A General Family of Two Step Runge-Kutta-Nyström Methods for $y'' = f(x, y)$ 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 $y'' = f(x, y)$, which provide approximation for the solution and its first derivative at the step point, and depend on the stage values at two consecutive step points. We derive the conditions to obtain methods within this family, which integrate algebraic polynomials exactly, describe a constructive technique and analyze the order of the resulting method.

1 Introduction

We are concerned with the analysis of a family of two step methods for the numerical integration of second order Ordinary Differential Equations, in which the first derivative does not appear explicitly,

$$y''(t) = f(t, y(t)), \quad y(t_0) = y_0, \quad y'(t_0) = y'_0, \qquad y(t), f(t, y) \in R^n, \tag{1}$$

having a periodic or an oscillatory solution. The initial value problem (1) often arises in applications of molecular dynamics, orbital mechanics, seismology. When 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, and therefore there is a great demand of efficient methods for the direct integration of problem (1).

Many methods with constant coefficients have already been derived for second order ODEs (1) with periodic or oscillatory solutions: see for example [5, 8, 11, 12, 14, 15] for an extensive bibliography.

In this paper we consider the following generalization of the two step Runge–Kutta–Nyström (TSRKN) methods introduced in [14], by introducing the stage values at two consecutive step points, in order to increase the order of the methods, as already done in [9] for first order ODEs:

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$$\begin{aligned}
Y_n^j &= u_{j1}y_{n-1} + u_{j2}y_n + h\left(\overline{u}_{j1}y'_{n-1} + \overline{u}_{j2}y'_n\right) + \\
&\quad + h^2 \textstyle\sum_{s=1}^m (a_{js} f(x_{n-1} + c_s h, Y_{n-1}^s) + b_{js} f(x_n + c_s h, Y_n^j)), \\
y_{n+1} &= \theta_1 y_{n-1} + \theta_2 y_n + h(\eta_1 y'_{n-1} + \eta_2 y'_n) + \\
&\quad h^2 \textstyle\sum_{j=1}^m (v_j f(x_{n-1} + c_j h, Y_{n-1}^j) + w_j f(x_n + c_j h, Y_n^j)), \\
h y'_{n+1} &= \theta'_1 y_{n-1} + \theta'_2 y_n + h(\eta'_1 y'_{n-1} + \eta'_2 y'_n) + \\
&\quad h^2 \textstyle\sum_{j=1}^m (v'_j f(x_{n-1} + c_j h, Y_{n-1}^j) + w'_j f(x_n + c_j h, Y_n^j)),
\end{aligned} \tag{2}$$

c_j, θ_1, θ_2, u_{j1}, u_{j2}, $\overline{u}_{j1}$, $\overline{u}_{j2}$, v'_j, w'_j, v_j, w_j, a_{js}, b_{js}, $j, s, = 1, \ldots, m$ are the coefficients of the methods, which can be represented by the following array:

$$\begin{array}{c|cc|c|c}
\mathbf{c} & \mathbf{u} & \bar{\mathbf{u}} & \mathbf{A} & \mathbf{B} \\
\hline
 & \theta & \eta & \mathbf{v}^{\mathbf{T}} & \mathbf{w}^{\mathbf{T}} \\
 & \theta' & \eta' & \mathbf{v}'^{\mathbf{T}} & \mathbf{w}'^{\mathbf{T}}
\end{array}$$

In [14] the TSRKN method was derived as an indirect method from the two step Runge–Kutta methods introduced in [9]. 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 alreay been evaluated in the previous step. Therefore the computational cost of the method depends on the matrix A, while the vectors $\mathbf{v}$ and $\bar{\mathbf{v}}$ add extra degrees of freedom.

Our aim is to analyze two step implicit methods of type (2) which integrate algebraic polynomials exactly. The main motivation for the development of implicit methods (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 (2), with the aim to derive the conditions for TSRKN methods to integrate algebraic polynomials exactly. In Section 3 we consider the collocation–based methods of type (2).

2 TSRKN Methods Based on Algebraic Polynomials

Let us consider the TSRKN methods (2). It is known that the method (2) is zero–stable if [14]

$$-1 < \theta \leq 1 \tag{3}$$

We treat formulas (2) by extending Albrecht's technique [1, 2] to the numerical method in concern, as we already have done in [11] for Runge–Kutta–Nyström methods, and in [13] for two step Runge–Kutta methods. According to this approach, we regard the two step Runge–Kutta–Nyström method (2) as a composite linear multistep scheme, but on a non–uniform grid.

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

$$\begin{aligned}&\mathcal{L}_j[z(x);h] = z(x+c_jh) - u_{j,1}z(x-h) - u_{j,2}z(x) -\\ &h\,(\overline{u}_{j,1}z'(x-h) + \quad \overline{u}_{j,2}z'(x)) - \\ &h^2\textstyle\sum_{s=1}^{m}(a_{js}z''(x+(c_s-1)h) + b_{js}z''(x+c_sh),\end{aligned} \tag{4}$$

for $j = 1,\ldots,m$, is associated with the internal stage Y_n^j of (2).

$$\begin{aligned}&\bar{\mathcal{L}}[z(x);h] = z(x+h) - \theta_1 z(x-h) - \theta_2 z(x) -\\ &h(\eta_1 z'(x-h) + \eta_2 z'(x)) -\\ &h^2\textstyle\sum_{j=1}^{m}(v_j z''(x+(c_j-1)h) + w_j z''(x+c_jh)),\end{aligned} \tag{5}$$

is associated with the stage y_{n+1} in (2). Finally

$$\begin{aligned}&\bar{\mathcal{L}}'[z(x);h] = hz'(x+h) - \theta_1' z(x-h) - \theta_2' z(x) -\\ &h(\eta_1' z'(x-h) + \eta_2' z'(x)) -\\ &h^2\textstyle\sum_{j=1}^{m}(v_j' z''(x+(c_j-1)h) + w_j' z''(x+c_jh))\end{aligned} \tag{6}$$

is associated with the final stage y'_{n+1} in (2).
Obviously the following relation holds:

$$\mathcal{L}_j[1;h] = 0, \quad j = 1,\ldots,m,$$

and

$$\bar{\mathcal{L}}[1;h] = \bar{\mathcal{L}}'[1;h] = 0$$

from which the parameters of the method have to satisfy the following relations:

$$u_{j,1} + u_{j,2} = 1, \quad j = 1,\ldots,m \tag{7}$$

$$\theta_1 + \theta_2 = 1, \qquad \theta_1' + \theta_2' = 0. \tag{8}$$

In order to have the *consistency* of the internal stages, the following relation hold:

$$\mathcal{L}_j[x;h] = 0, \quad j = 1,\ldots,m,$$

which holds if

$$c_j + u_{j1} = \overline{u}_{j,1} + \overline{u}_{j,2} \tag{9}.$$

(9) implies that $y(x_i + c_j h) - Y_i^j = O(h)$ for $h \to 0$. In the same way the final stages are consistent if $\bar{\mathcal{L}}[x;h] = \bar{\mathcal{L}}'[x;h] = \bar{\mathcal{L}}'[x^2;h] = 0$, that is

$$\begin{aligned} &1+\theta_1 = \eta_1 + \eta_2, \qquad 1+\theta_1' = \eta_1' + \eta_2', \\ &\textstyle\sum_{j=1}^m (v_j' + w_j') = \frac{2 - \theta_1' + 2\eta_1'}{2}. \end{aligned} \tag{10}$$

If (4) is identically equal to zero when $z(x) = x^p$, i.e. if $\mathcal{L}_j[x^p;h] = 0$, then it results:

$$\begin{aligned} &\textstyle\sum_{s=1}^m (a_{js}(c_s - 1)^{p-2} + b_{js} c_s^{p-2}) = \\ &= \frac{c_j^p - (-1)^p u_{j,1} - (-1)^{p-1} p\, \overline{u}_{j,1}}{p(p-1)}. \end{aligned} \tag{11}$$

Moreover, if (5) results equal to zero when $z(x) = x^p$, i.e. $\bar{\mathcal{L}}[x^p;h] = 0$, then

$$\begin{aligned} &\textstyle\sum_{j=1}^m (v_j(c_j - 1)^{p-2} + w_j c_j^{p-2}) = \\ &= \frac{1 - (-1)^p \theta_1 - (-1)^{p-1} p\, \eta_1}{p(p-1)}. \end{aligned} \tag{12}$$

Finally, if we annihilate (6) on the function $z(x) = x^{p+1}$, then from $\bar{\mathcal{L}}'[x^{p+1};h] = 0$, it follows that

$$\begin{aligned} &\textstyle\sum_{j=1}^m (v_j'(c_j - 1)^{p-1} + w_j' c_j^{p-1}) = \\ &= \frac{(p+1) - (-1)^{p+1}\theta_1' - (-1)^p (p+1)\, \eta_1'}{p(p+1)}. \end{aligned} \tag{13}$$

We can now give the following definitions:

Definition 1. *An m–stage TSRKN method (2) is said to satisfy the simplifying conditions $AB_2(p)$, $VW_2(p)$ and $V'W_2'(p)$ if its parameters satisfy respectively:*

Condition $AB_2(p)$:

$$\begin{aligned} &\textstyle\sum_{s=1}^m (a_{js}(c_s - 1)^{k-2} + b_{js} c_s^{k-2}) = \\ &= \frac{c_j^h - (-1)^k u_{j,1} - (-1)^{k-1} k\, \overline{u}_{j,1}}{k(k-1)} \end{aligned}$$

for $k = 1, \ldots, p,\ \ j = 1, \ldots, m$.

Condition $VW_2(p)$:

$$\sum_{j=1}^m (v_j(c_j - 1)^{k-2} + w_j c_j^{k-2}) = \frac{1 - (-1)^k \theta_1 - (-1)^{k-1} k\, \eta_1}{k(k-1)}$$

for $k = 1, \ldots, p$.

Condition $V'W_2'(p)$:

$$\textstyle\sum_{j=1}^{m}(v_j'(c_j-1)^{k-1}+w_j'c_j^{k-1}) =$$

$$= \frac{(k+1)-(-1)^{k+1}\theta_1'-(-1)^k(k+1)\,\eta_1'}{k(k+1)}.$$

for $k=1,\dots,p$.

$AB_2(p)$, $VW_2(p)$ and $V'W_2'(p)$ allow the reduction of order conditions of trees in the theory of two step RKN methods, which is under development by the authors of this paper; moreover 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].

As far as the order is concerned, we follow the classical definition of convergence of order p, related with the local truncation error. As a consequence, the conditions which we are going to formulate, are given *for exact starting values* y_1, y_1', Y_0^j, $j=1,\dots,m$, as already done, for instance, in [6].

Definition 2. *An m–stage TSRKN method (2) has order p if for sufficiently smooth problems (1), and for exact starting values* y_1, y_1', Y_0^j, $j=1,\dots,m$,

$$y(x_1+h)-y_1 = O(h^{p+1}),\ hy'(x_1+h)-hy_1' = O(h^{p+2}) \tag{14}$$

By using Albrecht's theory [1,2], it is easy to prove the following theorem:

Theorem 1. If $AB_2(p)$, $VW_2(p)$ and $VW_2'(p)$ hold, then for exact starting values the m–stage TSRKN method (2) has order of *convergence* p.

Proof. $AB_2(p)$, $VW_2(p)$ and $V'W_2'(p)$ imply that all the stages of the method have order p or, in Albrecht's terminology, that each stage in (4)–(6) 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 $AB_2(p)$, $VW_2(p)$ and $V'W_2'(p)$ are only sufficient conditions for the TSRKN method to have order p, but not necessary. 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 when the solutions of the system of ODEs (1) are algebraic polynomials. Moreover the simplifying conditions $AB_2(p)$, $VW_2(p)$ and $V'W_2'(p)$ are a constructive help for the derivation of new numerical methods within the family of TSRKN methods.

3 Collocation Methods

Let us generalize the Definition 3.2 of [7], in order to derive collocation methods for (1):

Definition 3. Consider m real numbers $c_1, \dots, c_m \in [0,1]$, the solution values y_n, y_{n-1} and the derivative values y'_n, y'_{n-1}. The *collocation polynomial* $P(x)$ of degree $2m+3$ is then defined by:

$$P(x_{n-1}) = y_{n-1}, \quad P(x_n) = y_n \tag{14}$$

$$P'(x_{n-1}) = y'_{n-1}, \quad P'(x_n) = y'_n \tag{15}$$

$$P''(x_{n-1} + c_i h) = f(x_{n-1} + c_i h, P(x_{n-1} + c_i h)), \tag{16}$$

$$P''(x_n + c_i h) = f(x_n + c_i h, P(x_n + c_i h)). \tag{17}$$

Then the numerical solution of (1) is given by

$$y_{n+1} = P(x_{n+1}), \quad y'_{n+1} = P'(x_{n+1}) \tag{18}$$

(14)–(18) constitute a Hermite interpolation problem with incomplete data, because the function values at $x_n + c_i h$ are missing. Following [7], to compute the *collocation polynomial* $P(x)$, we introduce the dimensionless coordinate $t = (x - x_n)/h$, $x = x_n + th$, with nodes $t_1 = -1, t_2 = 0$, and define the following polynomials, which constitute a generalized Lagrange basis:

– $\phi_i(t)$, $i = 1, 2$, of degree $2m+3$, defined by

$$\phi_i(t_j) = \delta_{ij}, \qquad \phi'_i(t_j) = 0, \quad i, j = 1, 2, \tag{19}$$

$$\phi''_i(c_j - 1) = 0,\ \phi''_i(c_j) = 0,\ i = 1, 2,\ \ j = 1, \dots, m, \tag{20}$$

– $\psi_i(t)$, $i = 1, 2$, of degree $2m+3$, defined by

$$\psi_i(t_j) = 0, \qquad \psi'(t_j) = \delta_{ij}, \quad i, j = 1, 2, \tag{21}$$

$$\psi''_i(c_j - 1) = 0, \quad \psi''_i(c_j) = 0,\ \ i = 1, 2,\ \ j = 1, \dots, m, \tag{22}$$

– $\chi_{i,n-1}(t)$ and $\chi_{i,n}(t)$, $i = 1, \dots, m$, of degree $2m+3$, defined by

$$\chi_{i,n-1}(t_j) = 0, \quad \chi_{i,n}(t_j) = 0, \quad i = 1, \dots, m,\ j = 1, 2 \tag{23}$$

$$\chi'_{i,n-1}(t_j) = 0, \quad \chi'_{i,n}(t_j) = 0, \quad i = 1, \dots, m,\ j = 1, 2 \tag{24}$$

$$\chi''_{i,n-1}(c_j - 1) = \delta_{ij}, \quad \chi''_{i,n-1}(c_j) = 0, \quad i, j = 1, \dots, m, \tag{25}$$

$$\chi''_{i,n}(c_j - 1) = 0, \quad \chi''_{i,n}(c_j) = \delta_{ij}, \quad i, j = 1, \dots, m. \tag{26}$$

δ_{ij} denotes the Kronecker tensor. Then the expression of the collocation polynomial $P(x)$ in terms of these polynomials is given by:

$$P(x_n + th) = \phi_1(t)\, y_{n-1} \;+\; \phi_2(t)\, y_n + h(\, \psi_1(t)\, y'_{n-1} +$$

$$\psi_2(t)\, y'_n) + \quad h^2 \textstyle\sum_{j=1}^{m} (\chi_{j,n-1}(t) \quad P''(x_{n-1} + c_j h) \quad +$$

$$+ \quad \chi_{j,n}(t)\;\, P''(x_n + c_j h)).$$

After constructing $\phi_i(t)$, $\psi_i(t)$, $\chi_{i,n-1}(t)$ and $\chi_{i,n}(t)$, by putting $t = c_i$, by writing $P(x_n + c_i h) = Y_n^i$ and by inserting the collocation conditions (14)–(17), we obtain the expression of the two step Runge–Kutta–Nyström (TSRKN) collocation method of type (2), where the parameters of the method are given by the following relations:

$$\theta_i = \phi_i(1), \quad u_{j,i} = \phi_i(c_j), \quad i = 1, 2,\;\; j = 1, \ldots, m$$

$$\eta_i = \psi_i(1), \quad \overline{u}_{j,i} = \psi_i(c_j), \quad i = 1, 2,\;\; j = 1, \ldots, m$$

$$v_j = \chi_{j,n-1}(1), \quad a_{js} = \chi_{j,n-1}(c_s), \quad j, s, = 1, \ldots, m,$$

$$w_j = \chi_{j,n}(1), \quad b_{js} = \chi_{j,n}(c_s), \quad j, s, = 1, \ldots, m$$

$$\theta'_i = \phi'_i(1), \quad \eta'_i = \psi'_i(1), \quad i = 1, 2,$$

$$v'_j = \chi'_{j,n-1}(1), \quad w'_j = \chi'_{j,n}(1), \quad j = 1, \ldots, m,$$

and $\phi_i(t)$, $\psi_i(t)$, $\chi_{i,n-1}(t)$ and $\chi_{i,n}(t)$ are the polynomials defined by conditions (19)–(26).

4 Conclusions

We have considered the family of TSRKN methods for $y'' = f(x, y)$ which integrate algebraic polynomials exactly. Following the procedure showed in this paper, that is annihilating the linear difference operators (4)–(6) on the set of power functions, and solving the arising systems $AB_2(p+1)$, $VW_2(p+1)$ and $V'W'_2(p)$, it is possible to derive TSRKN methods for ODEs (1) of order of convergence p. If $p = 2m + 2$, then the method is of collocation type.

Following the procedure showed in this paper, that is annihilating the linear difference operators (4)–(6) 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) 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 $\{1, \cos\omega x, \sin\omega x, \cos 2\omega x, \sin 2\omega x, \ldots\}$ for trigonometric polynomials, as already considered in [11, 13] 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 (2).

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