# ORDER CONDITIONS FOR CANONICAL RUNGE-KUTTA-NYSTRÖM METHODS

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#### Abstract.

We are concerned with Runge-Kutta-Nyström methods for the integration of second order systems of the special form  $d^2y/dt^2 = f(y)$ . If the function f is the gradient of a scalar field, then the system is Hamiltonian and it may be advantageous to integrate it by a so-called canonical Runge-Kutta-Nyström formula. We show that the equations that must be imposed on the coefficients of the method to ensure canonicity are simplifying assumptions that lower the number of independent order conditions. We count the number of order conditions, both for general and for canonical Runge-Kutta-Nyström formulae.

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## 1. Introduction.

The recent literature contains many items devoted to the numerical integration of Hamiltonian systems of differential equations by means of canonical or symplectic methods (see, among others, [1, 6–9, 12, 14–23]). Recall that Hamiltonian systems are of the form

(1.1) 
$$dp^{I}/dt = -\partial H/\partial q^{I}, \qquad dq^{I}/dt = \partial H/\partial p^{I}, \qquad 1 \le I \le d,$$

where the integer d is the number of degrees of freedom and the Hamiltonian  $H = H(p^1, ..., p^d, q^1, ..., q^d)$  is a sufficiently smooth, real function of 2d real variables. The main qualitative property of Hamiltonian systems is the preservation, by the corresponding flow, of the so-called symplectic structure in phase-space (i.e. in (p,q)-space) [2]. A one-step numerical integration method for (1.1) is said to be

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canonical or symplectic if it preserves this symplectic structure. Therefore canonical integrators mimic important qualitative features of (1.1) and can be expected to be better suited to the integration of Hamiltonian systems than their non-canonical counterparts [6, 12, 15, 19, 20].

In many applications, the Hamiltonian function has the form

(1.2) 
$$H = H(p,q) = T(p) + V(q), \qquad T(p) = \frac{1}{2}p^{T}p,$$

with V a given function of d variables. In mechanics, the q variables represent Lagrangian coordinates, the p variables the corresponding momenta, T is the kinetic energy, V the potential energy, and H the total energy. When the Hamiltonian is given by (1.2), the equations of motion (1.1) take the simple form

(1.3) 
$$dp^{I}/dt = -\partial V/\partial q^{I}, \qquad dq^{I}/dt = p^{I}, \qquad 1 \le I \le d,$$

a 2d-dimensional first order system equivalent to the d-dimensional second order system

(1.4) 
$$d^2q^I/dt^2 = -\partial V/\partial q^I, \qquad 1 \le I \le d.$$

For numerical purposes, second order systems of the special form

(1.5) 
$$d^2y/dt^2 = f(y), \qquad y = [y^1, \dots, y^d]^T,$$

can always be written in first-order form and integrated by, say, a standard Runge-Kutta formula. However, it is often advisable, on efficiency grounds, to retain the second-order formulation (1.5) and use a method for second-order problems (see e.g. [11], Section II.13). In this paper we are concerned with Runge-Kutta-Nyström (RKN) methods, of the form (a dot represents differentiation with respect to t)

(1.6)  

$$Y_{i} = y_{n} + h\gamma_{i}y_{n} + h^{2}\sum_{j=1}^{s} \alpha_{ij}f(Y_{j}),$$

$$y_{n+1} = y_{n} + h\sum_{i=1}^{s} b_{i}f(Y_{i}),$$

$$y_{n+1} = y_{n} + hy_{n} + h^{2}\sum_{i=1}^{s} \beta_{i}f(Y_{i}).$$

Here the subscript n numbers the steps and the vectors  $Y_i$  represent the s internal stages.

Suris [22] showed that the method (1.6) is canonical if

(1.7a) 
$$\beta_i = b_i(1 - \gamma_i), \qquad 1 \le i \le s,$$

(1.7b) 
$$b_i(\beta_j - \alpha_{ij}) = b_j(\beta_i - \alpha_{ji}), \qquad 1 \le i, j \le s,$$

(see also [16]). On the other hand, for *methods wihout equivalent stages*, (1.7) is also necessary for (1.6) to be canonical: a rigorous proof of this necessity can be found in [4] (cf, [1], Section 5). Recall that two stages  $Y_i$ ,  $Y_j$  of an RKN method are said to be

equivalent if  $Y_i = Y_j$  for sufficiently small *h* for all problems (1.5). A method with equivalent stages gives the same results as a method without equivalent stages where the redundant stages have been suppressed. In the remainder of this paper we shall use the expression "canonical RKN method" to refer to RKN methods that satisfy (1.7).

The condition in (1.7a) is well known from the standard theory of RKN methods: it is a *simplifying assumption* that lowers the number of relations that must be imposed on the method coefficients  $b_i$ ,  $\beta_i$ ,  $\gamma_i$ ,  $\alpha_{ij}$  to ensure order of consistency  $\geq p$ ([11], Chapter 2, Lemma 13.13). The main purpose of the present contribution is to show that the second condition (1.7b) is also a simplifying assumption. Section 2 contains the main result. Section 3 is devoted to counting the number of order conditions that are made redundant by the introduction of the canonicity condition. In particular, we give the number of order conditions that must be imposed for a *general* (i.e. not necessarily canonical) RKN method to have order  $\geq p$ , a result that does not seem to be available in the literature.

## 2. Main result.

We consider the application of the RKN method (1.6) to the system (1.5). Note that this system is *not* assumed to be Hamiltonian, i.e. we do not suppose that f is the gradient of a scalar function -V. Let us briefly recall the corresponding theory of order conditions, as given by Hairer *et al.* [11] (note however that our notation is sometimes different from that used in [11]). The theory uses so called *special* Nyström rooted trees. A special Nyström rooted tree  $\sigma v \rho \tau$  has vertices of two kinds, fat and meagre, that obey the following rules:

- (i) The root is fat.
- (ii) A fat vertex has only meagre sons.
- (iii) A meagre vertex has, at most, one son and this son is fat.

Figure 1 depicts the  $\sigma v \rho \tau$ 's with *order* (i.e. number of vertices)  $N(\sigma v \rho \tau) \leq 5$ . The vertex that plays the role of root has been indicated by attaching a cross to it. In this paper, we handle graphs by means of pictorial representations; a more rigourous treatment, like that in [21], is, of course, possible (but boring).

For (1.6) to have order of consistency  $\geq p$ , it is necessary and sufficient to impose simultaneously the following two sets of conditions ([11], Chapter II, Theorem 13.12).

I. For each  $\sigma v \rho \tau$  with order  $\leq p$ 

(2.1) 
$$\Phi(\sigma v \rho \tau) = 1/\gamma(\sigma v \rho \tau),$$

where  $\gamma(\sigma v \rho \tau)$ , the density, is an integer associated with  $\sigma v \rho \tau$  and  $\Phi(\sigma v \rho \tau)$  is the corresponding *elementary weight*. The density is defined recursively and ignoring the distinction between fat and meagre vertices. By definition, the density of

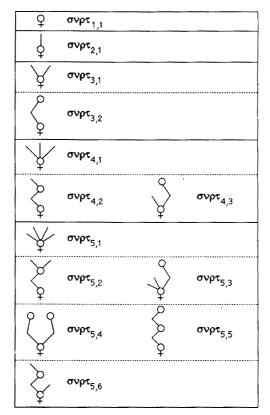


Fig. 1. Special Nyström rooted N-trees, N = 1, 2, 3, 4, 5.

a rooted tree with only one vertex is 1, and the density of a rooted tree with more than one vertex is the product of its order and the densities of the rooted trees that arise when the root is chopped off. On the other hand, the elementary weights are polynomials on the method coefficients. For instance for  $\sigma v \rho \tau_{5,3}$  in Figure 1, we have

$$\Phi(\sigma v \rho \tau_{5,3}) = \sum_{i,j=1}^{s} b_i \gamma_i^2 \alpha_{ij}$$

The general rule is that there are as many summation indices as fat vertices; if *i* is the summation index associated with the root, then to the (fat) root there corresponds to a factor  $b_i$ ; to a fat vertex with summation index *j* and *r* terminal meagre sons there corresponds a factor  $\gamma_j^r$ ; finally, to a fat vertex with index *j* that has a fat grandson with index *k* there corresponds a factor  $\alpha_{jk}$ .

II. For each  $\sigma v \rho \tau$  with order  $N(\sigma v \rho \tau) \leq p - 1$ 

(2.2) 
$$\Psi(\sigma v \rho \tau) = [(N(\sigma v \rho \tau) + 1)\gamma(\sigma v \rho \tau)]^{-1}.$$

Here the density  $\gamma$  appears again while  $\Psi$  is a second elementary weight obtained from  $\Phi$  by changing the factor  $b_i$ , associated with the root, into a factor  $\beta_i$ .

It is known ([11] Chapter II, Lemma 13.13), that (1.7a) is a simplifying assumption: when (1.7a) holds, set II of order conditions above is a consequence of set I, so that equations (2.2) need not be explicitly imposed. We are going to show that if, in addition to (1.7a), (1.7b) holds, then some of the conditions in set I above can be dispensed with.

We say that two different special Nyström rooted trees are equivalent if they have the same fat vertices and the same meagre vertices, connected by the same edges, so that they only differ in the choice of root (in the pictorial representation the cross is attached to different fat vertices). For instance, in Figure 1,  $\sigma v \rho \tau_{4,3}$  are equivalent, and so are the pairs  $\sigma v \rho \tau_{5,2}$  and  $\sigma v \rho \tau_{5,3}$  and the pairs  $\sigma v \rho \tau_{5,4}$  and  $\sigma v \rho \tau_{5,5}$ . We are now in a position to give the main result of this paper.

THEOREM 2.1. Assume that the RKM method is canonical and has, at least, order of consistency p - 1. Let  $\sigma v \rho \tau^*$  be two special Nyström rooted trees of order p that are equivalent in the sense just defined. Then the order conditions (2.1) corresponding to  $\sigma v \rho \tau$  and  $\sigma v \rho \tau^*$  are equivalent.

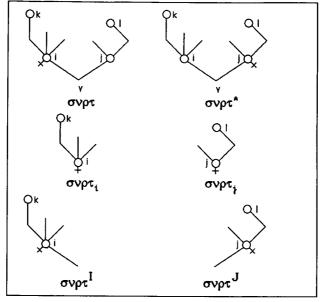


Fig. 2. Proof of Theorem 2.1.

**PROOF.** We first carry out the proof in the particular case where the vertices that play the role of roots in  $\sigma v \rho \tau$  and  $\sigma v \rho \tau^*$  are joined to each other via a meagre vertex v, as in Figure 2. Let us label the fat vertices of  $\sigma v \rho \tau$  and  $\sigma v \rho \tau^*$  with summation indices  $i, j, k, \ldots$  (see Figure 2) and suppose that the root of  $\sigma v \rho \tau$  has index *i* and the root of  $\sigma v \rho \tau^*$ 

has index j. Furthermore, let us consider four special Nyström rooted trees as follows. We denote by  $\sigma v \rho \tau_i$  (resp.  $\sigma v \rho \tau_j$ ) the special Nyström rooted tree arising by removing from  $\sigma v \rho \tau$  (resp.  $\sigma v \rho \tau^*$ ) all the vertices that can be joined to i (resp. j) through a path containing the meagre vertex v. Let  $\sigma v \rho \tau^I$  (resp.  $\sigma v \rho \tau^J$ ) be the special Nyström rooted tree obtained by grafting in the root of  $\sigma v \rho \tau_i$  (resp.  $\sigma v \rho \tau_j$ ) a (meagre) son (see Figure 2).

After these preliminaries, note that, by definition of elementary weight,

$$\Phi(\sigma v \rho \tau) = \sum b_i \alpha_{ij} \Pi(i) \Pi(j),$$

where the summation is extended to all the summation indices we have introduced. Here  $\Pi(i)$  and  $\Pi(j)$  are abbreviations for products of RKN coefficients. The factor  $\Pi(i)$  contains the contributions arising from the nodes that belong to  $\sigma v \rho \tau_i$  and  $\Pi(j)$  contains the contributions arising from the nodes that belong to  $\sigma v \rho \tau_j$ . In a similar manner

$$\Phi(\sigma v \rho \tau^*) = \sum b_j \alpha_{ji} \Pi(i) \Pi(j),$$

so that

(2.3)  $\Phi(\sigma \nu \rho \tau) - \Phi(\sigma \nu \rho \tau^*) = \sum (b_i \alpha_{ij} - b_j \alpha_{ji}) \Pi(i) \Pi(j).$ Now, on taking (1.7a) into (1.7b), we can write

$$b_i \alpha_{ij} - b_j \alpha_{ji} = b_i b_j (\gamma_i - \gamma_j), \qquad 1 \le i, j \le s,$$

an equality that combined with (2.3) yields

$$\begin{split} \Phi(\sigma \nu \rho \tau) &- \Phi(\sigma \nu \rho \tau^*) = \sum (b_i \gamma_i \Pi(i)) (b_j \Pi(j)) - \sum (b_i \Pi(i)) (b_j \gamma_j \Pi(j)) \\ &= \Phi(\sigma \nu \rho \tau^I) \Phi(\sigma \nu \rho \tau_j) - \Phi(\sigma \nu \rho \tau_i) \Phi(\sigma \nu \rho \tau^J). \end{split}$$

Since the method is at least of order p - 1, we conclude

(2.4) 
$$\Phi(\sigma \nu \rho \tau) - \Phi(\sigma \nu \rho \tau^*) = \frac{1}{\gamma(\sigma \nu \rho \tau^I)} \frac{1}{\gamma(\sigma \nu \rho \tau_j)} - \frac{1}{\gamma(\sigma \nu \rho \tau_i)} \frac{1}{\gamma(\sigma \nu \rho \tau^I)}.$$

On using the definition of  $\gamma$  given above, some easy manipulations reveal that the right hand side of (2.4) equals  $1/\gamma(\sigma\nu\rho\tau) - 1/\gamma(\sigma\nu\rho\tau^*)$ , and this proves that the order conditions for  $\sigma\nu\rho\tau$  and  $\sigma\nu\rho\tau^*$  are equivalent.

The general case where the roots of  $\sigma v \rho \tau$  and  $\sigma v \rho \tau^*$  are not necessarily joined through a single meagre vertex follows by induction from the particular case where the roots are joined via a single meagre vertex. For instance, in Figure 2, the order conditions for the trees with roots at vertices k and j are equivalent because each of them is equivalent, via the previous argument, to the order condition for the tree rooted at *i*.

The fact that the conditions for canonicity for RKN methods provide simplifying assumptions should not be surprising. In [21] and [1] similar results were proved for Runge-Kutta and partitioned Runge-Kutta methods respectively. The deep

reason for the reduction in the number of order conditions that occurs for canonical methods lies in the canonical theory of the order. It was shown in [21] that for any canonical one-step method, applied to Hamiltonian systems, consistency can be investigated in terms of the Taylor expansion of a suitable scalar function  $\Gamma$ , rather than in terms of the (vector-valued) standard local error. Now, the number of terms that arise when expanding  $\Gamma$  is lower than the number of terms that arise in a standard expansion of the local error. This explains why the number of independent order conditions for a canonical one-step method is smaller than the corresponding order for its non-canonical counterparts. The papers [21] and [1] mentioned above contain the canonical theory of the order for Runge-Kutta and partitioned Runge-Kutta methods respectively. The theory for RKN methods appears in [4] and for brevity is not reproduced here. However, it is perhaps useful to note that, if (1.6) is canonical, then the corresponding generating function ([2], [21]) is given by

$$S(p_n, q_{n+1}; h) = p_n^T q_{n+1} - h \sum_{i=1}^s b_i V(Q_i) - (h/2) p_n^T p_n + (h^3/2) \sum_{i,j=1}^s b_i (\beta_j - \alpha_{ij}) f(Q_i)^T f(Q_j),$$

where  $Q_i$  are the internal stages. We recall that the generating function is the key ingredient in the computation of the function  $\Gamma$  required in the canonical theory of order conditions.

## 3. Counting the number of order conditions.

In this section we investigate how many order conditions can be dispensed with when (1.7) holds. We begin by studying the number of order conditions that must be imposed on *general* RKN methods to have order of consistency  $\ge p$ . Strangely enough this number does not appear to be available in the literature ([3], [10]).

It is clearly sufficient to find the number  $m_N$  of special Nyström rooted trees of order N, N = 1, 2, ... Consider a special Nyström rooted tree  $\sigma v \rho \tau$  with N vertices and remove the root. This gives rise to, say,  $j_1$  graphs with one vertex,  $j_2$  graphs with two vertices, etc. For  $k \ge 2$ , each among the  $j_k$  graphs with k vertices consists of a meagre vertex (that was a son of the root in the original  $\sigma v \rho \tau$ ) followed by a special Nyström rooted tree of order k - 1. Hence, for  $k \ge 2$ , the  $j_k$  graphs with k vertices can be chosen in

$$\binom{m_{k-1}+j_k-1}{j_k}$$

different ways. There is only one way of choosing the  $j_1$  graphs with one meagre vertex and therefore

(3.1) 
$$m_N = \sum_{j_1+2j_2+\ldots+kj_k=N-1} \binom{m_1+j_2-1}{j_2} \binom{m_2+j_3-1}{j_3} \cdots \binom{m_{k-1}+j_k-1}{j_k},$$

a formula that makes it possible to compute  $m_N$  recursively.

Let us introduce the generating function M of  $m_N$ 

$$M(z):=\sum_{N=1}^{\infty}m_N z^N.$$

This satisfies

(3.2) 
$$M(z) = \frac{z}{(1-z)(1-z^2)^{m_1}\dots(1-z^k)^{m_{k-1}}\dots}.$$

To check (3.2) first expand each factor in the right hand side of (3.2) with the help of

$$\frac{1}{(1-z^r)^m} = \sum_{j=0}^{\infty} \binom{m+j-1}{j} z^{jr},$$

and then combine equal powers of z.

It is still possible to write the infinite product in (3.2) as the exponential of a series. This yields, after some algebra,

(3.3) 
$$M(z) = z \exp\left(z(1 + M(z)) + \frac{z^2}{2}(1 + M(z^2)) + \ldots + \frac{z^k}{k}(1 + M(z^k)) + \ldots\right),$$

an equation satisfied by M that allows recursive computation of  $m_N$ . The values of  $m_N$  for  $N \le 9$  are displayed in Table 1.

Table 1.

N	1	2	3	4	5	6	7	8	9
m <sub>N</sub> m <sup>*</sup> <sub>N</sub>		1 1	-		6 4	10 5	20 10	36 14	72 27

Let us now turn the attention to the number of order conditions for *canonical* RKN methods. After Theorem 2.1, the key quantity is the number  $m_N^*$  of equivalence classes of special Nyström rooted trees (under the equivalence relation introduced above). From Figure 1, we see that  $m_1^* = 1$ ,  $m_2^* = 1$ ,  $m_3^* = 2$ ,  $m_4^* = 2$ ,  $m_5^* = 4$ . To find the expression of  $m_N^*$  for general N, note that all the special Nyström rooted trees in a given equivalence class have the same *centroids* (see [13], Section 2.3.4.4 and [21]). Figure 3 depicts the equivalence classes for  $N \le 5$ ; the centroids have been indicated by attaching a star. For fixed N, the equivalence classes fall into the following disjoint cases.

(i) There is one centroid and it is meagre (in Figure 3, classes  $c_{3,1}$ ,  $c_{5,4}$ ). By chopping of the centroid, we obtain two special Nyström rooted trees (for  $c_{3,1}$  we obtain two copies of  $\sigma v \rho \tau_{1,1}$ ; for  $c_{5,4}$  two copies of  $\sigma v \rho \tau_{2,1}$ ). By definition of centroid, the special Nyström rooted trees obtained must have the same order *j*.

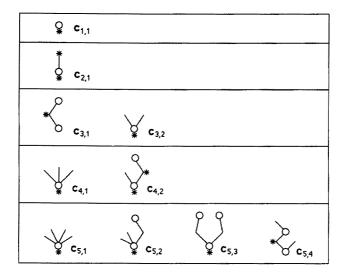


Fig. 3. Equivalence classes of special Nyström rooted trees.

Hence, in this case N must be odd and j = (N - 1)/2. Furthermore, when N is odd, there are

$$\binom{m_{(N-1)/2}+1}{2} = \frac{1}{2}m_{(N-1)/2}(m_{(N-1)/2}+1)$$

equivalence classes included in this case.

- (ii) There are two centroids (in Figure 3, the classes  $c_{2,1}, c_{4,2}$ ). These are necessarily adjacent and one of them fat and the other meagre. Furthermore N is even. We now chop off the meagre centroid, to get a special Nyström rooted tree of order N/2 and a special Nyström rooted tree with order N/2 1. Therefore this case comprises  $m_{N/2}m_{N/2-1}$  equivalence classes.
- (iii) There is one centroid and it is fat (in Figure 3, classes  $c_{1,1}, c_{3,2}, c_{4,1}, c_{5,1}, c_{5,2}, c_{5,3}$ ). By choosing the representative of the class that is rooted at the centroid, we see that there is a one-to-one correspondence between equivalence classes in this case and special Nyström rooted trees whose root is the only centroid. The number of such special Nyström rooted trees can be found to be, for N even,

$$m_N - (m_1 m_{N-2} + m_2 m_{N-3} + \ldots + m_{N/2-1} m_{N/2}) - m_{N/2} m_{N/2-1}$$

and, for N odd,

$$m_N - (m_1 m_{N-2} + m_2 m_{N-3} + \ldots + m_{(N-1)/2} m_{(N-1)/2})$$

These formulae can be proved by an argument similar to that used to obtain formula (8) in [13], Section 2.3.4.4: from the total number  $m_N$  of special Nyström rooted trees of order N we subtract the number of those for which the

root is not a centroid, and, if N is even, also the number of those with two centroids.

On combining these results we find, for N even,

(3.4a) 
$$m_N^* = m_N - (m_1 m_{N-2} + m_2 m_{N-3} + \ldots + m_{N/2-1} m_{N/2}),$$

and, for N odd,

(3.4b) 
$$m_N^* = m_N - (m_1 m_{N-2} + \dots + m_{(N-3)/2} m_{(N+1)/2}) - \frac{1}{2} m_{(N-1)/2} m_{(N-1)/2} + \frac{1}{2} m_{(N-1)/2}.$$

In terms of the generating functions, (3.4) reads

(3.5) 
$$M^*(z) = M(z) - \frac{1}{2}z(M(z)^2 - M(z^2)).$$

The number of equivalence classes for  $N \leq 9$  is given in Table 1.

For canonical methods, the advantages that derive from the reduction in number of order conditions are of course partly offset by the fact that one has to satisfy the equations (1.7). In order to gain some understanding of this point, we shall next consider in detail the case of *explicit* RKN methods. Assume that, following a standard practice, we restrict our attention to methods that satisfy the simplifying assumption (1.7a). Then, with s stages, we have, as free parameters, s coefficients  $b_i$ , s coefficients  $\gamma_i$  and s(s - 1)/2 coefficients  $\alpha_{ij}$  (the  $\beta_i$ 's are determined by (1.7a)). For order  $\geq p$ , there are  $m_1 + \ldots + m_p$  equations to be satisfied, so that the difference between the number of parameters and the number of equations is

$$F(p,s) = \frac{s^2}{2} + \frac{3s}{2} - m_1 - \ldots - m_p.$$

The function F(p, s) is tabulated in Table 2a, where the entries corresponding to negative values of F have not been given.

Let us now consider explicit canonical RKN methods. If a method of this kind has a coefficient  $b_i = 0$ , then, by (1.7*a*), the corresponding  $\beta_i$  also vanishes, and, by (1.7*b*),  $b_j \alpha_{ij} = 0$  for each *j*. Therefore the *i*-th stage plays no effective role in the computation and the method is equivalent to a method with fewer stages. Hence we may assume that  $b_i \neq 0$  for all *i*. Then (1.7b) reveals that  $\alpha_{ij} = b_j(\gamma_i - \gamma_j)$  for i > j, so that we have *s* values  $b_i$  and *s* values  $\gamma_i$  as only free parameters. For order  $\geq p$  there are  $m_1^* + \ldots + m_p^*$  equations, and the difference "parameters–equations" is now

$$F^*(p,s) = 2s - m_1^* - \ldots - m_p^*$$

The function  $F^*$  is tabulated in Table 2b. A comparison between F and  $F^*$  reveals that the class of explicit canonical RKN methods is just a small subclass of the family of explicit RKN methods. Nevertheless, we should stress that this is better than the situation for Runge-Kutta formulae, where the class of explicit methods contains no canonical formula.

	(a)									
p/s	1	2	3	4	5	6				
1	1	4	8	13	19	26				
2	0	3	7	12	18	25				
3	-	1	5	10	16	23				
4	-	-	2	7	13	20				
5	_	-	-	1	7	14				
6	-	-	-	—	-	4				
			(	b)						
1	1	3	5	7	9	11				
2	0	2	4	6	8	10				
3	-	0	2	4	6	8				
4	_	_	0	2	4	6				
5	_	_	-	_	0	2				
6	_	_	_	_	_	_				

Table 2. The functions F(p, s) (a) and  $F^*(p, s)$  (b)

As an example of the use of (1.7b) as a simplifying assumption let us consider the construction of explicit, canonical RKN methods of order 4. (Note that 4 is the minimum value of p for which  $m_p > m_p^*$ .) Upon choosing s = 5, Table 2 shows that there are 4 free parameters after imposing the order conditions. A good way of disposing of two of the free parameters is to set  $\gamma_1 = 0$  and  $\gamma_5 = 0$ : this ensures that the fifth stage of the current step is equal to the first stage in the next step (FSAL), so that effectively the method requires four function evaluations per step. The two remaining free parameters can be used to minimize the error constants in the local truncation error: this has been done in [5].

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