0 + \theta h)$ approximates $N(u(t_0 + \theta h))$ uniformly for $0 < \theta < 1$ to a given order. Replacing the exact problem with the approximate one, $\dot{v} = Lv + \bar{N}(t),\ v(t_0) = u_0$ one finds

$$u_1 := v(t_0 + h) = \mathrm{e}^{hL} u_0 + \sum_{r=1}^{s} b^r(hL) N_r, \quad \text{where } b^r(z) = \int_0^1 \mathrm{e}^{(1-\theta)z} w_r'(\theta)\,\mathrm{d}\theta.$$

We define the functions

$$\phi_k(z) = \int_0^1 \mathrm{e}^{(1-\theta)z} \theta^k\,\mathrm{d}\theta,\ k = 0, 1, \ldots. \tag{14}$$

Thus, here the function space $V_b = \mathrm{span}\{\phi_0, \ldots, \phi_{d-1}\}$, so $\psi_k = \phi_k$ and $K_b = d$ in (12). Cox and Matthews [4] presented a fourth order scheme using these basis functions with $K_b = 3$. Krogstad [9] also derived a variant of their method by using a continuous extension as just explained. In [16] Zennaro developed a theory which generalises the collocation polynomial idea to arbitrary Runge–Kutta schemes. The approach was called Natural Continuous Extensions (NCE). By making a slight modification to the approach of Zennaro, one can find a useful way of deriving exponential integrators as well as providing them with a continuous extension.

Suppose $w_1(\theta), \ldots, w_s(\theta)$ are given polynomials of degree d, and that the stage derivatives $N_1, \ldots, N_s$ of an exponential integrator are given from (2). We define the $d-1$ degree polynomial $\bar{N}(t)$ by (13)

Definition 3.3. We call $\bar{N}(t)$ of (13) a Natural Continuous N-Extension (NCNE) of degree d of the exponential integrator (2)–(3) if

1. $$w_r(0) = 0, \quad w_r(1) = b^r(0), \qquad r = 1, \ldots, s.$$

2. $$\max_{t_0 \le t \le t_1} |N(u(t)) - \bar{N}(t)| = \mathcal{O}(h^{d-1}) \tag{15}$$

   where $u(t)$ is the exact solution of (1) satisfying $u(t_0) = u_0$.

3. $$\int_{t_0}^{t_1} G(t)(N(u(t)) - \bar{N}(t))\,\mathrm{d}t = \mathcal{O}(h^{p+1}) \tag{16}$$

   for every smooth matrix-valued function $G(t)$.

It is important to note that the polynomial $\bar{N}(t)$ only depends on the stages N_r and the weights $b^r(0) = \beta^{r,0}$ corresponding to the underlying Runge–Kutta scheme. We also observe that since the $w_r(\theta)$ do not depend on L, an NCNE as defined above is also an NCE in the sense of Zennaro for the system $\dot{u} = N(u)$. Before discussing the existence of NCNEs, we motivate their usefulness in designing exponential integrators. Suppose an underlying Runge–Kutta method has been chosen, and that an NCNE has been found. Then we can determine the functions $b^r(z)$ in order to obtain an exponential Runge–Kutta method of the same order as the underlying scheme.

Theorem 3.4. *If $\bar{N}(t)$ defined from* (13) *is an NCNE of degree d for a pth order scheme, then the functions*

$$b^r(z) = \int_0^1 \mathrm{e}^{(1-\theta)z} w'(\theta)\,\mathrm{d}\theta = \beta^{r,0} + z \int_0^1 \mathrm{e}^{(1-\theta)z} w(\theta)\,\mathrm{d}\theta,$$

define the weights of an exponential integrator of order p.

Proof. The exponential integrator we consider, is obtained by replacing (1) by

$$\dot{v} = Lv + \bar{N}(t), \qquad v(t_0) = u_0 \tag{17}$$

over the interval $[t_0, t_1]$ and by solving (17) exactly. We subtract (17) from (1) to obtain

$$\dot{u} - \dot{v} = L(\dot{u} - \dot{v}) + \big(N(u) - \bar{N}(t)\big)$$

We may solve this equation to obtain

$$u(t_1) - v(t_1) = \int_{t_0}^{t_1} \mathrm{e}^{(t_1-t)L} \big(N(u(t)) - \bar{N}(t)\big)\,\mathrm{d}t = \mathcal{O}(h^{p+1}),$$

the last equality is thanks to (16). $\square$

A reinterpretation of a result by Zennaro [16] combined with Proposition 3.1 leads to the following statement

Theorem 3.5. *Suppose that an underlying Runge–Kutta scheme with coefficients $\alpha_r^{j,0}$ and $\beta^{r,0}$ of order p is given. Then it is possible to find a set of coefficient functions $a_r^j(z)$ with $a_r^j(0) = \alpha_r^{j,0}$ such that an NCNE of degree $d = \lfloor \frac{p+1}{2} \rfloor$ exists. Moreover, if $\bar{N}(t)$ is a NCNE of degree d then*

$$\left\lfloor \frac{p+1}{2} \right\rfloor \le d \le \min(\nu^*, p)$$

where ν^* is the number of distinct elements among $c_1, \ldots, c_s$.

Corollary 3.6. For every underlying Runge–Kutta scheme, there exists an exponential integrator whose coefficient functions $b^r(z)$ are in the linear span of the functions $\{\phi_0(z), \ldots, \phi_{d-1}(z)\}$ where $d = \lfloor \frac{p+1}{2} \rfloor$.

Note in particular that one can derive fourth order exponential integrators using linear combinations of just $\phi_0(z)$ and $\phi_1(z)$ for $b^r(z)$, which is one less than what Cox and Matthews use, we present a specific example in section 4.

3.2 Lower bounds for K_a and K_b

We start establishing lower bounds for the number of necessary basis functions ψ_k by proving an ancillary result.

Lemma 3.7. *Let $q \geq 0$ be a finite integer. The matrix $T_q \in \mathbf{R}^{d\times d}$ with elements*

$$(T_q)_{m+1,k+1} = \frac{m!\, k!}{(m+k+1+q)!}, \quad 0 \leq m, k \leq d-1$$

is invertible.

Proof. Consider the functions $\hat{\phi}_{k,q}(z)$ whose m'th derivative at $z=0$ is $(T_q)_{m+1,k+1}$. Representing these functions by their Taylor series we get

$$\hat{\phi}_{k,q}(z) = \sum_{m=0}^{\infty} \frac{\hat{\phi}_{k,q}^{(m)}(0)}{m!}\, z^m = \sum_{m=0}^{\infty} \frac{k!}{(m+k+1+q)!}\, z^m$$

from which we conclude that $\hat{\phi}_{k,q-1} = k\hat{\phi}_{k-1,q}(z)$. Solving this recurrence equation we then obtain the representation

$$\hat{\phi}_{k,q} = \frac{k!}{(k+q)!}\, \hat{\phi}_{k+q,0}.$$

Note that $\hat{\phi}_{k,0}$ are exactly the functions ϕ_k of equation (14). Consequently

$$\hat{\phi}_{k,q}(z) = \frac{k!}{(k+q)!} \int_0^1 \mathrm{e}^{z(1-\theta)}\, \theta^k\, w_q(\theta)\, \mathrm{d}\theta \quad \text{where} \quad w_q(\theta) = \theta^q. \tag{18}$$

Suppose there exists a non-zero $x = (x_0, \ldots, x_{d-1})^T$ such that $T_q x = 0$. Then the function $f_q(z) = \sum_{k=0}^{d-1} x_k\, \hat{\phi}_{k,q}(z)$ satisfies $f_q^{(m)}(0) = 0$ for $0 \leq m \leq d-1$. From (18) we have

$$f_q(z) = \int_0^1 \mathrm{e}^{z(1-\theta)}\, p_x^q(\theta)\, w_q(\theta)\, \mathrm{d}\theta \quad \text{where} \quad p_x^q(\theta) = \sum_{k=0}^{d-1} \frac{k!}{(k+q)!}\, x_k\, \theta^k, \tag{19}$$

so p_x^q is a non-zero polynomial of degree at most $d-1$. Differentiating (19) m times with respect to z and setting $z=0$, we find that $T_q x = 0$ if and only if

$$\int_0^1 (1-\theta)^m\, p_x^q(\theta)\, w_q(\theta)\, \mathrm{d}\theta = 0, \quad 0 \leq m \leq d-1.$$

In other words $T_q x = 0$ if and only if p_x^q is orthogonal with respect to the weight function w_q to every polynomial of degree $d-1$ on $[0,1]$. This implies $p_x^q \equiv 0$ which contradicts the assumption that x is non-zero. Therefore T_q is non-singular. □

We remark that as a part of the proof of this lemma we have also asserted that function spaces $V = \mathrm{span}(\phi_q, \ldots, \phi_{q+K-1}), q \geq 0$, with ϕ_k defined by (14), satisfy Assumption 3.2.

Theorem 3.8. *For an exponential integrator of order p, the dimension of the function spaces V_a and V_b are bounded from below as follows*

$$K_a = \dim V_a \geq \left\lfloor \frac{p}{2} \right\rfloor, \quad K_b = \dim V_b \geq \left\lfloor \frac{p+1}{2} \right\rfloor. \tag{20}$$

Proof. We will show that using smaller values of K_a or K_b than dictated by (20) is incompatible with the order conditions for a scheme of order p. Let V_a and V_b be arbitrary function spaces, satisfying Assumption 3.2, let V denote either of them, and let $d = \dim V$. If $f \in V$, then there are numbers $s_0, \ldots, s_{d-1}$ such that

$$f^{(d)}(0) = \sum_{m=0}^{d-1} s_m f^{(m)}(0) \tag{21}$$

Suppose now that $d_a := \dim V_a = \lfloor p/2 \rfloor - 1$ and $d_b := \dim V_b = \lfloor (p+1)/2 \rfloor - 1$. Consider the bicoloured trees $\tau_q^{m,k}$ defined by

$$\tau_q^{m,k} = B_+^q\big(W_+^m B_+(\overbrace{\bullet, \ldots, \bullet}^{k})\big)$$

which consist of a string of $q \geq 0$ black nodes followed by a string of $m > 0$ white nodes with a bushy tree of $k+1$ black nodes grafted onto the topmost leaf of the white nodes. We shall use these trees with $q = 0$ for proving the bound on K_b and with $q = 1$ for K_a. The density of $\tau_q^{m,k}$ is given by

$$\gamma(\tau_q^{m,k}) = \frac{(m+k+1+q)!}{k!}.$$

The trees corresponding to order conditions for a scheme of order p have at most p nodes, $|\tau_q^{m,k}| = q + m + 1 + k \leq p \Rightarrow 0 \leq k \leq p - m - 1 - q$. The definition of d_a and d_b implies that $p - 2 \geq 2d_a$ and $p - 1 \geq 2d_b$. If we set $q = 1, m = d_a$ we thus obtain conditions for $0 \leq k \leq d_a$, whereas $q = 0, m = d_b$ results in $0 \leq k \leq d_b$. The conditions corresponding to $\tau_1^{d_a,k}$ can be expressed as

$$\frac{1}{d_a!} \sum_{r,j=1}^{s} \beta^{r,0} (a_r^j)^{(d_a)}(0) c_j^k = \frac{k!}{(d_a+k+2)!}, \quad 0 \leq k \leq d_a$$

which, upon insertion of $(a_r^j)^{(d_a)}(0) = \sum s_m (a_r^j)^{(m)}(0)$ as in (21) yields

$$\frac{k!\; d_a!}{(k+d_a+2)!} = \sum_{m=0}^{d_a-1} s_m \Big(\sum_{r=1}^{s} \beta^{r,0} (a_r^j)^{(m)}(0) c_j^k\Big) = \sum_{m=0}^{d_a-1} s_m \frac{k!\; m!}{(k+m+2)!}.$$

The conditions for $\tau_0^{d_b,k}$ similarly yield

$$\frac{k!\; d_b!}{(k+d_b+1)!} = \sum_{m=0}^{d_b-1} s_m \Big(\sum_{r=1}^{s} (b^r)^{(m)}(0)\, c_r^k\Big) = \sum_{m=0}^{d_b-1} s_m \frac{k!\; m!}{(k+m+1)!}.$$

In both cases ($d = d_a$ or d_b) we end up with a $(d+1) \times d$ linear system of equations for determining $s_m, m = 0 \ldots, d-1$. This system is of the form

$$\sum_{m=0}^{d-1} \frac{k!\; m!}{(k+m+1+q)!} s_m = \frac{k!\; d!}{(k+d+1+q)!}, \quad 0 \leq k \leq d$$

for $q \in \{0, 1\}$ and is solvable only if the matrix with elements

$$(T_q)_{k+1,m+1} = \frac{k!\; m!}{(k+m+1+q)!}, \quad 0 \leq k, m \leq d$$

is singular. However, Lemma 3.7 implies that the matrix T_q is invertible so the linear system is inconsistent. It is hence not possible to choose $K_a = d_a$ or $K_b = d_b$. □

Some remarks regarding the implications of Theorem 3.8 are in order. First, note that the bounds in the theorem are not proved to be sharp, however Theorem 3.5 ensures that the lower bound is attainable for the dimension of V_b if a basis is given by the functions ϕ_k of (14). However, this result does not apply to the space V_a of the functions $a_r^j(z)$. For instance, in the case $p = 5$, one can prove that it is indeed possible to take $K_a = 2$, but V_a cannot be the span of ϕ_0 and ϕ_1. But an example of a feasible two-dimensional space is that with basis $\psi_0(z) = \phi_1(z)$ and $\psi_1(z) = \phi_1(\frac{3}{5}z)$. A particular scheme is given in Table 4. But the usefulness of the bounds are questionable in this particular example. Using, say $V_b = \mathrm{span}\{\phi_0, \phi_1, \phi_2\}$ combined with the above choice of V_a requires the computation with a total of 4 basis functions, whereas only 3 are necessary if one instead chooses $V_a = V_b$.

We furthermore note that the minimum attainable value of the parameters K_a and K_b depend only on the order p, of the underlying Runge–Kutta scheme and the choice of the basis functions ψ_k. Specifically, the coefficients of the underlying Runge–Kutta scheme do not influence the minimum values of K_a and K_b.

4 Examples of exponential integrators

The procedure we have used in constructing schemes may be summarised as follows

1. Choose an underlying Runge–Kutta scheme. This determines $\alpha_r^{j,0}$ and $\beta^{r,0}$.

2. Choose basis functions $\psi_k(z)$ for the coefficient functions and determine K_a and K_b.

3. Use the order conditions for the trees of the form $W_+^m(\tau_C)$ where τ_C is a tree with only black nodes, and determine $\beta^{r,m}$, for $1 \leq m \leq K_b - 1$. See also (11).

4. Identify order conditions which are linear in $c'_r = \sum_{j=1}^s \alpha_r^{j,1}$ and which otherwise depend only on $\beta_r^{j,m}$, $0 \leq m \leq K_b - 1$ and $\alpha_r^{j,0}$, and solve for c'_r.

5. Identify remaining conditions which depend linearly on $\alpha_r^{j,1}$. Solve for $\alpha_r^{j,1}$ together with $c'_r = \sum_{j=1}^s \alpha_r^{j,1}$. Repeat this procedure to solve for $\alpha_r^{j,m}$, $2 \leq m \leq K_a - 1$.

6. $\beta^{r,m}$ are now uniquely determined for $m \geq K_b$ and $\alpha_r^{j,m}$ for $m \geq K_a$ by (21). Verify all remaining order conditions for $\beta^{r,m}$, $K_b \leq m \leq p - 1$ and for $\alpha_r^{j,m}$, $K_a \leq m \leq p - 2$. If inconsistencies appear, the basis functions are not feasible.

7. Verify all remaining order conditions.

In most cases we have considered, once $\alpha_r^{j,0}$ and $\beta^{r,0}$ have been chosen, one can find the remaining $\alpha_r^{j,m}$ independently of the $\beta^{r,m}$. Most of the exponential integrators we find in the literature are based on the classical fourth order scheme of Kutta, and it is typical that one can combine $a_r^j(z)$ from one scheme with $b^r(z)$ from another scheme and still get overall order four.

In the class of ETD schemes, proposed by Cox and Matthews [4] and Krogstad [9], the space V_b is spanned by the three functions ϕ_0, ϕ_1, ϕ_2 of (14). However in the former reference, $\dim V_a = 2$ with a basis $\{\phi_0(z/2), z\phi_0(z/2)^2\}$. This V_a coincides with the one used in [2], given in Table 1(b).

Another choice is to use $\phi_k(z)$ of (14) both for V_a and V_b. In Table 3 we characterise all resulting schemes with $K_a = 2$ and $K_b = 3$. It is interesting to note that Theorem 3.8

predicts $K_a \geq 2$ and $K_b \geq 2$, and indeed, by choosing $\gamma_1 = \frac{1}{3}$ and $\gamma_2 = -\frac{1}{3}$, we see that ϕ_2 disappears from the $b^r(z)$-functions. Choosing $\gamma_1 = \gamma_2 = 0$, we recover the $b^r(z)$-functions obtained in [4]. Letting V_b, be spanned by $\psi_0(z) = \phi_0(z)$ and $\psi_1(z) = \phi_0(z/2)$, one obtains

$$
\begin{aligned}
a_2^1(z) &= -(\tfrac{1}{2} + \rho_1)\phi_0(z) + (2\rho_1 + 2)\phi_1(z) \\
a_3^1(z) &= (1 + \rho_1 - \tfrac{1}{4}(\rho_2 + \rho_3))\phi_0(z) + (-2 - 2\rho_1 + \tfrac{1}{2}(\rho_2 + \rho_3))\phi_1(z) \\
a_3^2(z) &= (-1 + \tfrac{1}{4}(\rho_2 + \rho_3))\phi_0(z) + (3 - \tfrac{1}{2}(\rho_2 + \rho_3)\phi_1(z) \\
a_4^1(z) &= \tfrac{1}{2}(\rho_2 + \rho_3)\phi_0(z) - (\rho_2 + \rho_3)\phi_1(z) \\
a_4^2(z) &= -\frac{\rho_2}{2}\phi_0(z) + \rho_2\phi_1(z) \\
a_4^3(z) &= (1 - \tfrac{1}{2}\rho_3)\phi_0(z) + \rho_3\phi_1(z)
\end{aligned}
$$

$$
\begin{aligned}
b^1(z) &= (1 + \gamma_2)\,\phi_0(z) + (-3 - 6\gamma_2)\,\phi_1(z) + (6\gamma_2 + 2)\,\phi_2(z) \\
b^2(z) &= (-\gamma_1 - 2\gamma_2)\,\phi_0(z) + (6\gamma_1 + 12\gamma_2 + 2)\phi_1(z) + (-6\gamma_1 - 12\gamma_2 - 2)\,\phi_2(z) \\
b^3(z) &= \gamma_1\,\phi_0(z) + (-6\gamma_1 + 2)\,\phi_1(z) + (6\gamma_1 - 2)\,\phi_2(z) \\
b^4(z) &= \gamma_2\,\phi_0(z) + (-6\gamma_2 - 1)\,\phi_1(z) + (6\gamma_2 + 2)\,\phi_2(z)
\end{aligned}
$$

Table 3: Coefficient function for a fourth order ETD scheme with classical RK4 as underlying scheme. Basis functions given by (14).

the unique solution

$$
\begin{aligned}
b^1(z) &= \tfrac{1}{2}\phi_0(z) - \tfrac{1}{3}\phi_0(z/2) \\
b^2(z) &= b^3(z) = \tfrac{1}{3}\phi_0(z) \\
b^4(z) &= -\tfrac{1}{6}\phi_0(z) + \tfrac{1}{3}\phi_0(z/2).
\end{aligned}
\tag{22}
$$

These weights coincide with the ones derived in the fourth order scheme in [2], given in Table 1(b). Yet another choice is to let V_b consist of functions of the form $p(z)\phi_0(z)$ where $p(z)$ is a polynomial of degree 1, and we recover $b^r(z)$ as in Table 1(a).

Finally, we give an example of a fifth order exponential integrator based on a scheme of Fehlberg. As indicated in Section 3.2 we take $\dim V_a = 2$ with basis $\psi_0(z) = \phi_1(z)$, $\psi_1(z) = \phi_1(\frac{3}{5}z)$. For V_b we use the basis $\psi_k(z) = \phi_k(z)$. The resulting coefficient functions are given in Table 4.

In summary, this paper presents a complete order theory for exponential integrators of the form (2)–(3). From deriving order conditions by means of bicoloured trees to proving bounds for the lowest possible number of basis functions, the results presented herein provide a general framework for constructing schemes of this type. A number of issues are, however, not addressed in the present paper. These include systematically choosing basis functions ψ_k, and how to construct schemes with low error constants.

Exponential integrators are interesting from the point of view of handling unbounded or stiff operators, yet the order theory does not say anything about what happens for large eigenmodes of L in (1). Determining conditions for favorable behaviour in light of such operators should be an arena for future work.

5 Acknowledgements

Thanks to Christian Bower for advice regarding the enumeration of bicoloured trees.

$$
\begin{array}{c|cccccc}
0 & & & & & & \\
\frac{2}{9} & -\frac{2}{3}\phi_1 + \frac{10}{9}\hat{\phi}_1 & & & & & \\
\frac{1}{3} & \frac{569}{11544}\phi_1 + \frac{1355}{11544}\hat{\phi}_1 & -\frac{831}{3848}\phi_1 + \frac{2755}{3848}\hat{\phi}_1 & & & & \\
\frac{3}{4} & -\frac{77157}{61568}\phi_1 + \frac{143535}{61568}\hat{\phi}_1 & \frac{587979}{61568}\phi_1 - \frac{821745}{61568}\hat{\phi}_1 & -\frac{405}{64}\phi_1 + \frac{675}{64}\hat{\phi}_1 & & & \\
1 & \frac{655263}{7696}\phi_1 - \frac{2031205}{23088}\hat{\phi}_1 & -\frac{1148769}{7696}\phi_1 + \frac{1252665}{7696}\hat{\phi}_1 & \frac{1593}{40}\phi_1 - \frac{405}{8}\hat{\phi}_1 & \frac{144}{5}\phi_1 - \frac{80}{3}\hat{\phi}_1 & & \\
\frac{5}{6} & -\frac{2212835}{277056}\phi_1 + \frac{6888625}{831168}\hat{\phi}_1 & \frac{477285}{30784}\phi_1 - \frac{496525}{30784}\hat{\phi}_1 & -\frac{39}{16}\phi_1 + \frac{65}{16}\hat{\phi}_1 & -\frac{4}{9}\phi_1 + \frac{20}{27}\hat{\phi}_1 & -\frac{185}{96}\phi_1 + \frac{575}{288}\hat{\phi}_1 & \\
\hline
 & b^1(z) & b^2(z) & b^3(z) & b^4(z) & b^5(z) & b^6(z)
\end{array}
$$

$$
\begin{aligned}
b^1(z) &= \tfrac{47}{150}\phi_0 - \tfrac{188}{75}\phi_1 + \tfrac{47}{15}\phi_2 \\
b^2(z) &= 0 \\
b^3(z) &= -\tfrac{43}{25}\phi_0 + \tfrac{132}{5}\phi_1 - 33\phi_2 \\
b^4(z) &= \tfrac{4124}{75}\phi_0 - \tfrac{6152}{15}\phi_1 + \tfrac{1352}{3}\phi_2 \\
b^5(z) &= \tfrac{189}{10}\phi_0 - \tfrac{662}{5}\phi_1 + 142\phi_2 \\
b^6(z) &= -\tfrac{1787}{25}\phi_0 + \tfrac{12966}{25}\phi_1 - \tfrac{2814}{5}\phi_2
\end{aligned}
$$

Table 4: Coefficient functions for a fifth order exponential integrator with Fehlbergs fifth order RK as the underlying scheme. Here $\hat{\phi}_1(z) = \phi_1(\frac{3}{5}z)$.

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