

Two step Runge-Kutta-Nyström methods based on algebraic polynomials

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ABSTRACT: *We consider the new family of two step Runge-Kutta-Nyström methods for the numerical integration of $y'' = f(x, y)$. We derive the conditions to obtain two step Runge-Kutta-Nyström methods which integrate algebraic polynomials exactly and analyze the one-stage case.*

1 – Introduction

We are concerned with second order Ordinary Differential Equations, in which the first derivative does not appear explicitly,

$$(1.1) \quad y''(t) = f(t, y(t)), \quad y(t_0) = y_0, \quad y'(t_0) = y'_0, \quad y(t), f(t, y) \in R^n,$$

having a periodic or an oscillatory solution. These initial value problems often arise in applications of molecular dynamics, orbital mechanics, seismology, and they are usually considered as a difficult integration problem. Indeed standard numerical methods can require a huge number of time-steps to track the oscillations. In many situations, when the problem has a large dimension, or the evaluation of the right-hand side function is

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very costly, or the response time is extremely important, for example in simulation processes, there is the need of obtaining an accurate solution in a reasonable time frame. Therefore there is a great demand of efficient methods for problem (1.1).

Although the system (1.1) may be reduced into a first order system, the development of numerical methods for its direct integration seems more natural. Many methods with constant coefficients have already been derived for second order ODEs (1.1) with periodic or oscillatory solutions. Linear multistep methods, hybrid and one step methods appeared in the literature: see for example [5], [6], [10], [13] for an extensive bibliography.

In [12] we introduced the two step Runge-Kutta-Nyström (TSRKN) methods

$$\begin{aligned}
 Y_{i-1}^j &= y_{i-1} + hc_j y'_{i-1} + h^2 \sum_{s=1}^m a_{js} f(x_{i-1} + c_s h, Y_{i-1}^s), \quad j = 1, \dots, m \\
 Y_i^j &= y_i + hc_j y'_i + h^2 \sum_{s=1}^m a_{js} f(x_i + c_s h, Y_i^s), \quad j = 1, \dots, m, \\
 (1.2) \quad y_{i+1} &= (1 - \theta)y_i + \theta y_{i-1} + h \sum_{j=1}^m v_j y'_{i-1} + h \sum_{j=1}^m w_j y'_i + \\
 &\quad + h^2 \sum_{j=1}^m (\bar{v}_j f(x_{i-1} + c_j h, Y_{i-1}^j) + \bar{w}_j f(x_i + c_j h, Y_i^j)), \\
 y'_{i+1} &= (1 - \theta)y'_i + \theta y'_{i-1} + h \sum_{j=1}^m (v_j f(x_{i-1} + c_j h, Y_{i-1}^j) + \\
 &\quad + w_j f(x_i + c_j h, Y_i^j)),
 \end{aligned}$$

for the direct numerical integration of (1.1). $\theta, \bar{v}_j, \bar{w}_j, v_j, w_j, a_{js}, b_{js}, j, s, = 1, \dots, m$ are the coefficients of the methods, which can be represented by the following array:

$$(1.3) \quad \begin{array}{c|c} \mathbf{c} & \mathbf{A} \\ \hline & \bar{\mathbf{v}} \\ \theta & \bar{\mathbf{w}} \\ & \mathbf{v} \\ & \mathbf{w}. \end{array}$$

For an m -stage TSRKN method, A is a $m \times m$ real matrix; c, \bar{v}, \bar{w}, v and w are real vectors of length m .

In [12] the TSRKN method was derived as an indirect method from the two step Runge-Kutta methods introduced in [7]. The reason of interest in methods TSRKN (1.2) lies in the fact that, advancing from x_i to x_{i+1} we only have to compute Y_i , because Y_{i-1} has already been evaluated in the previous step. Therefore the computational cost of the method depends on the matrix A , while the vectors v and \bar{v} add extra degrees of freedom.

Our aim is to analyze two step implicit methods of type (1.2) which integrate algebraic polynomials exactly. The main motivation for the development of implicit methods (1.2), as those considered in the present paper, is their property of having a high stage order which make them suitable for stiff systems, also because their implicitness. Collocation-based methods also belong to this class.

In Section 2 we extend Albrecht's approach [1], [2] to the family (1.2), with the aim to derive the conditions for TSRKN methods to integrate algebraic polynomials exactly.

In Section 3 we perform the linear stability analysis. In Section 4 we consider the case of one stage methods.

2 – TSRKN methods based on algebraic polynomials

Let us consider the TSRKN methods (1.2). It is known that the method (1.2) is zero-stable if [12]

$$(2.1) \quad -1 < \theta \leq 1.$$

We treat formulas (1.2) by extending Albrecht's technique [1], [2] to the numerical method in concern, as we already done in [9] for Runge-Kutta-Nyström methods, and in [11] for two step Runge-Kutta methods. According to this approach, we regard the two step Runge-Kutta-Nyström method (1.2) as a composite linear multistep scheme, but on a not equidistant grid.

Adopting the $m + 1$ linear stage representation, which is used in Albrecht's theory for Runge-Kutta, we slightly modify the notation of (1.2)

in the following way:

$$\begin{aligned}
 y_{i-1+c_j} &= y_{i-1} + hc_j y'_{i-1} + h^2 \sum_{s=1}^m a_{js} f(x_{i-1} + c_s h, y_{i-1+c_s}), \\
 & \qquad \qquad \qquad j = 1, \dots, m \\
 y_{i+c_j} &= y_i + hc_j y'_i + h^2 \sum_{s=1}^m a_{js} f(x_i + c_s h, y_{i+c_s}), \quad j = 1, \dots, m, \\
 (2.2) \quad y_{i+1} &= (1 - \theta)y_i + \theta y_{i-1} + h \sum_{j=1}^m v_j y'_{i-1} + h \sum_{j=1}^m w_j y'_i + \\
 & \quad + h^2 \sum_{j=1}^m (\bar{v}_j f(x_{i-1} + c_j h, y_{i-1+c_j}) + \bar{w}_j f(x_i + c_j h, y_{i+c_j})), \\
 y'_{i+1} &= (1 - \theta)y'_i + \theta y'_{i-1} + h \sum_{j=1}^m (v_j f(x_{i-1} + c_j h, y_{i-1+c_j}) + \\
 & \quad + w_j f(x_i + c_j h, y_{i+c_j})),
 \end{aligned}$$

y_{i-1+c_j} and y_{i+c_j} in (2.2) are the *internal stages*; y_{i+1} and y'_{i+1} are the *final stages*, which give the approximation of the solution and of the derivative of the solution in the step point x_i .

We associate a linear difference operator with each stage, in the following way:

$$(2.3) \quad \mathcal{L}_j[z(x); h] = z(x + c_j h) - z(x) - hc_j z'(x) - h^2 \sum_{s=1}^m (a_{js} z''(x + c_s h)),$$

for $j = 1, \dots, m$ is associated with the internal stage y_{i+c_j} of (2.2);

$$\begin{aligned}
 (2.4) \quad \bar{\mathcal{L}}[z(x); h] &= z(x+h) - (1-\theta)z(x) - \theta z(x-h) - h \left(\sum_{j=1}^m v_j z'(x-h) + \right. \\
 & \quad \left. + \sum_{j=1}^m w_j z'(x) \right) - h^2 \sum_{j=1}^m (\bar{v}_j z''(x + (c_j - 1)h) + \bar{w}_j z''(x + c_j h)),
 \end{aligned}$$

is associated with the stage y_{i+1} in (2.2).

$$\begin{aligned}
 (2.5) \quad \bar{\mathcal{L}}'[z(x); h] &= z'(x+h) - (1-\theta)z'(x) - \theta z'(x-h) + \\
 & \quad - h \sum_{j=1}^m (v_j z''(x + (c_j - 1)h) + w_j z''(x + c_j h)),
 \end{aligned}$$

is associated with the final stage y'_{i+1} in (2.3).

It results:

$$\begin{aligned}\mathcal{L}_j[1; h] &= \mathcal{L}_j[x; h] = 0, \quad j = 1, \dots, m, \\ \overline{\mathcal{L}}[1; h] &= \overline{\mathcal{L}}'[1; h] = \overline{\mathcal{L}}'[x; h] = 0, \quad j = 1, \dots, m.\end{aligned}$$

If we annihilate (2.4) on the function $z(x) = x$, then from $\overline{\mathcal{L}}[x; h] = 0$, it follows that

$$(2.6) \quad \sum_{j=1}^m (v_j + w_j) = 1 + \theta$$

which represents the consistency condition already derived in [7].

The condition (2.6) implies that the method (1.2) is consistent [7] and, together with (2.1), it ensures that the TSRKN is convergent with order at least one.

If (2.3) is identically equal to zero when $z(x) = x^p$, i.e. if $\mathcal{L}_j[x^p; h] = 0$, then it results:

$$(2.7) \quad \sum_{s=1}^m a_{js} c_s^{p-2} = \frac{c_j^p}{p(p-1)}, \quad j = 1, \dots, m.$$

Moreover, if (2.4) results equal to zero when $z(x) = x^p$, i.e. $\overline{\mathcal{L}}[x^p; h] = 0$, then

$$(2.8) \quad \sum_{j=1}^m (\bar{v}_j (c_j - 1)^{p-2} + \bar{w}_j c_j^{p-2}) = \frac{1 - (-1)^p \theta}{p(p-1)} - \frac{(-1)^{p-1}}{p-1} \sum_{j=1}^m v_j.$$

Finally, if we annihilate (2.5) on the function $z(x) = x^p$, then from $\overline{\mathcal{L}}'[x^p; h] = 0$, it follows that

$$(2.9) \quad \sum_{j=1}^m (v_j (c_j - 1)^{p-2} + w_j c_j^{p-2}) = \frac{1 - (-1)^{p-1} \theta}{(p-1)}.$$

We can now give the following definitions:

DEFINITION 1. An m-stage TSRKN method is said to satisfy the simplifying conditions $C_2(p)$ if its parameters satisfy

$$\sum_{s=1}^m a_{js} c_s^{k-2} = \frac{c_j^k}{k(k-1)}, \quad j = 1, \dots, m, \quad k = 1, \dots, p.$$

DEFINITION 2. An m -stage TSRKN method is said to satisfy the simplifying conditions $B_2(p)$ if its parameters satisfy

$$\sum_{j=1}^m (\bar{v}_j (c_j - 1)^{k-2} + \bar{w}_j c_j^{k-2}) = \frac{1 - (-1)^k \theta}{k(k-1)} - \frac{(-1)^{k-1}}{k-1} \sum_{j=1}^m v_j, \\ j = 1, \dots, m, \quad k = 1, \dots, p.$$

DEFINITION 3. An m -stage TSRKN method is said to satisfy the simplifying conditions $B'_2(p)$ if its parameters satisfy

$$\sum_{j=1}^m (v_j (c_j - 1)^{k-2} + w_j c_j^{k-2}) = \frac{1 - (-1)^{k-1} \theta}{(k-1)}, \quad k = 1, \dots, p.$$

$C_2(p)$, $B_2(p)$ and $B'_2(p)$ not only allow the reduction of order conditions of trees in the theory of two step RKN methods, which is under development by the author of this paper, but they also mean that all the quadrature formulas represented by the TSRKN method have order at least p , similarly as it happens in the theory of Runge-Kutta methods [3].

Now we prove the following theorem by using Albrecht's theory [1], [2]:

THEOREM 1. *If $C_2(p)$, $B_2(p)$ and $B'_2(p)$ hold, then the m -stage TSRKN method (1.2) has order of convergence p .*

PROOF. $C_2(p)$, $B_2(p)$ and $B'_2(p)$ imply that all the stages of the method have order p or, in Albrecht's terminology, that each stage in (2.2) has order of *consistency* p , so that the method has order of *consistency* p . In this case the method converges with order at least p .

It is worth mentioning that the conditions $C_2(p)$, $B_2(p)$ and $B'_2(p)$ are only sufficient conditions for the TSRKN method to have order p . Indeed the final stage must certainly have order of *consistency* p , which is the condition $B'_2(p)$, but it is not necessary that also the internal stages have order of *consistency* p . Therefore $C_2(p)$ and $B_2(p)$ are not necessary conditions for the method to have order p .

If all the stages have order of *consistency* p , then all the stages are exact on any linear combination of the power set $\{1, x, x^2, \dots, x^p\}$, and this implies that the TSRKN method results exact on algebraic polynomials. Moreover the simplifying conditions $C_2(p)$, $B_2(p)$ and $B'_2(p)$ are

a constructive help for the derivation of new numerical methods within the family of TSRKN methods.

3 – Linear stability analysis

The linear stability analysis for numerical methods for second order ODEs (1.1) is performed by applying the method to the linear homogeneous test equation [12]

$$(3.1) \quad y'' = -\omega^2 y, \quad \omega \in \mathbf{R}.$$

The following recursion results for methods (1.2):

$$(3.2) \quad \begin{pmatrix} y_i \\ y_{i+1} \\ h y'_i \\ h y'_{i+1} \end{pmatrix} = M(z^2) \begin{pmatrix} y_{i-1} \\ y_i \\ h y'_{i-1} \\ h y'_i \end{pmatrix}$$

with

$$(3.3) \quad M(z^2) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ \theta - z^2 \bar{\mathbf{v}}^T \mathbf{N}^{-1} \mathbf{e} & 1 - \theta - z^2 \bar{\mathbf{w}}^T \mathbf{N}^{-1} \mathbf{e} & \mathbf{v}^T \mathbf{e} - z^2 \bar{\mathbf{v}}^T \mathbf{N}^{-1} \mathbf{c} & \mathbf{w}^T \mathbf{e} - z^2 \bar{\mathbf{w}}^T \mathbf{N}^{-1} \mathbf{c} \\ 0 & 0 & 0 & 1 \\ -z^2 \mathbf{v}^T \mathbf{N}^{-1} \mathbf{e} & -z^2 \mathbf{w}^T \mathbf{N}^{-1} \mathbf{e} & \theta - z^2 \mathbf{v}^T \mathbf{N}^{-1} \mathbf{c} & 1 - \theta - z^2 \mathbf{w}^T \mathbf{N}^{-1} \mathbf{c} \end{pmatrix},$$

where $z = \omega h$, $\mathbf{e} = (1, \dots, 1)^T$, $N = I + z^2 A$.

$M(z^2)$ in (3.2)-(3.3) is the *stability* or *amplification* matrix for the two-step RKN methods (1.2). The stability properties of the method depend on the eigenvalues of the amplification matrix, i.e. they depend on the roots of the stability polynomial,

$$(3.4) \quad \pi(\lambda) = \det(M(z^2) - \lambda I),$$

whose coefficients are rational functions of the parameters of the method. For the sake of completeness, we recall now the following two definitions.

DEFINITION 4. $(0, H_0^2)$ is interval of periodicity for the two step RKN method if, $\forall z^2 \in (0, H_0^2)$, the roots of the stability polynomial $\pi(\lambda)$ satisfy:

$$r_1 = e^{i\phi(z)}, \quad r_2 = e^{-i\phi(z)}, \quad |r_{3,4}| \leq 1$$

with $\phi(z)$ real.

DEFINITION 5. The two step RKN method is P -stable if its interval of periodicity is $(0, +\infty)$.

For an A -stable method the eigenvalues of the amplification matrix are within the unit circle for all stepsizes and any choice of frequency in the test equations, and this ensures that the amplitude of the numerical solution of the test equation does not increase with time. If, what's more, there isn't numerical dissipation, that is if the principal eigenvalues of the amplification matrix lie on the unit circle, then the method is P -stable [12].

4 – One stage TSRKN method

Let us consider now the one stage TSRKN method (1.2) represented by the following Butcher array

$$(4.1) \quad \begin{array}{c|c} c & a \\ \hline & \bar{v} \\ \theta & \bar{w} \\ & v \\ & w. \end{array}$$

The method (4.1) has all the stages of order 2 if $C_2(2)$, $B_2(2)$ and $B_2'(2)$ hold, that is if the parameters in (4.1) satisfy

$$(4.2) \quad a = \frac{1}{2}c^2, \quad v + w = 1 + \theta, \quad \bar{v} + \bar{w} - v = \frac{1 - \theta}{2}.$$

Solving (4.2) leaving c, θ, \bar{w}, v as free parameters, the resulting method has all the stages of order 2 if

$$(4.3) \quad a = \frac{1}{2}c^2, \quad w = 1 + \theta - v, \quad \bar{v} = \frac{1 - \theta}{2} - \bar{w} + v.$$

A necessary condition to obtain a method with a not-empty interval of periodicity is that the characteristic polynomial (3.4) of the method (4.1), with parameters given by (4.3), is symmetric. In this case, if λ is an eigenvalue of $M(z^2)$, then also $\frac{1}{\lambda}$ is eigenvalue and any stability interval is also an interval of periodicity.

The analytical study shows that for no values of the free parameters the characteristic polynomial (3.4) can be symmetric. This implies that the one-stage TSRKN method (4.1), having all stages of order 2, does not possess interval of periodicity. An extensive numerical search proved that there exist methods with large interval of stability. The interval of stability is defined in a natural way to be the interval $(0, Z^2)$, where the roots of the stability polynomial $\pi(\lambda)$ are in modulus less than unity $\forall z^2 \in (0, Z^2)$. The values of the free parameters which maximize the interval of stability can be determined by using the symbolic package which is described in [4], that analyzes the stability properties of a large variety of numerical methods for ODEs by considering the associated stability functions.

An alternative approach to maximize the interval of stability $(0, Z^2)$, consists in analyzing for which values of the free parameters the characteristic polynomial (3.4) results to be a Schur polynomial, according to the definition given in [8], that is for which values for c, θ, v, \bar{w} in (4.3) the roots of (3.4) result to lie within the unit circle. For this analysis we solved the set of inequalities produced by the Routh-Hurwitz criterion [8], which is known to be a criterion for the roots of a polynomial to lie in the left half-plane.

The characteristic polynomial (3.4) has the following form for the one stage method (4.1)-(4.3):

$$(4.4) \quad \pi(\lambda) = \frac{P_0(z^2) + P_1(z^2)\lambda + P_2(z^2)\lambda^2 + P_3(z^2)\lambda^3 + P_4(z^2)\lambda^4}{2 + c^2z^2}$$

with

$$\begin{aligned}
 P_0(z^2) &= 2v^2z^2 - \theta(1 + 2(1 + c)v - 2\bar{w})z^2 + \theta^2(2 + z^2 + c^2z^2), \\
 P_1(z^2) &= (-1 - 2(-1 + c)v - 4v^2 + 2\bar{w})z^2 - \theta^2(4 + z^2 + 2cz^2 + \\
 &\quad + 2c^2z^2) + 2\theta(2 + (1 - c + c^2 + 3v + 2cv - 2\bar{w})z^2), \\
 P_2(z^2) &= 2 + (3 - 2c + c^2 - 2v + 4cv + 2v^2 - 4\bar{w})z^2 + \theta^2(2 + \\
 &\quad + (2 + 2c + c^2)z^2) - \theta(8 + (-3 + 4c^2 + 4v + 2cv - 2\bar{w})z^2), \\
 P_3(z^2) &= 2(-2 - c^2z^2 + \bar{w}z^2 + \theta(2 + cz^2 + c^2z^2) + c(z^2 - vz^2)), \\
 P_4(z^2) &= 2 + c^2z^2.
 \end{aligned}$$

Following [8], we perform the transformation

$$(4.5) \quad \lambda = \frac{1+r}{1-r}$$

which maps the interior of the circle $|\lambda| = 1$ onto the left half-plane $\operatorname{Re} r < 0$. The following polynomial

$$Q(r) = a_0r^4 + a_1r^3 + a_2r^2 + a_3r + a_4$$

arises from (4.4) after the transformation (4.5). Then the necessary and sufficient conditions for $\pi(\lambda)$ in (4.4) to be a Schur polynomial, are that the principal minors of the following 4×4 matrix

$$K = \begin{pmatrix} a_1 & a_3 & 0 & 0 \\ a_0 & a_2 & a_4 & 0 \\ 0 & a_1 & a_3 & 0 \\ 0 & a_0 & a_2 & a_4 \end{pmatrix}$$

be positive. By omitting the details, a set of inequalities follows which we solved numerically, finding many methods with large intervals of stability. Some of the largest intervals are found, for instance, with the following values of the free parameters:

$$\begin{aligned}
 \theta &= -\frac{1}{2}, & c &= 1, & v &= -1, & \bar{w} &= \frac{1}{2}, & (0, Z^2) &= (0, 16) \\
 \theta &= -\frac{1}{2}, & c &= \frac{7}{8}, & v &= -\frac{3}{4}, & \bar{w} &= -\frac{1}{2}, & (0, Z^2) &= (0, 10).
 \end{aligned}$$

Of course all the free parameters have influence on the amplitude of the interval of stability; but in particular, for the one-stage method (4.1), the intervals of stability are going to become larger when the c -value goes towards 1.

5 – Conclusions

We have considered the family of TSRKN methods for $y'' = f(x, y)$ which integrate algebraic polynomials exactly. Within this family we do not find methods possessing interval of periodicity, but methods with large interval of stability, which can be used in the numerical treatment of stiff systems. The work containing the derivation of the Butcher arrays for methods up to three stages is forthcoming. It is worth mentioning that, if we let down the request of obtaining an high stage order, we can find zero-dissipative stable two step Runge-Kutta Nyström methods; indeed the existence of P -stable methods within family (1.2) has been proved in [12].

Following the procedure showed in this paper, that is annihilating the linear difference operators (2.3)-(2.5) on different basis of functions, it is possible to derive TSRKN methods for ODEs having solutions with an already known behaviour. For example, it is worth considering TSRKN methods for ODEs (1.1) having periodic or oscillatory solution, for which the dominant frequency ω is known in advance; in this case a proper set of functions is the basis for trigonometric polynomial $\{1, \cos \omega x, \sin \omega x, \cos 2\omega x, \sin 2\omega x, \dots\}$, as already considered in [9], [11] for Runge-Kutta-Nyström and two step Runge-Kutta methods. The technique used in this paper can also be applied for the construction of collocation methods within family (1.2).

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