Order conditions for multistep Runge-Kutta methods

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1 Review of Order Conditions for Runge–Kutta Methods

In this section we review the derivation of order conditions for Runge-Kutta methods via the approach due to Albrecht [Albrecht, 1996]. The basic notation is defined in section 1.1. A formula for the global error in terms of the method coefficients is derived in section 1.2. This leads to a recursion for determining the order conditions, as explained in section 3.1.

1.1 Notation

Write the nth step of a Runge–Kutta method as

$$\mathbf{y}^n = u^n\mathbf{e} + \Delta t\mathbf{A}\mathbf{f}^n \tag{1a}$$

$$u^{n+1} = u^n + \Delta t\mathbf{b}^{\mathrm{T}}\mathbf{f}^n \tag{1b}$$

where

$$\begin{aligned}\mathbf{y}^n &= [y_1^n, \dots, y_s^n],\\ \mathbf{f}^n &= [F(y_1^n), \dots, F(y_s^n)]\end{aligned}$$

are the vector of stage values and stage derivatives, respectively. Let $\tilde{u}(t)$ denote the exact solution at time t and define the vectors of exact stage solution values and exact stage derivatives:

$$\begin{aligned}\tilde{\mathbf{y}}^n &= [\tilde{u}(t_n + c_1\Delta t), \dots, \tilde{u}(t_n + c_s\Delta t)],\\ \tilde{\mathbf{f}}^n &= [F(\tilde{u}(t_n + c_1\Delta t)), \dots, F(\tilde{u}(t_n + c_s\Delta t))].\end{aligned}$$

Next define the *truncation error* τ^n and *stage truncation errors* $\boldsymbol{\tau}^n$ by

$$\tilde{\mathbf{y}}^n = \tilde{u}^n\mathbf{e} + \Delta t\mathbf{A}\tilde{\mathbf{f}}^n + \Delta t\boldsymbol{\tau}^n \tag{2a}$$

$$\tilde{u}(t_{n+1}) = \tilde{u}^n + \Delta t\mathbf{b}^{\mathrm{T}}\tilde{\mathbf{f}}^n + \Delta t\tau^n. \tag{2b}$$

1.2 Global error formulas

To find formulas for the truncation errors, we make use of the Taylor expansions

$$\tilde{u}(t_n + c_i\Delta t) = \sum_{k=0}^{\infty} \frac{1}{k!}\Delta t^k c_i^k \tilde{u}^{(k)}(t_n) \tag{3a}$$

$$F(\tilde{u}(t_n + c_i\Delta t)) = \sum_{k=1}^{\infty} \frac{1}{(k-1)!}\Delta t^{k-1} c_i^{k-1} \tilde{u}^{(k)}(t_n) \tag{3b}$$

Substitution of (3) into (2) gives

$$\boldsymbol{\tau}^n = \sum_{k=1}^{\infty} \left(\frac{1}{k!}\mathbf{c}^k - \frac{1}{(k-1)!}\mathbf{A}\mathbf{c}^{k-1}\right) \Delta t^{k-1}\tilde{u}^{(k)}(t_n) = \sum_{k=1}^{\infty} \boldsymbol{\tau}_k \Delta t^{k-1}\tilde{u}^{(k)}(t_n) \tag{4a}$$

$$\tau^n = \sum_{k=1}^{\infty} \left(\frac{1}{k!} - \frac{1}{(k-1)!}\mathbf{b}^{\mathrm{T}}\mathbf{c}^{k-1}\right) \Delta t^{k-1}\tilde{u}^{(k)}(t_n) = \sum_{k=1}^{\infty} \tau_k \Delta t^{k-1}\tilde{u}^{(k)}(t_n) \tag{4b}$$

where

$$\boldsymbol{\tau}_k = \frac{1}{k!}\mathbf{c}^k - \frac{1}{(k-1)!}\mathbf{A}\mathbf{c}^{k-1} \tag{5a}$$

$$\tau_k = \frac{1}{k!} - \frac{1}{(k-1)!}\mathbf{b}^{\mathrm{T}}\mathbf{c}^{k-1} \tag{5b}$$

Subtracting (2) from (1) gives

$$\boldsymbol{\epsilon}^n = \epsilon^n \mathbf{e} + \Delta t \mathbf{A}\boldsymbol{\delta}^n - \Delta t \boldsymbol{\tau}^n \tag{6a}$$

$$\epsilon^{n+1} = \epsilon^n + \Delta t \mathbf{b}^{\mathrm{T}}\boldsymbol{\delta}^n - \Delta t \tau^n, \tag{6b}$$

where $\epsilon^{n+1} = u^{n+1} - \tilde{u}(t_{n+1})$ is the global error, $\boldsymbol{\epsilon}^n = \mathbf{y}^n - \tilde{\mathbf{y}^n}$, is the global stage error, and $\boldsymbol{\delta}^n = \mathbf{f}^n - \tilde{\mathbf{f}}^n$ is the stage derivative error.

Next assume expansions for the stage derivative errors $\boldsymbol{\delta}^n$ and stage errors $\boldsymbol{\epsilon}^n$ as a power series in Δt:

$$\boldsymbol{\delta}^n = \sum_{k=0}^{\infty} \boldsymbol{\delta}_k^n \Delta t^k, \tag{7a}$$

$$\boldsymbol{\epsilon}^n = \sum_{k=0}^{\infty} \boldsymbol{\epsilon}_k^n \Delta t^k. \tag{7b}$$

Then substituting the expansions (7a) and (4) into the global error formula (7b) yields

$$\boldsymbol{\epsilon}^n = \epsilon^n \mathbf{e} + \sum_{k=0}^{p-1} \mathbf{A}\boldsymbol{\delta}_k^n \Delta t^{k+1} - \sum_{k=1}^{p} \boldsymbol{\tau}_k \tilde{u}^{(k)}(t_n)\Delta t^k + \mathcal{O}(\Delta t^{p+1}) \tag{8a}$$

$$\epsilon^{n+1} = \epsilon^n + \sum_{k=0}^{p-1} \mathbf{b}^{\mathrm{T}}\boldsymbol{\delta}_{k-1}^n \Delta t^{k+1} - \sum_{k=1}^{p} \tau_k \tilde{u}^{(k)}(t_n)\Delta t^k + \mathcal{O}(\Delta t^{p+1}) \tag{8b}$$

Assuming stable propagation of errors, we have global accuracy of order p if the following conditions hold:

$$\begin{aligned} \tau_k &= 0 && \text{for } 0 \le k \le p \\ \mathbf{b}^{\mathrm{T}}\boldsymbol{\delta}_k^n &= 0 && \text{for } 0 \le k \le p-1. \end{aligned}$$

It remains to determine the vectors $\boldsymbol{\delta}_k^n$. In fact, we can relate these recursively to the global stage error vectors $\boldsymbol{\epsilon}_k$. First define

$$\begin{aligned} \mathbf{t}_n &= t_n \mathbf{e} + \mathbf{c}\Delta t, \\ \mathbf{F}(\mathbf{y}, \mathbf{t}) &= [F(y_1(t_1)), \dots, F(y_s(t_s))]^{\mathrm{T}}. \end{aligned}$$

Then we have the Taylor series

$$\begin{aligned} \mathbf{f}^n = \mathbf{F}(\mathbf{y}^n, \mathbf{t}_n) &= \tilde{\mathbf{f}}^n + \sum_{j=1}^{\infty} \frac{1}{j!}(\mathbf{y}^n - \tilde{\mathbf{y}}^n)^j \cdot \mathbf{F}^{(j)}(\tilde{\mathbf{y}}^n, \mathbf{t}_n) \\ &= \tilde{\mathbf{f}}^n + \sum_{j=1}^{\infty} \frac{1}{j!}(\boldsymbol{\epsilon}^n)^j \cdot \mathbf{g}_j(\mathbf{t}_n), \end{aligned}$$

where

$$\begin{aligned} \mathbf{F}^{(j)}(\mathbf{y}, \mathbf{t}) &= [F^{(j)}(y_1(t_1)), \dots, F^{(j)}(y_s(t_s))]^{\mathrm{T}}, \\ \mathbf{g}_j(\mathbf{t}) &= [F^{(j)}(y(t_1)), \dots, F^{(j)}(y(t_s))]^{\mathrm{T}}, \end{aligned}$$

and the dot product denotes componentwise multiplication. Thus

$$\boldsymbol{\delta}^n = \mathbf{f}^n - \tilde{\mathbf{f}}^n = \sum_{j=1}^{\infty} \frac{1}{j!}(\boldsymbol{\epsilon}^n)^j \cdot \mathbf{g}_j(t_n \mathbf{e} + \mathbf{c}\Delta t). \tag{9}$$

Since

$$\mathbf{g}_j(t_n\mathbf{e}+\mathbf{c}) = \sum_{l=0}^{\infty} \frac{\Delta t^l}{l!}\mathbf{C}^l \mathbf{g}_j^{(l)}(t_n), \tag{10}$$

where $\mathbf{C} = \mathrm{diag}(\mathbf{c})$, we finally obtain the desired expansion:

$$\boldsymbol{\delta}^n = \sum_{j=1}^{\infty}\sum_{l=0}^{\infty} \frac{\Delta t^l}{j!l!}\mathbf{C}^l (\boldsymbol{\epsilon}^n)^j \cdot \mathbf{g}_j^{(l)}(t_n). \tag{11}$$

1.3 Generation of stage derivative error vectors

Combining (7b) with (8a) and equating coefficients of powers of Δt gives (for $k \geq 1$)

$$\boldsymbol{\epsilon}_k^n = \mathbf{A}\boldsymbol{\delta}_{k-1}^n - \boldsymbol{\tau}_k \tilde{u}^{(k)}(t_n). \tag{12}$$

To determine the coefficients $\boldsymbol{\delta}_k$, we alternate recursively between (11) and (12). Typically, the abscissas $\mathbf{c}$ are chosen as $\mathbf{Ae}$ so that $\boldsymbol{\tau}_1 = 0$; we will assume this since it simplifies the conditions considerably.

The terms appearing in the $\boldsymbol{\delta}_k$ involve products of certain constants with derivatives of $\tilde{u}$ and the Butcher coefficients. In order for $\mathbf{b}^{\mathrm{T}}\delta_k$ to vanish for arbitrary $\tilde{u}$, it must be that $\mathbf{b}^{\mathrm{T}}\mathbf{v} = 0$ for each vector $\mathbf{v}$ appearing in $\boldsymbol{\delta}_k$. Since this latter condition does not depend on $|\mathbf{v}|$, the constants and the derivatives of $\tilde{u}$ can be neglected in our analysis. Hence we focus solely on the vectors appearing in $\boldsymbol{\delta}_k$ depending on the Butcher coefficients. We use the symbol $\bar{\boldsymbol{\delta}}_k$ to denote the set of these vectors. Then the order conditions for order p can be summarized as follows:

$$\frac{1}{k!} = \frac{1}{(k-1)!}\mathbf{b}^{\mathrm{T}}\mathbf{c}^{k-1} \qquad \text{for } 1 \leq k \leq p \tag{13a}$$

$$\mathbf{b}^{\mathrm{T}}\mathbf{v} = 0 \qquad \text{for all } \mathbf{v} \in \bar{\boldsymbol{\delta}}_k, \quad \text{for } 1 \leq k \leq p-1. \tag{13b}$$

The conditions (13a) are referred to as *bushy-tree order conditions* because they are associated with the bushy trees in Butcher's approach [Butcher, 2003]. It is convenient to refer to the order conditions (13b) as *non-bushy-tree order conditions*; the remainder of the section focuses on the task of determining these explicitly. Also $\boldsymbol{\delta}_0 = 0$ for any consistent method. Then taking $k = 1$ in (12) gives $\boldsymbol{\epsilon}_1 = 0$. Plugging this into (11) yields $\boldsymbol{\delta}_1 = 0$.

Taking $k = 2$ in (12), we see that the factor $\boldsymbol{\tau}_2$ appears in $\boldsymbol{\epsilon}_2$. Plugging this into (11), we see that $\boldsymbol{\tau}_2$ appears in $\bar{\boldsymbol{\delta}}_2$. Using this (with $k = 3$) in (12), we have that $\mathbf{A}\boldsymbol{\tau}_2$ and $\boldsymbol{\tau}_3$ appear in $\boldsymbol{\epsilon}_3$. Substituting this into (11) reveals that terms proportional to $\mathbf{C}\boldsymbol{\tau}_2, \mathbf{A}\boldsymbol{\tau}_2, \boldsymbol{\tau}_3$ appear in $\bar{\boldsymbol{\delta}}_3$.

Proceeding in this manner, the order conditions for any order of accuracy can be derived.

2 Enumeration of conditions

In this section we write out explicitly (for reference) the result of applying the recursion derived in the previous section.

2.1 Terms appearing in the error vectors

Here we enumerate the terms generated by the recursion outlined above. As before, we assume $\mathbf{c} = \mathbf{A}\mathbf{e}$ so that $\boldsymbol{\tau}_1 = 0$.

- Terms appearing in $\bar{\boldsymbol{\delta}}_1$: $\emptyset$
- Terms appearing in $\boldsymbol{\epsilon}_2$: $\boldsymbol{\tau}_2$
- Terms appearing in $\bar{\boldsymbol{\delta}}_2$: $\boldsymbol{\tau}_2$
- Terms appearing in $\boldsymbol{\epsilon}_3$: $\mathbf{A}\boldsymbol{\tau}_2, \boldsymbol{\tau}_3$
- Terms appearing in $\bar{\boldsymbol{\delta}}_3$: $\mathbf{C}\boldsymbol{\tau}_2, \mathbf{A}\boldsymbol{\tau}_2, \boldsymbol{\tau}_3$
- Terms appearing in $\boldsymbol{\epsilon}_4$: $\mathbf{AC}\boldsymbol{\tau}_2, \mathbf{A}^2\boldsymbol{\tau}_2, \mathbf{A}\boldsymbol{\tau}_3, \boldsymbol{\tau}_4$
- Terms appearing in $\bar{\boldsymbol{\delta}}_4$: $\mathbf{AC}\boldsymbol{\tau}_2, \mathbf{A}^2\boldsymbol{\tau}_2, \mathbf{A}\boldsymbol{\tau}_3, \boldsymbol{\tau}_4, \mathbf{CA}\boldsymbol{\tau}_2, \mathbf{C}\boldsymbol{\tau}_3, \mathbf{C}^2\boldsymbol{\tau}_2, \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_2$
- Terms appearing in $\boldsymbol{\epsilon}_5$:
  $\mathbf{A}^2\mathbf{C}\boldsymbol{\tau}_2, \mathbf{A}^3\boldsymbol{\tau}_2, \mathbf{A}^2\boldsymbol{\tau}_3, \mathbf{A}\boldsymbol{\tau}_4, \mathbf{ACA}\boldsymbol{\tau}_2, \mathbf{AC}\boldsymbol{\tau}_3, \mathbf{AC}^2\boldsymbol{\tau}_2, \mathbf{A}(\boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_2), \boldsymbol{\tau}_5$
- Terms appearing in $\bar{\boldsymbol{\delta}}_5$:
  $\mathbf{A}^2\mathbf{C}\boldsymbol{\tau}_2, \mathbf{A}^3\boldsymbol{\tau}_2, \mathbf{A}^2\boldsymbol{\tau}_3, \mathbf{A}\boldsymbol{\tau}_4, \mathbf{ACA}\boldsymbol{\tau}_2, \mathbf{AC}\boldsymbol{\tau}_3, \mathbf{AC}^2\boldsymbol{\tau}_2, \mathbf{A}(\boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_2), \boldsymbol{\tau}_5,$
  $\mathbf{CAC}\boldsymbol{\tau}_2, \mathbf{CA}^2\boldsymbol{\tau}_2, \mathbf{CA}\boldsymbol{\tau}_3, \mathbf{C}\boldsymbol{\tau}_4,$
  $\mathbf{C}^2\mathbf{A}\boldsymbol{\tau}_2, \mathbf{C}^2\boldsymbol{\tau}_3, \mathbf{C}^3\boldsymbol{\tau}_2, \mathbf{C}(\boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_2), \boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3, \boldsymbol{\tau}_2 \cdot (\mathbf{A}\boldsymbol{\tau}_2)$
- Terms appearing in $\boldsymbol{\epsilon}_6$:
  $\mathbf{A}^3\mathbf{C}\boldsymbol{\tau}_2, \mathbf{A}^4\boldsymbol{\tau}_2, \mathbf{A}^3\boldsymbol{\tau}_3, \mathbf{A}^2\boldsymbol{\tau}_4, \mathbf{ACA}^2\boldsymbol{\tau}_2, \mathbf{A}^2\mathbf{C}\boldsymbol{\tau}_3, \mathbf{A}^2\mathbf{C}^2\boldsymbol{\tau}_2, \mathbf{A}^2(\boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_2), \mathbf{A}\boldsymbol{\tau}_5,$
  $\mathbf{ACAC}\boldsymbol{\tau}_2, \mathbf{ACA}^2\boldsymbol{\tau}_2, \mathbf{ACA}\boldsymbol{\tau}_3, \mathbf{AC}\boldsymbol{\tau}_4,$
  $\mathbf{AC}^2\mathbf{A}\boldsymbol{\tau}_2, \mathbf{AC}^2\boldsymbol{\tau}_3, \mathbf{AC}^3\boldsymbol{\tau}_2, \mathbf{AC}(\boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_2), \mathbf{A}(\boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3), \mathbf{A}(\boldsymbol{\tau}_2 \cdot (\mathbf{A}\boldsymbol{\tau}_2)), \boldsymbol{\tau}_6$
- Terms appearing in $\bar{\boldsymbol{\delta}}_6$:
  $\mathbf{A}^3\mathbf{C}\boldsymbol{\tau}_2, \mathbf{A}^4\boldsymbol{\tau}_2, \mathbf{A}^3\boldsymbol{\tau}_3, \mathbf{A}^2\boldsymbol{\tau}_4, \mathbf{ACA}^2\boldsymbol{\tau}_2, \mathbf{A}^2\mathbf{C}\boldsymbol{\tau}_3, \mathbf{A}^2\mathbf{C}^2\boldsymbol{\tau}_2, \mathbf{A}^2(\boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_2), \mathbf{A}\boldsymbol{\tau}_5,$
  $\mathbf{ACAC}\boldsymbol{\tau}_2, \mathbf{ACA}^2\boldsymbol{\tau}_2, \mathbf{ACA}\boldsymbol{\tau}_3, \mathbf{AC}\boldsymbol{\tau}_4,$
  $\mathbf{AC}^2\mathbf{A}\boldsymbol{\tau}_2, \mathbf{AC}^2\boldsymbol{\tau}_3, \mathbf{AC}^3\boldsymbol{\tau}_2, \mathbf{AC}(\boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_2), \mathbf{A}(\boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3), \mathbf{A}(\boldsymbol{\tau}_2 \cdot (\mathbf{A}\boldsymbol{\tau}_2)), \boldsymbol{\tau}_6,$

$\mathbf{C}\mathbf{A}^2\mathbf{C}\boldsymbol{\tau}_2, \mathbf{C}\mathbf{A}^3\boldsymbol{\tau}_2, \mathbf{C}\mathbf{A}^2\boldsymbol{\tau}_3, \mathbf{C}\mathbf{A}\boldsymbol{\tau}_4, \mathbf{C}\mathbf{A}C\mathbf{A}\boldsymbol{\tau}_2, \mathbf{C}\mathbf{A}C\boldsymbol{\tau}_3, \mathbf{C}\mathbf{A}C^2\boldsymbol{\tau}_2, \mathbf{C}\mathbf{A}(\boldsymbol{\tau}_2\cdot\boldsymbol{\tau}_2), \mathbf{C}\boldsymbol{\tau}_5,$
$\mathbf{C}^2\mathbf{A}C\boldsymbol{\tau}_2, \mathbf{C}^2\mathbf{A}^2\boldsymbol{\tau}_2, \mathbf{C}^2\mathbf{A}\boldsymbol{\tau}_3, \mathbf{C}^2\boldsymbol{\tau}_4, \mathbf{C}^3\mathbf{A}\boldsymbol{\tau}_2, \mathbf{C}^3\boldsymbol{\tau}_3, \mathbf{C}^4\boldsymbol{\tau}_2,$
$\mathbf{C}^2\boldsymbol{\tau}_2^2, \mathbf{C}(\boldsymbol{\tau}_2\cdot\boldsymbol{\tau}_3), \mathbf{C}(\boldsymbol{\tau}_2\cdot(\mathbf{A}\boldsymbol{\tau}_2)), \boldsymbol{\tau}_2\cdot(\mathbf{A}\mathbf{C}\boldsymbol{\tau}_2), \boldsymbol{\tau}_2\cdot(\mathbf{A}^2\boldsymbol{\tau}_2), \boldsymbol{\tau}_2\cdot(\mathbf{A}\boldsymbol{\tau}_3), \boldsymbol{\tau}_2\cdot\boldsymbol{\tau}_4,$
$(\mathbf{A}\boldsymbol{\tau}_2)^2, \boldsymbol{\tau}_3^2$

The number of order conditions grows rapidly with k. The number of conditions that must be considered can be reduced dramatically if the method is assumed to have higher stage order. So far we have assumed only that $\boldsymbol{\tau}_1 = 0$, i.e. stage order one. Assumption of stage order q means simply that $\boldsymbol{\tau}_k = 0$ for $1 \le k \le q$. For example, assuming stage order three, we now give the order conditions for order seven.

- Terms appearing in $\boldsymbol{\epsilon}_7$ that do not involve $\boldsymbol{\tau}_2$ or $\boldsymbol{\tau}_3$:
  $\mathbf{A}^3\boldsymbol{\tau}_4, \mathbf{A}^2\boldsymbol{\tau}_5, \mathbf{A}^2\mathbf{C}\boldsymbol{\tau}_4, \mathbf{A}\boldsymbol{\tau}_6, \mathbf{A}\mathbf{C}\mathbf{A}\boldsymbol{\tau}_4, \mathbf{A}\mathbf{C}\boldsymbol{\tau}_5, \mathbf{A}\mathbf{C}^2\boldsymbol{\tau}_4, \boldsymbol{\tau}_7$
- Terms appearing in $\bar{\boldsymbol{\delta}}_7$ that do not involve $\boldsymbol{\tau}_2$ or $\boldsymbol{\tau}_3$:
  $\mathbf{A}^3\boldsymbol{\tau}_4, \mathbf{A}^2\boldsymbol{\tau}_5, \mathbf{A}^2\mathbf{C}\boldsymbol{\tau}_4, \mathbf{A}\boldsymbol{\tau}_6, \mathbf{A}\mathbf{C}\mathbf{A}\boldsymbol{\tau}_4, \mathbf{A}\mathbf{C}\boldsymbol{\tau}_5, \mathbf{A}\mathbf{C}^2\boldsymbol{\tau}_4, \boldsymbol{\tau}_7,$
  $\mathbf{C}\mathbf{A}^2\boldsymbol{\tau}_4, \mathbf{C}\mathbf{A}\boldsymbol{\tau}_5, \mathbf{C}\mathbf{A}\mathbf{C}\boldsymbol{\tau}_4, \mathbf{C}\boldsymbol{\tau}_6, \mathbf{C}^2\mathbf{A}\boldsymbol{\tau}_4, \mathbf{C}^2\boldsymbol{\tau}_5, \mathbf{C}^3\boldsymbol{\tau}_4$

2.2 Order conditions

Here we enumerate the order conditions themselves.

- Order $p = 1$: $\mathbf{b}^{\mathrm{T}}\mathbf{e} = 1$
- Order $p = 2$:
  - $\mathbf{b}^{\mathrm{T}}\mathbf{c} = \frac{1}{2}$
- Order $p = 3$:
  - $\mathbf{b}^{\mathrm{T}}\mathbf{c}^2 = \frac{1}{3}$
  - $\mathbf{b}^{\mathrm{T}}\boldsymbol{\tau}_2 = 0$
- Order $p = 4$:
  - $\mathbf{b}^{\mathrm{T}}\mathbf{c}^3 = \frac{1}{4}$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{C}\boldsymbol{\tau}_2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{A}\boldsymbol{\tau}_2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\boldsymbol{\tau}_3 = 0$

- Order $p = 5$:
  - $\mathbf{b}^{\mathrm{T}}\mathbf{c}^4 = \frac{1}{5}$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{A}\mathbf{C}\boldsymbol{\tau}_2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{A}^2\boldsymbol{\tau}_2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{A}\boldsymbol{\tau}_3 = 0$
  - $\mathbf{b}^{\mathrm{T}}\boldsymbol{\tau}_4 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{C}\mathbf{A}\boldsymbol{\tau}_2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{C}\boldsymbol{\tau}_3 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{C}^2\boldsymbol{\tau}_2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\boldsymbol{\tau}_2^2 = 0$
- Order $p = 6$:
  - $\mathbf{b}^{\mathrm{T}}\mathbf{c}^5 = \frac{1}{6}$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{A}^2\mathbf{C}\boldsymbol{\tau}_2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{A}^3\boldsymbol{\tau}_2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{A}^2\boldsymbol{\tau}_3 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{A}\boldsymbol{\tau}_4 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{A}\mathbf{C}\mathbf{A}\boldsymbol{\tau}_2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{A}\mathbf{C}\boldsymbol{\tau}_3 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{A}\mathbf{C}^2\boldsymbol{\tau}_2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{A}\boldsymbol{\tau}_2^2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\boldsymbol{\tau}_5 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{C}\mathbf{A}\mathbf{C}\boldsymbol{\tau}_2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{C}\mathbf{A}^2\boldsymbol{\tau}_2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{C}\mathbf{A}\boldsymbol{\tau}_3 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{C}\boldsymbol{\tau}_4 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{C}^2\mathbf{A}\boldsymbol{\tau}_2 = 0$
  - $\mathbf{b}^{\mathrm{T}}\mathbf{C}^2\boldsymbol{\tau}_3 = 0$

- $\mathbf{b}^{\mathrm{T}}\mathbf{C}^3\boldsymbol{\tau}_2 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{C}\boldsymbol{\tau}_2^2 = 0$
- $\mathbf{b}^{\mathrm{T}}(\boldsymbol{\tau}_2 \cdot \boldsymbol{\tau}_3) = 0$
- $\mathbf{b}^{\mathrm{T}}(\boldsymbol{\tau}_2 \cdot (\mathbf{A}\boldsymbol{\tau}_2)) = 0$

The list of conditions that must be considered is smaller for methods with higher stage order. For instance, if we assume stage order two then the conditions for fifth order are just

- $\mathbf{b}^{\mathrm{T}}\mathbf{e} = 1$
- $\mathbf{b}^{\mathrm{T}}\mathbf{c} = \frac{1}{2}$
- $\mathbf{b}^{\mathrm{T}}\mathbf{c}^2 = \frac{1}{3}$
- $\mathbf{b}^{\mathrm{T}}\mathbf{c}^3 = \frac{1}{4}$
- $\mathbf{b}^{\mathrm{T}}\boldsymbol{\tau}_3 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{c}^4 = \frac{1}{5}$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}\boldsymbol{\tau}_3 = 0$
- $\mathbf{b}^{\mathrm{T}}\boldsymbol{\tau}_4 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{C}\boldsymbol{\tau}_3 = 0$

For stage order two methods, the additional conditions for 6th order are just

- $\mathbf{b}^{\mathrm{T}}\mathbf{c}^5 = \frac{1}{6}$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}^2\boldsymbol{\tau}_3 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}\boldsymbol{\tau}_4 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}\mathbf{C}\boldsymbol{\tau}_3 = 0$
- $\mathbf{b}^{\mathrm{T}}\boldsymbol{\tau}_5 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{C}\mathbf{A}\boldsymbol{\tau}_3 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{C}\boldsymbol{\tau}_4 = 0$

- $\mathbf{b}^{\mathrm{T}}\mathbf{C}^2\boldsymbol{\tau}_3 = 0$

For stage order three methods, the additional conditions for 7th order are just

- $\mathbf{b}^{\mathrm{T}}\mathbf{c}^6 = \frac{1}{7}$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}^2\boldsymbol{\tau}_4 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}\boldsymbol{\tau}_5 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}\mathbf{C}\boldsymbol{\tau}_4 = 0$
- $\mathbf{b}^{\mathrm{T}}\boldsymbol{\tau}_6 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{C}\mathbf{A}\boldsymbol{\tau}_4 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{C}\boldsymbol{\tau}_5 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{C}^2\tau_4 = 0$

and the additional conditions for 8th order are just

- $\mathbf{b}^{\mathrm{T}}\mathbf{c}^7 = \frac{1}{8}$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}^3\boldsymbol{\tau}_4 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}^2\boldsymbol{\tau}_5 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}^2\mathbf{C}\boldsymbol{\tau}_4 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}\boldsymbol{\tau}_6 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}\mathbf{C}\mathbf{A}\boldsymbol{\tau}_4 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}\mathbf{C}\boldsymbol{\tau}_5 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{A}\mathbf{C}^2\boldsymbol{\tau}_4 = 0$
- $\mathbf{b}^{\mathrm{T}}\boldsymbol{\tau}_7 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{C}\mathbf{A}^2\boldsymbol{\tau}_4 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{C}\mathbf{A}\boldsymbol{\tau}_5 = 0$

- $\mathbf{b}^{\mathrm{T}}\mathbf{CAC}\boldsymbol{\tau}_4 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{C}\boldsymbol{\tau}_6 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{C}^2\mathbf{A}\boldsymbol{\tau}_4 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{C}^2\boldsymbol{\tau}_5 = 0$
- $\mathbf{b}^{\mathrm{T}}\mathbf{C}^3\boldsymbol{\tau}_4 = 0$

3 Multistep Runge–Kutta Methods of Type I

We consider multistep Runge–Kutta methods of the form

$$y_i^n = \sum_{l=1}^{k} d_{il} u^{n-k+l} + \Delta t \sum_{j=1}^{s} a_{ij} F(y_j^n) \tag{14a}$$

$$u^{n+1} = \sum_{l=1}^{k} \theta_l u^{n-k+l} + \Delta t \sum_{j=1}^{s} b_j F(y_j^n), \tag{14b}$$

where it is assumed that (for consistency)

$$\sum_{l=1}^{k} d_{il} = 1 \qquad \sum_{l=1}^{k} \theta_l = 1.$$

This form includes both Type I and Type II methods, but it must be remembered that s is not an accurate indication of the cost of the method for Type II methods in this form. More specifically, it is possible to include terms such as $F(u^{n-1})$ by having one of the stages equal to u^{n-1} identically (like the Type II TSRK methods from our paper), and that in this case the cost of the method is generally less than s function evaluations.

We write method (14) as

$$\mathbf{y}^n = \mathbf{D}\mathbf{u}^n + h\mathbf{A}\mathbf{f}^n \tag{15a}$$

$$u^{n+1} = \boldsymbol{\theta}\mathbf{u}^n + h\mathbf{b}^{\mathrm{T}}\mathbf{f}^n \tag{15b}$$

where $\mathbf{u}$ is the vector of previous step values

$$\mathbf{u} = [u^{n-k+1}, u^{n-k+2}, \ldots, u^n].$$

Then the true solution satisfies

$$\tilde{\mathbf{y}}^n = \mathbf{D}\tilde{\mathbf{u}}^n + h\mathbf{A}\tilde{\mathbf{f}}^n + h\boldsymbol{\tau}^n \tag{16a}$$

$$\tilde{u}^{n+1} = \boldsymbol{\theta}\tilde{\mathbf{u}}^n + h\mathbf{b}^{\mathrm{T}}\tilde{\mathbf{f}}^n + h\tau^n. \tag{16b}$$

Using the Taylor expansions above, as well as

$$\begin{aligned}\tilde{u}(t_{n-1-r}) &= \tilde{u}(t_{n-1}) - rh\tilde{u}'(t_{n-1}) + \frac{1}{2}h^2r^2\tilde{u}''(t_{n-1}) + \cdots \\ &= \sum_{k=0}^{\infty}\frac{1}{k!}h^k(-r)^k\tilde{u}^{(k)}(t_{n-1}),\end{aligned}$$

substitution gives

$$\boldsymbol{\tau} = \sum_{k=1}^{\infty}\boldsymbol{\tau}_k h^{k-1}\tilde{u}^{(k)}(t_{n-1}) \tag{17a}$$

$$\tau^n = \sum_{k=1}^{\infty}\tau_k h^{k-1}\tilde{u}^{(k)}(t_{n-1}) \tag{17b}$$

where

$$\boldsymbol{\tau}_k = \frac{1}{k!}\left(\mathbf{c}^k - \mathbf{D}(-\boldsymbol{l})^k\right) - \frac{1}{(k-1)!}\mathbf{A}\mathbf{c}^{k-1} \tag{18a}$$

$$\tau_k = \frac{1}{k!}\left(1 - \boldsymbol{\theta}^{\mathrm{T}}(-\boldsymbol{l})^k\right) - \frac{1}{(k-1)!}\mathbf{b}^{\mathrm{T}}\mathbf{c}^{k-1} \tag{18b}$$

and $\boldsymbol{l} = [k-1, k-2, \ldots, 0]$. We assume consistency of the stages, which means $\boldsymbol{\tau}_1 = 0$. We take this condition to define the abscissas, which means we have stage order at least equal to one:

$$\mathbf{c} = \mathbf{A}\mathbf{e} - \mathbf{D}\boldsymbol{l}. \tag{19}$$

Subtracting (16) from (15) gives

$$\boldsymbol{\epsilon}^n = \mathbf{D}\bar{\boldsymbol{\epsilon}}^n + h\mathbf{A}\boldsymbol{\delta}^n - h\boldsymbol{\tau}^n \tag{20a}$$

$$\epsilon^{n+1} = \boldsymbol{\theta}^{\mathrm{T}}\bar{\boldsymbol{\epsilon}}^n + h\mathbf{b}^{\mathrm{T}}\boldsymbol{\delta}^n - h\tau^n \tag{20b}$$

where $\bar{\boldsymbol{\epsilon}}^n = [\epsilon^{n-1}, \epsilon^{n-2}, \ldots, \epsilon^{n-k}]$.

Now we seek expressions for the global stage errors $\boldsymbol{\epsilon}$ and the stage derivative errors $\boldsymbol{\delta}$ of the form (7). Substituting (7a) and (17) into (20) yields

$$\boldsymbol{\epsilon}^n = \mathbf{D}\bar{\boldsymbol{\epsilon}}^n + \sum_{k=0}^{p-1} \mathbf{A}\boldsymbol{\delta}_k^n \Delta t^{k+1} - \sum_{k=1}^{p} \boldsymbol{\tau}_k \tilde{u}^{(k)}(t_n)\Delta t^k + \mathcal{O}(\Delta t^{p+1}) \tag{21a}$$

$$\epsilon^{n+1} = \boldsymbol{\theta}^{\mathrm{T}}\bar{\boldsymbol{\epsilon}}^n + \sum_{k=0}^{p-1} \mathbf{b}^{\mathrm{T}}\boldsymbol{\delta}_{k-1}^n \Delta t^{k+1} - \sum_{k=1}^{p} \tau_k \tilde{u}^{(k)}(t_n)\Delta t^k + \mathcal{O}(\Delta t^{p+1}) \tag{21b}$$

with $\boldsymbol{\tau}_k$ given by (18a). Assuming stable propagation of errors, we again have global accuracy of order p if

$$\begin{aligned} \tau_k &= 0 && \text{for } 0 \le k \le p \\ \mathbf{b}^{\mathrm{T}}\boldsymbol{\delta}_k^n &= 0 && \text{for } 0 \le k \le p-1. \end{aligned}$$

Furthermore, we still have the expression (11) for $\boldsymbol{\delta}$.

3.1 Generation of stage derivative error vectors

Combining (7b) with (21a) and equating coefficients of powers of Δt gives again (12). Hence we can again determine the vectors appearing in $\boldsymbol{\delta}_k$ recursively using (11) and (12). The only difference is that the stage truncation error vectors are now given by (18a). Hence the non-bushy tree order conditions for these methods are the same as those for Runge-Kutta methods, as enumerated in Section 2, except that the definitions of the stage truncation errors $\boldsymbol{\tau}_k, \tau_k$, and of the abscissas $\mathbf{c}$ are given by (18a), (18b), and (19), respectively. Meanwhile, the bushy tree order conditions for order p are (from (18b)):

$$\frac{1}{k!}\left(1 - \boldsymbol{\theta}^{\mathrm{T}}(-\boldsymbol{l})^k\right) = \frac{1}{(k-1)!}\mathbf{b}^{\mathrm{T}}\mathbf{c}^{k-1} \qquad \text{for } 1 \le k \le p.$$

4 Spijker forms

The Spijker form for the Type I methods of the last section is

$$\mathbf{x} = \left[u^{n-k+1}, u^{n-k+2}, \ldots, u^{n-1}, u^n\right] \tag{22}$$

$$\mathbf{y} = \left[u^{n-k+1}, u^{n-k+2}, \ldots, u^{n-1}, u^n, y_1, \ldots, y_s, u^{n+1}\right] \tag{23}$$

$$\mathbf{S} = \begin{pmatrix} \mathbf{I} \\ \mathbf{D} \\ \boldsymbol{\theta}^{\mathrm{T}} \end{pmatrix} \qquad \mathbf{T} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & 0 \\ \mathbf{0} & \mathbf{A} & \mathbf{0} \\ \mathbf{0} & \mathbf{b}^{\mathrm{T}} & 0 \end{pmatrix}. \tag{24}$$

We are also interested in Type II methods, which take the form

$$y_i^n = \sum_{l=1}^{k} d_{il} u^{n-k+l} + \Delta t \sum_{l=1}^{k-1} \hat{a}_{il} F(u^{n-k+l}) + \Delta t \sum_{j=1}^{s} a_{ij} F(y_j^n) \tag{25a}$$

$$u^{n+1} = \sum_{l=1}^{k} \theta_l u^{n-k+l} + \Delta t \sum_{l=1}^{k-1} \hat{b}_l F(u^{n-k+l}) + \Delta t \sum_{j=1}^{s} b_j F(y_j^n), \tag{25b}$$

where $y_1^n = u^n$. These admit the Spijker form

$$\mathbf{x} = \left[u^{n-k+1}, u^{n-k+2}, \ldots, u^{n-1}, u^n\right] \tag{26}$$

$$\mathbf{y} = \left[u^{n-k+1}, u^{n-k+2}, \ldots, u^{n-1}, u^n, y_1 = u^n, y_2, \ldots, y_s, u^{n+1}\right] \tag{27}$$

$$\mathbf{S} = \begin{pmatrix} \mathbf{I}\ \mathbf{0} \\ \mathbf{D} \\ \boldsymbol{\theta}^{\mathrm{T}} \end{pmatrix} \qquad \mathbf{T} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & 0 \\ \hat{\mathbf{A}} & \mathbf{A} & \mathbf{0} \\ \hat{\mathbf{b}}^{\mathrm{T}} & \mathbf{b}^{\mathrm{T}} & 0 \end{pmatrix}. \tag{28}$$

Here the first row of $\mathbf{D}$ is $(0, 0, \ldots, 0, 1)$ and the first row of $\mathbf{A}, \hat{\mathbf{A}}$ is identically zero. The order conditions presented above can also be applied to these Type II methods by writing them as Type I methods (simply introduce additional stages that are equal to the old steps). **David can write this last bit up if necessary.**

5 Methods for linear problems

In this section we consider only linear problems of the form

$$u_t = Lu,$$

so that the order conditions simplify considerably. This case is of interest for several reasons. First, linear problems are of interest in many cases (cite Bernardo Cockburn), and it is possible to include a time-dependent forcing term or boundary condition while maintaining the order of the method. Second, up to second order the order conditions for linear and nonlinear problems are the same. Thus, this approach will provide results for second order multi-step multi-stage methods, which gives us a picture of the size of the time-step for higher order nonlinear methods. Finally, the time-step restriction for the linear high order methods serves as an upper bound for that of nonlinear high order methods.

5.1 Tall Tree Order conditions for Multistep Runge–Kutta methods

For k-step Runge-Kutta methods of Type II, applying the method to the linear scalar homogeneous test equation, we find that it reduces to the iteration

$$u^{n+1} = \left(\boldsymbol{\theta}^{\mathrm{T}} + z\hat{\mathbf{b}}^{\mathrm{T}} + z\mathbf{b}^{\mathrm{T}}(I - z\mathbf{A})^{-1}(\mathbf{D} + z\hat{\mathbf{A}})\right)\mathbf{u} \tag{29}$$

where

$$\mathbf{u} = \left(u^{n-k+1}, u^{n-k+2}, \dots, u^{n}\right)^{T} \tag{30}$$

and $\hat{\mathbf{A}}, \hat{\mathbf{b}}^{\mathrm{T}}$ each have k columns but the last column is zero. Using the Taylor expansions

$$(\mathbf{I} - z\mathbf{A})^{-1} = \sum_{j=0}^{\infty} z^j \mathbf{A}^j \tag{31a}$$

$$u^{n-\boldsymbol{l}} = e^{-\boldsymbol{l}\Delta t}u^n = u^n \sum_{j=0}^{\infty} \frac{1}{j!} z^j (-l)^j \tag{31b}$$

we obtain the tall tree order conditions for linear problems. These are given by equating coefficients in

$$\begin{aligned} e^z + \mathcal{O}(z^{p+1}) &= \left[\boldsymbol{\theta}^{\mathrm{T}} + z\hat{\mathbf{b}}^{\mathrm{T}} + z\mathbf{b}^{\mathrm{T}}\left(\sum_{j=0}^{\infty} z^j\mathbf{A}^j\right)(z + \mathbf{D}\hat{\mathbf{A}})\right]\left(\sum_{j=0}^{\infty}\frac{1}{j!}z^j(-\boldsymbol{l})^j\right) \\ &= \sum_{j=0}^{\infty} z^j \Big(\frac{(-1)^j}{j!}\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{l}^j + \frac{(-1)^{j-1}}{(j-1)!}\hat{\mathbf{b}}^{\mathrm{T}}\boldsymbol{l}^{j-1} \\ &+ \mathbf{b}^{\mathrm{T}}\sum_{i=0}^{j-1}\frac{(-1)^i}{i!}\mathbf{A}^{j-i-1}\mathbf{D}\boldsymbol{l}^i + \frac{(-1)^{i-1}}{(i-1)!}\mathbf{A}^{j-i}\hat{\mathbf{A}}\boldsymbol{l}^{i-1}\Big) \end{aligned} \tag{32}$$

where $\boldsymbol{l} = (k-1, k-2, \dots, 0)^{\mathrm{T}}$. *need to add something about terms with negative exponents being understood to be zero here*

The resulting conditions are (given our assumption that $\mathbf{De} = \mathbf{e}$ and $\boldsymbol{\theta}^{\mathrm{T}}\mathbf{e} = 1$):

$$(\mathbf{b}^{\mathrm{T}} + \hat{\mathbf{b}}^{\mathrm{T}})\mathbf{e} - \boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{l} = 1 \tag{33a}$$

$$\mathbf{b}^{\mathrm{T}}\mathbf{c} - \hat{\mathbf{b}}^{\mathrm{T}}\boldsymbol{l} + \frac{1}{2}\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{l}^2 = \frac{1}{2} \tag{33b}$$

$$\mathbf{b}^{\mathrm{T}}(\mathbf{Ac} + \frac{1}{2}\mathbf{D}\boldsymbol{l}^2 - \hat{\mathbf{A}}\boldsymbol{l}) + \frac{1}{2}\hat{\mathbf{b}}^{\mathrm{T}}\boldsymbol{l}^2 - \frac{1}{6}\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{l}^3 = \frac{1}{6} \tag{33c}$$

s k	2	3	4	5
2	0.707	0.809	0.860	
3	0.817	0.879	0.911*	
4	0.866	0.911	0.934	
5	0.894	0.930		

Table 1: Effective SSP coefficients $\mathcal{C}_{\text{eff}}$ of optimal explicit 2nd order k-step Runge-Kutta methods of type (explicit with a zero row) (for both linear and nonlinear problems).

where

$$\mathbf{c} = (\mathbf{A} + \hat{\mathbf{A}})\mathbf{e} - \mathbf{D}\boldsymbol{l}.$$

For k-step Runge-Kutta methods of Type I, the analysis is the same as that above, but with $\hat{\mathbf{b}} = \hat{\mathbf{A}} = 0$. The first five order conditions in this case reduce to

$$\mathbf{b}^T\mathbf{e} - \boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{l} = 1, \tag{34a}$$

$$\mathbf{b}^T\mathbf{c} + \frac{1}{2}\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{l}^2 = \frac{1}{2}, \tag{34b}$$

$$\mathbf{b}^{\mathrm{T}}\left(\mathbf{A}\mathbf{c} + \frac{1}{2}\mathbf{D}\boldsymbol{l}^2\right) - \frac{1}{6}\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{l}^3 = \frac{1}{6} \tag{34c}$$

$$\mathbf{b}^{\mathrm{T}}\left(\mathbf{A}^2\mathbf{c} + \frac{1}{2}\mathbf{A}\mathbf{D}\boldsymbol{l}^2 - \frac{1}{6}\mathbf{D}\boldsymbol{l}^3\right) + \frac{1}{24}\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{l}^4 = \frac{1}{24} \tag{34d}$$

$$\mathbf{b}^{\mathrm{T}}\left(\mathbf{A}^3\mathbf{c} + \frac{1}{2}\mathbf{A}^2\mathbf{D}\boldsymbol{l}^2 - \frac{1}{6}\mathbf{A}\mathbf{D}\boldsymbol{l}^3 + \frac{1}{24}\mathbf{D}\boldsymbol{l}^4\right) - \frac{1}{120}\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{l}^5 = \frac{1}{120} \tag{34e}$$

where $\mathbf{c} = \mathbf{A}\mathbf{e} - \mathbf{D}\boldsymbol{l}$.

5.2 Optimal SSP Multistep Runge–Kutta methods for linear problems

These are David's old results from 2007-2008. SSP coefficients for optimal explicit methods of Type II are shown in Tables 1-2.

We have solved numerically the optimization problem of maximizing r subject to (34) and (**??**) for various values of s, k with $p = 2$ (i.e., implicit methods of Type I). It appears (after some `fmincon` searches) that the optimal 2nd order SSP implicit Runge-Kutta methods given in [**?**, **?**] are actually optimal over all second order k-step, 2-stage methods.

s k	2	3	4	5
2	0.366	0.556	0.622	0.622
3	0.550	0.667*	0.667	
4	0.627			
5	0.677	0.679	0.679	
6	0.705	0.705	0.705	

Table 2: Effective SSP coefficients $\mathcal{C}_{\text{eff}}$ of optimal explicit 3rd order k-step Runge-Kutta methods of type (explicit with a zero row) for linear problems.

References

[Albrecht, 1996] Albrecht, P. (1996). The Runge-Kutta Theory in a Nutshell. *SIAM Journal on Numerical Analysis*, 33(5):1712 – 1735.

[Butcher, 2003] Butcher, J. (2003). *Numerical Methods for Ordinary Differential Equations*.