CANONICAL RUNGE-KUTTA-NYSTRÖM METHODS OF ORDERS 5 AND 6*

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Abstract. In this paper, we construct canonical explicit 5-stage and 7-stage Runge-Kutta-Nyström methods of orders 5 and 6, respectively, for Hamiltonian dynamical systems.

Key Words: Hamiltonian systems, canonical integrators, symplectic integrators, Runge-Kutta-Nyström methods.

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1. Introduction. There has been much recent interest in deriving for Hamiltonian systems

$$\frac{dq}{dt} = \frac{\partial H(q,p)}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H(q,p)}{\partial q}, \tag{1}$$

higher order numerical integrators which retain the canonical (or symplectic) property of the flow of the original system. Of particular interest have been explicit Runge-Kutta-Nyström methods(RKN) for the special separable Hamiltonian

$$H(q,p) = \frac{1}{2}p^{\mathrm{T}}M^{-1}p + V(q), \tag{2}$$

where q and p are vectors representing, respectively, the positions and momenta and where M is a diagonal matrix. The function $V(q)$ is associated with the potential energy and H the total energy.

Ruth[9] was the first to publish results about canonical numerical integrators. He showed that the 2nd-order 1-stage leapfrog/Störmer/Verlet method was canonical and discovered a 3-stage canonical RKN method of order 3. Ruth's work was followed by considerable research in the area of constructing higher order canonical integrators[3, 6, 10, 2, 11, 12]. Forest and Ruth[3] derived an explicit 3-stage canonical integrator of order 4. Yoshida[12] was the first to prove the existence of canonical integrators of arbitrarily high order. He showed how to construct a 3^k-stage method having order $2k+2$ using a composition of canonical 1-stage method of order 2. He derived numerically 7- and 15-stage canonical integrators, respectively of orders 6 and 8 using a Lie group approach. Low stage number is desirable because of greater convenience (such as the generation of more closely spaced output values).

Still much is unknown about the possibilities for higher order canonical methods—information that is useful in the search for practical methods. In this paper we derive

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numerically 5th-order, 5-stage RKN methods and symmetric 6th-order, 7-stage RKN methods in section 3. A total of four 5th-order, 5-stage RKN methods are reported. Sixteen symmetric 6th-order, 7-stage RKN methods were obtained, three of these are equivalent (in the sense used in [6]) to the canonical integrators constructed by Yoshida[12] for general separable Hamiltonians.

2. Order and Canonical Conditions. An s-stage Runge-Kutta-Nyström method for a system with the Hamiltonian (2) is given by

$$\begin{aligned} y_i &= q_n + c_i h\dot{q}_n + h^2 \sum_{j=1}^{s} a_{ij} f(y_j), \quad i = 1, 2, \dots, s, \\ q_{n+1} &= q_n + h\dot{q}_n + h^2 \sum_{i=1}^{s} b_i f(y_i), \\ \dot{q}_{n+1} &= \dot{q}_n + h \sum_{i=1}^{s} B_i f(y_i). \end{aligned} \tag{3}$$

where $\dot{q}_n = M^{-1}p_n$ and $f(q) = -M^{-1}\nabla V(q)$. The method (3) is explicit if $a_{ij} = 0$ for $j \geq i$. An explicit s-stage RKN method without redundant stages is canonical if [6, 7, 11]

$$b_i = B_i(1 - c_i), \quad 1 \leq i \leq s, \tag{4}$$

$$a_{ij} = B_j(c_i - c_j), \quad j < i. \tag{5}$$

If we assume that the conditions in (4) and (5) are satisfied, we have[4] the following order conditions for RKN methods of order ≤ 5

$$t_1 \ : \ \sum_i B_i = 1, \quad t_2 \ : \ \sum_i B_i c_i = \frac{1}{2},$$

$$t_3 \ : \ \sum_i B_i c_i^2 = \frac{1}{3}, \quad t_4 \ : \ \sum_i \sum_{j<i} B_i B_j (c_i - c_j) = \frac{1}{6},$$

$$t_5 \ : \ \sum_i B_i c_i^3 = \frac{1}{4}, \quad t_6 \ : \ \sum_i \sum_{j<i} B_i B_j c_i (c_i - c_j) = \frac{1}{8},$$

$$t_7 \ : \ \sum_i \sum_{j<i} B_i B_j (c_i - c_j) c_j = \frac{1}{24}, \quad t_8 \ : \ \sum_i B_i c_i^4 = \frac{1}{5},$$

$$t_9 \ : \ \sum_i \sum_{j<i} B_i B_j c_i^2 (c_i - c_j) = \frac{1}{10}, \quad t_{10} \ : \ \sum_i \sum_{j<i} \sum_{l<i} B_i B_j B_l (c_i - c_j)(c_i - c_l) = \frac{1}{20},$$

$$t_{11} \ : \ \sum_i \sum_{j<i} B_i B_j c_i c_j (c_i - c_j) = \frac{1}{30}, \quad t_{12} \ : \ \sum_i \sum_{j<i} B_i B_j c_j^2 (c_i - c_j) = \frac{1}{60},$$

$$t_{13} \quad : \quad \sum_i \sum_{j<i} \sum_{l<j} B_i B_j B_l (c_i - c_j)(c_j - c_l) = \frac{1}{120}.$$

The condition t_7 is redundant (see Okunbor and Skeel [6]). We use a similar approach as in [6] to show that t_{12} and t_{13} are also redundant:

$$\begin{aligned}
\text{lhs of } t_{12} &= \sum_i \sum_{j<i} B_i B_j c_j^2 (c_i - c_j) \\
&= -\sum_i \sum_{j>i} B_i B_j c_i^2 (c_i - c_j) \\
&= \sum_i \sum_{j<i} B_i B_j c_i^2 (c_i - c_j) - \sum_i \sum_j B_i B_j c_i^2 (c_i - c_j) \\
&= \frac{1}{10} - (\sum_i \sum_j B_i B_j c_i^3 - \sum_j \sum_i B_i B_j c_i^2) \\
&= \frac{1}{10} - (\frac{1}{4} \cdot 1 - \frac{1}{3} \cdot \frac{1}{2}) \\
&= \frac{1}{60} = \text{ rhs of } t_{12},
\end{aligned}$$

$$\begin{aligned}
\text{lhs of } t_{13} &= \sum_i \sum_{j<i} \sum_{l<j} B_i B_j B_l (c_i - c_j)(c_j - c_l) \\
&= -\sum_i \sum_{j>i} \sum_{l<i} B_i B_j B_l (c_i - c_j)(c_i - c_l) \\
&= \sum_i \sum_{j<i} \sum_{l<i} B_i B_j B_l (c_i - c_j)(c_i - c_l) - \sum_i \sum_j \sum_{l<i} B_i B_j B_l (c_i - c_j)(c_i - c_l) \\
&= \frac{1}{20} - \sum_j B_j [\sum_i \sum_{l<i} B_i B_l (c_i - c_l) c_i - \sum_i \sum_{l<i} B_i B_l (c_i - c_l) c_j] \\
&= \frac{1}{20} - [1 \cdot \frac{1}{8} - \sum_j B_j c_j \sum_l \sum_{l<i} B_i B_l (c_i - c_l)] \\
&= \frac{1}{20} - (1 \cdot \frac{1}{8} - \frac{1}{2} \cdot \frac{1}{6}) \\
&= \frac{1}{120} = \text{ rhs of } t_{13}.
\end{aligned}$$

The above results illustrate the proposition of Calvo and Sanz-Serna[1] that states that if two Nyström trees that are equivalent (see definition in the Appendix), then the Φ (see Appendix) that corresponds to one can be expressed in terms of Φ's of the other and trees of lower orders. In our case, the trees, $f[z^2, f]$ and $f[f[z^2]]$ in our special notation (see Appendix) that result respectively, from t_9 and t_{12} are equivalent. The same is true for trees, $f[f[z]^2]$ and $f[f[f]]$ that result respectively, from t_{10} and t_{13}.

3. Canonical Runge-Kutta-Nyström methods.

3.1. 5th-Order 5-Stage Methods. In section 2, we showed that t_7, t_{12} and t_{13} are redundant for a canonical RKN method of 5th-order, leaving us with 10 conditions involving 10 parameters. These conditions were then solved for B_i and c_i. We resorted

Method	B_i	c_i
1	−1.67080892327314312060	0.69491389107017931259
	1.22143909230997538270	0.63707199676998338411
	0.08849515813253908125	−0.02055756998211598005
	0.95997088013770159876	0.79586189634575355001
	0.40090379269297793385	0.30116624272377778837
2	0.22116193442417902970	0.77070344943939539384
	1.00218471521051766260	0.24564166478370674795
	0.20420286893045538901	0.87295101556657583863
	−0.82437756359543068463	0.13352418017438366649
	0.39682804503028051846	0.03827009985427366062
3	0.40090379269664777606	0.69883375727544694289
	0.95997088013412390506	0.20413810365459889029
	0.08849515812721633901	1.02055757000418534370
	1.22143909234910252870	0.36292800323075291580
	−1.67080892330709041000	0.30508610893167564804
4	0.39682804502748120212	0.96172990014637649292
	−0.82437756359000080586	0.86647581982605526019
	0.20420286893142899909	0.12704898443392728669
	1.00218471520794616400	0.75435833521637640775
	0.22116193442314432960	0.22929655056040595951

TABLE 1
5th-order 5-stage Runge-Kutta-Nyström Methods

to an iterative procedure because these conditions involve complicated expressions in B_i and c_i. We used the subroutines HYBRD1 and HYBRJ1 of MINPACK obtained from Netlib for determining the solution. HYBRD1 combines Powell's method for optimization, QR factorization and the finite divided difference method for computing the Jacobian matrix. HYBRJ1 is the same as HYBRD1 except that exact Jacobian matrix is used. The initial guesses were obtained randomly from a Gaussian distribution with mean 0 and standard deviation 1. About 10,000 different initial guesses were tried and only four methods were obtained. These four methods, obtained using HYBRD1 were used as initial solutions for the HYBRJ1 program to improve the accuracy of method coefficients. These four methods are shown in Table 1. The 2-norm of residuals in all 13 order conditions is 10^{-13} for method 1, 10^{-14} for methods 2, 10^{-15} for method 3 and 4. As is obvious method 3 is the adjoint of method 1, and 4 the adjoint of 2. The adjoint of a method is obtained by interchanging h, q_n and $\dot{q}_n$, respectively, with $-h$, q_{n+1} and $\dot{q}_{n+1}$. The slight differences in coefficients, indicates the error in these values. We speculate that these are the only methods with real coefficients considering the magnitude of the number of initial guesses tried. Very recently, we also found these methods in [8].

3.2. 6th-Order 6-Stage Methods. To construct symmetric methods of order 6, we start with a 6-stage RKN method with the following conditions

$$B_1 = B_6, \quad B_2 = B_5, \quad B_3 = B_4,$$

$$c_1 = 1 - c_6, \quad c_2 = 1 - c_5, \quad c_3 = 1 - c_4.$$

With these conditions t_1, t_3, t_4 and t_7 can be written as

$$t_1 \quad : B_4 + B_5 + B_6 = \frac{1}{2},$$

$$t_3 \quad : B_4 c_4(1-c_4) + B_5 c_5(1-c_5) + B_6 c_6(1-c_6) = \frac{1}{12},$$

$$t_4 \quad : \quad B_5 c_5(B_4 + B_5) + B_6 c_6(1-B_6) + B_4(B_4 c_4 + B_5 c_5) = \frac{5}{24},$$

$$t_8 \quad : B_4 c_4^2(1-c_4)^2 + B_5 c_5^2(1-c_5)^2 + B_6 c_6^2(1-c_6)^2 = \frac{1}{60}.$$

The conditions t_2, t_5 and t_6 are redundant given t_1, t_3, t_4 and the symmetry conditions. For details, see [5]. The conditions t_9, t_{10} and t_{11} have complicated expressions even after they have been simplified and they are omitted here. For a symmetric 6-stage RKN method, it turns out that t_1, t_3, t_4, t_8 and two of t_9, t_{10}, t_{11} are enough to find B_4, B_5, B_6, c_4, c_5 and c_6. In all, there are 3 possible sets of equations, namely

$$t_1,\ t_3,\ t_4,\ t_8,\ t_9,\ t_{10};$$

$$t_1,\ t_3,\ t_4,\ t_8,\ t_9,\ t_{11};$$

$$t_1,\ t_3,\ t_4,\ t_8,\ t_{10},\ t_{11}.$$

The three sets were solved by HYBRD1 and all solutions obtained from each set never satisfied the missing equation after trying 1000 initial guesses. We therefore state the following conjecture.

Conjecture 1. *There is no symmetric 6-stage RKN method of order 6.*

3.3. 6th-Order 7-Stage Methods. The negative result above motivated us to search for symmetric 7-stage methods of order 6. The symmetry conditions in this case are

$$B_1 = B_7, \quad B_2 = B_6, \quad B_3 = B_5,$$

$$c_1 = 1 - c_7, \quad c_2 = 1 - c_6, \quad c_3 = 1 - c_5, \quad c_4 = \frac{1}{2}.$$

With these conditions t_1, t_3, t_4 and t_7 can now be written as

$$t_1 \quad : \quad \frac{1}{2}B_4 + B_5 + B_6 + B_7 = \frac{1}{2},$$

$$t_3 \quad : \quad \frac{1}{8}B_4 + B_5 c_5(1-c_5) + B_6 c_6(1-c_6) + B_7 c_7(1-c_7) = \frac{1}{12},$$

$$t_4 \quad : \quad \frac{1}{8}B_4^2 + B_5 c_5(B_4 + B_5) + B_6 c_6(1-B_6) + B_7 c_7(1-B_7) - 2B_6 B_7 c_6 = \frac{5}{24},$$

$$t_8 \quad : \quad \frac{1}{16}B_4 + 2B_5c_5^2(1-c_5)^2 + 2B_6c_6^2(1-c_6)^2 + 2B_7c_7^2(1-c_7)^2 = \frac{1}{30}.$$

The unknowns in this case are B_4, B_5, B_6, B_7, c_5, c_6 and c_7. This makes it likely that the conditions t_1, t_3, t_4,t_8, t_9, t_{10} and t_{11} can be solved uniquely for those parameters. Again, we used the routine HYBRD1. After trying 1000 different initial guesses, we obtained 16 different methods as indicated in Tables 2(a) and 2(b). The numbers in brackets represent the 2-norms of the residuals of all twenty-three order conditions. We did not use HYBRJ1 to improve the accuracy of method coefficients as we did in section 3.1. The 6th-order conditions are given in the appendix for verification purpose. These methods which include the methods constructed by Yoshida are 7-stage all of order 6, counterexamples to what is suggested by Calvo and Sanz-Serna[1].

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Method	$1(10^{-18})$	$2(10^{-11})$
B_4	0.26987577187133640373	3.5928607443524524644
$B_5 = B_3$	0.92161977504885189358	−15.107332703974111230
$B_6 = B_2$	0.13118241020105280626	12.863477709969692675 0
$B_7 = B_1$	−0.68774007118557290171	0.9474246218281922159
c_4	0.50000000000000000000	0.5000000000000000000
$c_5 = 1 - c_3$	0.06520862987680341024	0.6183748743920897662
$c_6 = 1 - c_2$	0.65373769483744778901	0.6157971577674397523
$c_7 = 1 - c_1$	0.05586607811787376572	0.2078328848108624420
Method	$3(10^{-10})$	$4(10^{-13})$
B_4	0.00024286040977501724	0.05051938039496037400
$B_5 = B_3$	0.08191385007043372004	−0.19724296189815250792
$B_6 = B_2$	−0.23158642248235284281	0.29421383710950594204
$B_7 = B_1$	0.64955114220703161414	0.37776943459116637888
c_4	0.50000000000000000000	0.50000000000000000000
$c_5 = 1 - c_3$	1.43531315933193655010	0.17400697317940588248
$c_6 = 1 - c_2$	−0.24517048359575719767	0.35112157438498342180
$c_7 = 1 - c_1$	0.88961673353684493504	0.88538450585116639129
Method	$5(10^{-14})$	$6(10^{-14})$
B_4	0.53433276576163783988	−1.17551592085151988540
$B_5 = B_3$	0.26761229791037091471	0.18255582404490564371
$B_6 = B_2$	−0.11049289984863524218	0.90437790353606192425
$B_7 = B_1$	0.07571421905744540753	0.00082423284479237473
c_4	0.50000000000000000000	0.50000000000000000000
$c_5 = 1 - c_3$	0.89004117238340154310	0.08339934196578745364
$c_6 = 1 - c_2$	0.38649500090554366120	0.60111926613307930040
$c_7 = 1 - c_1$	0.32278696952656012456	−0.44472255124612840218
Method	$7(10^{-12})$	$8(10^{-12})$
B_4	0.00932218673977119732	1.83115871043482115980
$B_5 = B_3$	0.32498572599945862848	−1.60893178391505317150
$B_6 = B_2$	−0.88165912535231663693	0.78644114551518701850
$B_7 = B_1$	0.01052012305982972410	0.40691128318245557316
c_4	0.50000000000000000000	0.50000000000000000000
$c_5 = 1 - c_3$	−0.48459939249170722986	0.64281876387138123413
$c_6 = 1 - c_2$	1.31770114865711416950	0.19374710559145964916
$c_7 = 1 - c_1$	−0.04817222754723789332	0.45783632321785344125

Table 2

(a) 6th-order 7-stage Runge-Kutta-Nyström methods

Appendix

Appendix A. Order Six Conditions. Using the notation in [4], we have that an RKN method applied to a problem of the form $y'' = f(y)$ is order p if and only if

(6) $$\sum b_i \Phi_i(t) = \frac{1}{(\rho(t)+1)\gamma(t)}, \quad \text{for Nyström trees with } \rho(t) \le p-1$$

(7) $$\sum B_i \Phi_i(t) = \frac{1}{\gamma(t)}, \quad \text{for Nyström trees with } \rho(t) \le p$$

Method	9(10^{-18})	10(10^{-11})
B_4	0.17870556351604306204	1.31518632072133272890
$B_5 = B_3$	−0.70725865603123129122	−1.17767998419672486520
$B_6 = B_2$	0.52154603876818645804	0.23557321336789232463
$B_7 = B_1$	0.59635983550502330216	0.78451361046816617611
c_4	0.50000000000000000000	0.50000000000000000000
$c_5 = 1 - c_3$	0.19372673677147641095	0.56875316825018557554
$c_6 = 1 - c_2$	0.12281363909397727225	0.09769978284560674493
$c_7 = 1 - c_1$	0.73810405290506590652	0.60774319475878124335
Method	11(10^{-14})	12(10^{-10})
B_4	2.37635274430775195470	2.38944778326077997980
$B_5 = B_3$	−2.13228522200145071250	0.00152886228323448038
$B_6 = B_2$	0.00426068187079227608	−2.14403531631696198820
$B_7 = B_1$	1.43984816797678245910	1.44778256240333751790
c_4	0.50000000000000000000	0.50000000000000000000
$c_5 = 1 - c_3$	0.62203376115315070111	1.69548832271598027000
$c_6 = 1 - c_2$	−0.44197850891210198213	0.62423509575146441018
$c_7 = 1 - c_1$	0.28007591601160846049	0.27610871880122885876
Method	13(10^{-12})	14(10^{-16})
B_4	0.38064159097019513586	−1.17241029106097547350
$B_5 = B_3$	0.68913741186280925274	0.00086271011462916579
$B_6 = B_2$	−0.37962421427441621893	0.18278954099977372197
$B_7 = B_1$	0.00016600692650939825	0.90255289441608484900
c_4	0.50000000000000000000	0.50000000000000000000
$c_5 = 1 - c_3$	0.84399425728108029845	1.40898136623592965580
$c_6 = 1 - c_2$	0.82565840518543383652	0.082185108932481825795
$c_7 = 1 - c_1$	2.01308797898817647120	0.60010457532587368429
Method	15(10^{-13})	16(10^{-12})
B_4	−1.19948849633588912820	0.40373333538947505081
$B_5 = B_3$	0.18573478166656658757	0.00883814004797850015
$B_6 = B_2$	0.00455888416048774229	0.69312512248770876197
$B_7 = B_1$	0.90945058234089023426	−0.40382993023042478752
c_4	0.50000000000000000000	0.50000000000000000000
$c_5 = 1 - c_3$	0.08589899029079409324	1.13151603666090087950
$c_6 = 1 - c_2$	1.12994507963609089810	0.83551090965247561460
$c_7 = 1 - c_1$	0.59383562925528326251	0.81425812752434768871

TABLE 2
(b) 6th-order 7-stage Runge-Kutta-Nyström methods

where $\rho(t)$ is the order of the tree, $\gamma(t)$ is the density of the tree and $\Phi_i(t)$ corresponds to the elementary weight of the Nyström tree. If conditions (4) combine with (7) then conditions (6) are superfluous. Therefore, we concentrate on the conditions (7). First, we let $z = y'$ and then use a special notation (similar to what was used in our Mathematica program) to represent the trees or the elementary differentials. We give here the correspondence between the elementary differentials in our notation and the Nyström trees for a few of the elementary differentials. The "fat" node correspond to derivative of z and the "meagre" node, to the derivative of the y. The bottom node is the root of the tree. Two Nyström trees are *equivalent* in the sense defined in Calvo and Sanz-Serna[1], if they have equal number of fat nodes, equal number of meagre nodes and identical branches and differs only in their roots. The order 6 conditions are given in Table 3, where $\alpha(t)$ is the weight of the elementary differential.

FIGURE MISSING

t	$\rho(t)$	$\alpha(t)$	$\gamma(t)$	$\Phi_i(t)$
$f[z^5]$	6	1	6	c_i^5
$f[f^2, z]$	6	15	24	$\sum_j \sum_k a_{ij} a_{ik} c_i$
$f[f, z^3]$	6	10	12	$\sum_j a_{ij} c_i^3$
$f[z, f[f]]$	6	5	144	$\sum_j \sum_k a_{ij} a_{jk} c_i$
$f[f, f[z]]$	6	10	72	$\sum_j \sum_k a_{ij} a_{ik} c_k$
$f[z^2, f[z]]$	6	10	36	$\sum_j a_{ij} c_i^2 c_j$
$f[f[f, z]]$	6	3	240	$\sum_j \sum_k a_{ij} a_{jk} c_j$
$f[z, f[z^2]]$	6	5	72	$\sum_j a_{ij} c_i c_j^2$
$f[f[z^3]]$	6	1	120	$\sum_j a_{ij} c_j^3$
$f[f[f[z]]]$	6	1	720	$\sum_j \sum_k a_{ij} a_{jk} c_k$

TABLE 3
Order Six Conditions