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Order conditions for General Linear Nyström methods

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**Dedicated to John C. Butcher,
in occasion of his 80th birthday**

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Abstract The purpose of this paper is to analyze the algebraic theory of order for the family of general linear Nyström (GLN) methods introduced in [20] with the aim to provide a general framework for the representation and analysis of numerical methods solving initial value problems based on second order ordinary differential equations (ODEs). Our investigation is carried out by suitably extending the theory of B-series for second order ODEs to the case of GLN methods, which leads to a general set of order conditions. This allows to recover the order conditions of numerical methods already known in the literature, but also to assess a general approach to study the order conditions of new methods, simply regarding them as GLN methods: the obtained results are indeed applied to both known and new methods for second order ODEs.

Keywords Second order ordinary differential equations · General Linear methods · Nyström methods · order conditions · B-series.

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1 Introduction

This paper is devoted to the numerical solution of Hadamard well-posed initial value problems based on special second order Ordinary Differential Equations (ODEs)

$$\begin{cases} y''(t) = f(y(t)), \quad t \in [t_0, T], \\ y(t_0) = y_0 \in \mathbb{R}^d, \\ y'(t_0) = y'_0 \in \mathbb{R}^d. \end{cases} \tag{1}$$

It is well known that problem (1) admits an equivalent representation as a first order system of ODEs but with doubled dimension, thus the direct numerical integration of the second order version results to be more efficient.

We focus our attention on the family of General Linear Methods for second order ODEs (1)

$$\begin{aligned} Y_i^{[n]} &= h^2 \sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}) + h \sum_{j=1}^{r'} p_{ij} {y'}_j^{[n-1]} + \sum_{j=1}^{r} u_{ij} y_j^{[n-1]}, \quad i = 1, ..., s, \\ h{y'}_i^{[n]} &= h^2 \sum_{j=1}^{s} c_{ij} f(Y_j^{[n]}) + h \sum_{j=1}^{r'} r_{ij} {y'}_j^{[n-1]} + \sum_{j=1}^{r} w_{ij} y_j^{[n-1]}, \quad i = 1, ..., r', \\ y_i^{[n]} &= h^2 \sum_{j=1}^{s} b_{ij} f(Y_j^{[n]}) + h \sum_{j=1}^{r'} q_{ij} {y'}_j^{[n-1]} + \sum_{j=1}^{r} v_{ij} y_j^{[n-1]}, \quad i = 1, ..., r, \end{aligned} \tag{2}$$

introduced in [20], here denoted as General Linear Nyström (GLN) methods. The supervectors

$$y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix} \in \mathbb{R}^{rd}, \ {y'}^{[n-1]} = \begin{bmatrix} {y'}_1^{[n-1]} \\ {y'}_2^{[n-1]} \\ \vdots \\ {y'}_{r'}^{[n-1]} \end{bmatrix} \in \mathbb{R}^{r'd}, \ Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ Y_2^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix} \in \mathbb{R}^{sd}$$

are respectively denoted as input vector of the *external approximations*, input vector of the *first derivative approximations* and *internal stage* vector. The vector $y^{[n-1]}$ is denoted as *input vector* of the external stages, and contains all the informations transferred advancing from the point t_{n-1} to the point t_n of the grid. It is important to observe that such a vector could also contain not only approximations to the solution of the problem in the grid points inherited from the previous steps, but also other informations computed in the past that we want to use in the integration process. The vector ${y'}^{[n-1]}$ instead contains previous approximations to the first derivative of the solution computed in previous step points, while the values $Y_j^{[n-1]}$, denoted as *internal stage* values, provide an approximation to the solution in the internal points $t_{n-1} + c_j h$, $j = 1, 2, \ldots, s$, where $\mathbf{c} = [c_1, c_2, \ldots, c_s]$ is the vector of the abscissae of the method.

Formulation (2) of GLMs for second order ODEs involves nine coefficient matrices $\mathbf{A} \in \mathbb{R}^{s\times s}$, $\mathbf{P} \in \mathbb{R}^{s\times r'}$, $\mathbf{U} \in \mathbb{R}^{s\times r}$, $\mathbf{C} \in \mathbb{R}^{r'\times s}$, $\mathbf{R} \in \mathbb{R}^{r'\times r'}$, $\mathbf{W} \in \mathbb{R}^{r'\times r}$, $\mathbf{B} \in \mathbb{R}^{r\times s}$, $\mathbf{Q} \in \mathbb{R}^{r\times r'}$, $\mathbf{V} \in \mathbb{R}^{r\times r}$, which are put together in the following partitioned $(s + r' + r) \times (s + r' + r)$ matrix

$$\left[\begin{array}{c|c|c} \mathbf{A} & \mathbf{P} & \mathbf{U} \\ \hline \mathbf{C} & \mathbf{R} & \mathbf{W} \\ \hline \mathbf{B} & \mathbf{Q} & \mathbf{V} \end{array}\right], \tag{3}$$

denoted as the Butcher tableau of the GLM. Using these notations, a GLM for second order ODEs can then be expressed as follows:

$$\begin{aligned} Y^{[n]} &= h^2(\mathbf{A} \otimes \mathbf{I})F^{[n]} + h(\mathbf{P} \otimes \mathbf{I})y'^{[n-1]} + (\mathbf{U} \otimes \mathbf{I})y^{[n-1]}, \\ hy'^{[n]} &= h^2(\mathbf{C} \otimes \mathbf{I})F^{[n]} + h(\mathbf{R} \otimes \mathbf{I})y'^{[n-1]} + (\mathbf{W} \otimes \mathbf{I})y^{[n-1]}, \\ y^{[n]} &= h^2(\mathbf{B} \otimes \mathbf{I})F^{[n]} + h(\mathbf{Q} \otimes \mathbf{I})y'^{[n-1]} + (\mathbf{V} \otimes \mathbf{I})y^{[n-1]}, \end{aligned} \tag{4}$$

where $\otimes$ denotes the usual Kronecker tensor product, $\mathbf{I}$ is the identity matrix in $\mathbb{R}^{d\times d}$ and $F^{[n]} = [f(Y_1^{[n]}), f(Y_2^{[n]}), \ldots, f(Y_s^{[n]})]^\intercal$. This representation is in line with the one usually proposed in the literature regarding multistage numerical methods for second order ODEs: this is typical, for instance, of Runge-Kutta-Nyström methods (see [25]).

The specific purpose of this paper is the formulation of order conditions for GLN methods (2), by means of a suitable generalization of the algebraic theory of order (compare [5, 25]) described in the remainder of the paper. The treatise is organized as follows: Section 2 reviews the needed framework to develop order conditions for second order ODEs, i.e. Nyström trees and related operators; these tools are then employed in Section 3 to derive order conditions for GLN methods (2) which, due to their generalities, also recover the order conditions of already known numerical methods for (1). Section 4 is devoted to provide an example of application of the results on order conditions to derive a new method of order 4.

2 Framework

It is well known from the literature that the algebraic theory of order of multistage/multivalue numerical methods for ODEs (compare [3–9, 25] and references therein) is based on the representation of the exact and numerical solutions in terms of functions on the set of rooted trees

$T = \{$  $, \ldots\}$.

Rooted trees provide an essential tool to analyze the properties of numerical methods for evolutionary problems, thanks to a smart intuition of John C. Butcher, who introduced an algebraic theory of order for Runge-Kutta and general linear methods (compare [5] and references therein) for first order

ODEs which is nowadays used in many different context, not only related to the numerical solution of functional equations. In fact, Connes and Kreimer [12] observed that the Hopf algebra of rooted trees that, also known as Butcher group (compare [5,7]), independently arose in their own work on renormalization in quantum field theory. This Connes-Kreimer algebra, is equivalent to the Butcher group, because its dual is the universal enveloping algebra of the Lie algebra of the Butcher group (compare [1]).

For second order equations, due to the presence of the derivative of the exact solution, we need a more general set of rooted trees, namely bi-coloured trees, defined as follows (compare [25])

$NT = \{\bullet,\ \circ,$  $\ldots\}.$

The vertices $\tau_1 = \bullet$ and $\tau_2 = \circ$ are combined according to following the rules

1. the root of $t \in NT$ is always fat;
2. a meagre vertex has at most one son which has to be fat.

Following [10,25], we adapt the theory of N-trees and of N-series introduced by Hairer and Wanner in [23] to the special problem

$$y''(x) = f(y(x)). \tag{5}$$

By calculating the derivatives of the exact solution of problem (5)

$$y''' = \frac{\partial f}{\partial y} y', \quad y^{(iv)} = \frac{\partial^2 f}{\partial y^2} y'^2 + \frac{\partial f}{\partial y} y'', \quad y^{(v)} = \frac{\partial^3 f}{\partial y^3} y'^3 + 3 \frac{\partial^2 f}{\partial y^2} y' f + \frac{\partial f}{\partial y} y''', \quad \ldots$$

we observe that the terms including the derivative of f with respect to y' disappear, producing a smaller set of trees called Special N-trees (SNT) set [25]

$SNT = \{\bullet,\ \circ,$  $\ldots\}.$

2.1 Composition and decomposition rules, elementary differentials and functions on SNT

By combining the formalisms introduced in [10,23], a composition rule of special Nyström trees is given according to the following scheme. We consider $t_1, \ldots, t_k \in SNT$ and a new root τ_2. Then,

1. if $t_i \neq \tau_1$, then its root is connected to a new meagre node, linked to the new root;
2. if $t_i = \tau_1$, then it is connected to the new root via a new branch.

The resulting SN-tree is denoted as $t = [t_1, \ldots, t_k]$. Inversely, cutting the branches leaving from the root of a given $t \in SNT$, let u_1, u_2, ..., u_k be the resulting subtrees. For any $u_i \neq \tau_1$, we cut off the branch leaving from its root τ_1 and denote the remaining part as t_i. For the remaining u_i, we set $t_i = \tau_1$. Then, the tree is decomposed as $t = [t_1, \ldots, t_k]$.

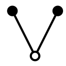
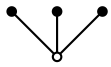
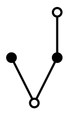
$\rho(t)$	t	$F(t)$	$\alpha(t)$
1	$\bullet$	y'	1
2	$\circ$	f	1
3		$f'y'$	1
4		$f''(y',y')$	1
		$f'f$	1
5		$f'''(y',y',y')$	1
		$f''(y',f)$	3
		$f'f'y'$	1

Table 1 Special Nyström trees up to order 5 and associated elementary differentials

Given these rules, we can extend the definition of elementary differential given in [5,25] to the special problem (5). For a given $t = [t_1, \dots, t_k] \in SNT$, we recursively define the elementary differentials as follows

$$
\begin{aligned}
F(\bullet)(y,y') &= y', \\
F(\circ)(y,y') &= y'' = f, \\
F(t)(y,y') &= f^{(k)}\left(F(t_1)(y,y'), \dots, F(t_k)(y,y')\right).
\end{aligned}
$$

Moreover, for a given tree $t = [t_1^{\mu_1}, t_2^{\mu_2}, \ldots, t_k^{\mu_k}]$, we recursively define the following useful functions ρ and α (compare [10,23])

$$\begin{aligned} &\rho(\bullet) = 1, \quad \rho(\circ) = 2, \quad \rho(t) = 2 + \sum_{i=1}^{k} \mu_i \rho(t_i), \\ &\alpha(\bullet) = \alpha(\circ) = 1, \quad \alpha(t) = (\rho(t) - 2)! \prod_{i=1}^{k} \frac{1}{\mu_i!} \left(\frac{\alpha(t_i)}{\rho(t_i)} \right)^{\mu_i}. \end{aligned} \tag{6}$$

2.2 N-Series

Following [23], we define a SN-series as

$$SN(a, y, y') = \sum_{t \in SNT} \frac{h^{\rho(t)}}{\rho(t)!} \alpha(t) a(t) F(t)(y, y'). \tag{7}$$

We observe that both the exact solution of (5) and its first derivative can be formally written as SN-series, whose coefficients are calculated in next sections.

The following theorem, useful in the remainder of the paper, provides a representation form for the composition of a SN-series with the function f in (5) (compare [23]).

Theorem 1 *For a given map $a : SNT \mapsto \mathbb{R}$ satisfying $a(\emptyset) = 1$, we have*

$$f(SN(a, y, y')) = \sum_{t \in SNT} \frac{h^{\rho(t)-2}}{(\rho(t) - 2)!} \alpha(t) a''(t) F(t)(y, y') \tag{8}$$

with

$$a''(t) = \begin{cases} 0, & \text{if } t = \emptyset, \tau_1, \\ 1, & \text{if } t = \tau_2, \\ a(t_1) \cdots a(t_k), & \text{if } t = [t_1, \ldots, t_k]. \end{cases} \tag{9}$$

3 Order Conditions for GLNs

We now employ the theory of SN-series above recalled, to derive a general set of order conditions for the family of GLN methods (2). First of all, let us assume that the input vector is a SN-series of the form

$$y_i^{[0]} = \sum_{t \in SNT} \frac{h^{\rho(t)}}{\rho(t)!} \alpha(t) \xi_i(t) F(t)(y, y'), \tag{10}$$

and, analogously, that

$$Y_i^{[0]} = \sum_{t \in SNT} \frac{h^{\rho(t)}}{\rho(t)!} \alpha(t) \eta_i(t) F(t)(y, y'). \tag{11}$$

We need to establish how terms like $h^2 f(Y_i)$ and $hy'^{[0]}_i$ can be expressed as SN-series. Theorem 1 allows us to write $h^2 f(Y_i)$ as SN-series (7) of coefficients

$$\overline{\eta}_i(t) = \eta''_i(t) \cdot \rho(t) \cdot (\rho(t) - 1)\,, \tag{12}$$

while, if $y'^{[0]}_i$ is a formal series of the form

$$y'^{[0]}_i = \sum_{t \in SNT} \frac{h^{\rho(t)-1}}{(\rho(t)-1)!} \alpha(t) \xi'_i(t) F(t)(y, y'), \tag{13}$$

$hy'^{[0]}_i$ is a SN-series (7) of coefficients

$$\delta_i(t) = \xi'_i(t) \cdot \rho(t)$$

With abuse of notation, we have denoted the coefficients of the SN-series (13) by $\xi'_i(t)$, even if they are not actually the first derivatives of $\xi_i(t)$ in (10).

We can now suitably extend the strategy proposed in [5], in order to develop an algebraic theory of order for GLNs. To this purpose, we insert the derived SN-series in the method formulation (4), obtaining

$$SN(\eta_i, y, y') = \sum_{j=1}^{s} a_{ij} SN(\overline{\eta}_j, y, y') + \sum_{j=1}^{r'} p_{ij} SN(\delta_j, y, y') + \sum_{j=1}^{r} u_{ij} SN(\xi_j, y, y'),$$

$i = 1, 2, \dots s$, which leads to

$$SN(\eta_i, y, y') = SN\left(\sum_{j=1}^{s} a_{ij} \overline{\eta}_j + \sum_{j=1}^{r'} p_{ij} \delta_j + \sum_{j=1}^{r} u_{ij} \xi_j, y, y' \right), \quad i = 1, \dots s.$$

Thus,

$$\eta_i(t) = \sum_{j=1}^{s} a_{ij} \overline{\eta}_j(t) + \sum_{j=1}^{r'} p_{ij} \delta_j(t) + \sum_{j=1}^{r} u_{ij} \xi_j(t), \quad i = 1, \dots s. \tag{14}$$

In analogous way, we obtain the following equations for the external approximations

$$\widehat{\xi}_i(t) = \sum_{j=1}^{s} b_{ij} \overline{\eta}_j(t) + \sum_{j=1}^{r'} q_{ij} \delta_j(t) + \sum_{j=1}^{r} v_{ij} \xi_j(t), \quad i = 1, \dots r, \tag{15}$$

$$\widehat{\delta}_i(t) = \sum_{j=1}^{s} c_{ij} \overline{\eta}_j(t) + \sum_{j=1}^{r'} r_{ij} \delta_j(t) + \sum_{j=1}^{r} w_{ij} \xi_j(t), \quad i = 1, \dots r'. \tag{16}$$

Collecting the left-hand sides of (14), (15) and (16) in the vectors $\eta \in \mathbb{R}^s$, $\xi \in \mathbb{R}^r$ and $\delta \in \mathbb{R}^{r'}$, respectively, leads to the following matrix representation

$$\begin{cases} \eta = \mathbf{A}\overline{\eta} + \mathbf{P}\delta + \mathbf{U}\xi, \\ \widehat{\xi} = \mathbf{B}\overline{\eta} + \mathbf{Q}\delta + \mathbf{V}\xi, \\ \widehat{\delta} = \mathbf{C}\overline{\eta} + \mathbf{R}\delta + \mathbf{W}\xi. \end{cases} \tag{17}$$

As a consequence, the following result holds.

Proposition 1 *If the operators $\widehat{\xi}$ and $\widehat{\delta}$ in* (17) *of a given GLN* (2) *are such that $\widehat{\xi}_i(t)$ and $\widehat{\delta}_i(t)$ coincide with the correspoding coefficients $E\xi_i(t)$ and $E\delta_i(t)$ in the Taylor series expansions of the exact values approximated by $y_i^{[n]}$ and $y'^{[n]}_i$ for any $t \in SNT$ of order $\rho(t) \leq p$ and $\rho(t) \leq p+1$ respectively, then the method has order p, i.e.*

$$\begin{cases} E\xi = \mathbf{B}\overline{\eta} + \mathbf{Q}\delta + \mathbf{V}\xi, & \rho(t) \leq p, \\ E\delta = \mathbf{C}\overline{\eta} + \mathbf{R}\delta + \mathbf{W}\xi, & \rho(t) \leq p+1. \end{cases} \tag{18}$$

Moreover, the method has stage order q if the operators $\eta_i(t)$, $i = 1, \ldots, s$, in (17) *coincide with the coefficients $E\eta_i$ of the Taylor series expansion of $y(x_0 + c_i h)$, for any $t \in SNT$ of order $\rho(t) \leq q+1$, i.e.*

$$E\eta = \mathbf{A}\overline{\eta} + \mathbf{P}\delta + \mathbf{U}\xi. \tag{19}$$

By applying the result derived in Proposition 1, we derive the expressions of the operators (18) and (19) in correspondence of the trees up to order 4 for a GLN method (2). We observe that the algebraic conditions (18) and (19) in Proposition 1 have to be solved recursively by means of the decomposition rule given in Section 2.1, according to Theorem 1. We first consider (18) and (19) corresponding to the trees $\emptyset$, τ_1 and τ_2, which provide the base case of the recursion, obtaining

$\emptyset$

$$\begin{aligned} \eta_i(\emptyset) &= \sum_{j=1}^{r} u_{ij}\xi_j(\emptyset), \quad i = 1, \ldots, s, \\ E\delta_i(\emptyset) &= \sum_{j=1}^{r} w_{ij}\xi_j(\emptyset), \quad i = 1, \ldots, r', \\ E\xi_i(\emptyset) &= \sum_{j=1}^{r} v_{ij}\xi_j(\emptyset), \quad i = 1, \ldots, r, \end{aligned} \tag{20}$$

$\bullet$

$$\begin{aligned} \eta_i(\bullet) &= \sum_{j=1}^{r'} p_{ij}\xi'_j(\bullet) + \sum_{j=1}^{r} u_{ij}\xi_j(\bullet), \quad i = 1, \ldots, s, \\ E\delta_i(\bullet) &= \sum_{j=1}^{r'} r_{ij}\xi'_j(\bullet) + \sum_{j=1}^{r} w_{ij}\xi_j(\bullet), \quad i = 1, \ldots, r', \\ E\xi_i(\bullet) &= \sum_{j=1}^{r'} q_{ij}\xi'_j(\bullet) + \sum_{j=1}^{r} v_{ij}\xi_j(\bullet), \quad i = 1, \ldots, r, \end{aligned} \tag{21}$$

$\circ$

$$
\begin{aligned}
\eta_i(\circ) &= 2\sum_{j=1}^{s} a_{ij}\eta_j(\emptyset) + 2\sum_{j=1}^{r'} p_{ij}\xi'_j(\circ) + \sum_{j=1}^{r} u_{ij}\xi_j(\circ), \quad i=1,\dots,s,\\
E\delta_i(\circ) &= 2\sum_{j=1}^{s} c_{ij}\eta_j(\emptyset) + 2\sum_{j=1}^{r'} r_{ij}\xi'_j(\circ) + \sum_{j=1}^{r} w_{ij}\xi_j(\circ), \quad i=1,\dots,r',\\
E\xi_i(\circ) &= 2\sum_{j=1}^{s} b_{ij}\eta_j(\emptyset) + 2\sum_{j=1}^{r'} q_{ij}\xi'_j(\circ) + \sum_{j=1}^{r} v_{ij}\xi_j(\circ), \quad i=1,\dots,r.
\end{aligned}
\tag{22}
$$

Once the base case is provided, the operators evaluated in the trees of order 2, 3 and 4 are recursively derived according to Theorem 1, leading to

$\overset{\bullet}{\circ}$

$$
\begin{aligned}
E\delta_i(\overset{\bullet}{\circ}) &= 6\sum_{j=1}^{s} c_{ij}\eta_j(\bullet) + 3\sum_{j=1}^{r'} r_{ij}\xi'_j(\overset{\bullet}{\circ}) + \sum_{j=1}^{r} w_{ij}\xi_j(\overset{\bullet}{\circ}), \quad i=1,\dots,r',\\
E\xi_i(\overset{\bullet}{\circ}) &= 6\sum_{j=1}^{s} b_{ij}\eta_j(\bullet) + 3\sum_{j=1}^{r'} q_{ij}\xi'_j(\overset{\bullet}{\circ}) + \sum_{j=1}^{r} v_{ij}\xi_j(\overset{\bullet}{\circ}), \quad i=1,\dots,r,
\end{aligned}
\tag{23}
$$

$\overset{\bullet\,\bullet}{\circ}$

$$
\begin{aligned}
E\delta_i(\overset{\bullet\,\bullet}{\circ}) &= 12\sum_{j=1}^{s} c_{ij}\eta_j(\bullet)^2 + 4\sum_{j=1}^{r'} r_{ij}\xi'_j(\overset{\bullet\,\bullet}{\circ}) + \sum_{j=1}^{r} w_{ij}\xi_j(\overset{\bullet\,\bullet}{\circ}), \quad i=1,\dots,r',\\
E\xi_i(\overset{\bullet\,\bullet}{\circ}) &= 12\sum_{j=1}^{s} b_{ij}\eta_j(\bullet)^2 + 4\sum_{j=1}^{r'} q_{ij}\xi'_j(\overset{\bullet\,\bullet}{\circ}) + \sum_{j=1}^{r} v_{ij}\xi_j(\overset{\bullet\,\bullet}{\circ}), \quad i=1,\dots,r,
\end{aligned}
\tag{24}
$$

$\overset{\circ}{\overset{\bullet}{\circ}}$

$$
\begin{aligned}
E\delta_i(\overset{\circ}{\overset{\bullet}{\circ}}) &= 12\sum_{j=1}^{s} c_{ij}\eta_j(\circ) + 4\sum_{j=1}^{r'} r_{ij}\xi'_j(\overset{\circ}{\overset{\bullet}{\circ}}) + \sum_{j=1}^{r} w_{ij}\xi_j(\overset{\circ}{\overset{\bullet}{\circ}}), \quad i=1,\dots,r',\\
E\xi_i(\overset{\circ}{\overset{\bullet}{\circ}}) &= 12\sum_{j=1}^{s} b_{ij}\eta_j(\circ) + 4\sum_{j=1}^{r'} q_{ij}\xi'_j(\overset{\circ}{\overset{\bullet}{\circ}}) + \sum_{j=1}^{r} v_{ij}\xi_j(\overset{\circ}{\overset{\bullet}{\circ}}), \quad i=1,\dots,r,
\end{aligned}
\tag{25}
$$

$\overset{\bullet\bullet\bullet}{\circ}$

$$
\begin{aligned}
E\delta_i(\overset{\bullet\bullet\bullet}{\circ}) &= 20\sum_{j=1}^{s} c_{ij}\eta_j(\bullet)^3 + 5\sum_{j=1}^{r'} r_{ij}\xi'_j(\overset{\bullet\bullet\bullet}{\circ}) + \sum_{j=1}^{r} w_{ij}\xi_j(\overset{\bullet\bullet\bullet}{\circ}), \quad i=1,\dots,r',\\
E\xi_i(\overset{\bullet\bullet\bullet}{\circ}) &= 20\sum_{j=1}^{s} b_{ij}\eta_j(\bullet)^3 + 5\sum_{j=1}^{r'} q_{ij}\xi'_j(\overset{\bullet\bullet\bullet}{\circ}) + \sum_{j=1}^{r} v_{ij}\xi_j(\overset{\bullet\bullet\bullet}{\circ}), \quad i=1,\dots,r,
\end{aligned}
\tag{26}
$$

$$E\delta_i(\;) = 20\sum_{j=1}^{s} c_{ij}\eta_j(\bullet)\eta_j(\circ) + 5\sum_{j=1}^{r'} r_{ij}\xi'_j(\;) + \sum_{j=1}^{r} w_{ij}\xi_j(\;), \quad i = 1,\dots,r',$$
$$E\xi_i(\;) = 20\sum_{j=1}^{s} b_{ij}\eta_j(\bullet)\eta_j(\circ) + 5\sum_{j=1}^{r'} q_{ij}\xi'_j(\;) + \sum_{j=1}^{r} v_{ij}\xi_j(\;), \quad i = 1,\dots,r, \tag{27}$$

$$E\delta_i(\;) = 20\sum_{j=1}^{s} c_{ij}\eta_j(\;) + 5\sum_{j=1}^{r'} r_{ij}\xi'_j(\;) + \sum_{j=1}^{r} w_{ij}\xi_j(\;), \quad i = 1,\dots,r',$$
$$E\xi_i(\;) = 20\sum_{j=1}^{s} b_{ij}\eta_j(\;) + 5\sum_{j=1}^{r'} q_{ij}\xi'_j(\;) + \sum_{j=1}^{r} v_{ij}\xi_j(\;), \quad i = 1,\dots,r, \tag{28}$$

where $\eta_i(\;) = 6\sum_{j=1}^{s} a_{ij}\eta_j(\bullet) + 3\sum_{j=1}^{r'} p_{ij}\xi'_j(\;) + \sum_{j=1}^{r} u_{ij}\xi_j(\;)$, $i = 1,\dots,s$.

3.1 Recovering the order conditions of classical methods

The family of GLN methods (2) properly contains many known classes of numerical methods for (1). Analogously, the order conditions above derived are general, hence it is possible to recover through them the order conditions of numerical methods already considered in the literature. To make this possible, we need to regard these methods as GLN methods and specialize the operators $E\delta$ and $E\xi$ on the case by case basis. This is clarified in the following examples.

RKN methods
Runge-Kutta-Nyström methods (see [25,27])

$$Y_i = y_{n-1} + c_i h y'_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j), \quad i = 1,...,s,$$
$$h y'_n = h y'_{n-1} + h^2 \sum_{j=1}^{s} b'_j f(Y_j), \tag{29}$$
$$y_n = y_{n-1} + h y'_{n-1} + h^2 \sum_{j=1}^{s} b_j f(Y_j),$$

can be recasted as GLN methods (2) with $r = r' = 1$, in correspondence to the tableau (3)

$$\left[\begin{array}{c|c|c} \mathbf{A} & \mathbf{P} & \mathbf{U} \\ \hline \mathbf{C} & \mathbf{R} & \mathbf{W} \\ \hline \mathbf{B} & \mathbf{Q} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|c|c} A & c & e \\ \hline b'^{\intercal} & 1 & 0 \\ \hline b^{\intercal} & 1 & 1 \end{array}\right],$$

where e is the unit vector in $\mathbb{R}^s$, and the input vectors $y^{[n-1]} = [y_{n-1}]$, $y'^{[n-1]} = [y'_{n-1}]$. Correspondingly, the set of order and stage order conditions (18)-(19) assumes the form

$$\begin{cases} E\eta = A\overline{\eta} + c\delta + e\xi, \\ E\delta = b'^{\intercal}\overline{\eta} + \delta, \\ E\xi = b^{\intercal}\overline{\eta} + \delta + \xi. \end{cases} \tag{30}$$

The values of $E\eta$, $E\delta$ and $E\xi$ are reported in Table 2. We observe that these conditions match the classical ones (compare [23,25]).

tree	$E\xi(t)$	$E\delta(t)$	$E\eta_i(t)$
$\emptyset$	1	0	1
$\bullet$	1	1	c_i
$\circ$	1	2	c_i^2
	1	3	c_i^3
$\vdots$	$\vdots$	$\vdots$	$\vdots$
t	1	$\rho(t)$	$c_i^{\rho(t)}$

Table 2 Values of $E\eta_i$, $E\delta$ and $E\xi$ for RKN methods regarded as GLN methods

Coleman hybrid methods
We now consider the following class of methods

$$\begin{aligned} Y_i &= (1 + c_i)y_{n-1} - c_i y_{n-2} + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j), \quad i = 1, ..., s, \\ y_n &= 2y_{n-1} - y_{n-2} + h^2 \sum_{j=1}^{s} b_j f(Y_j), \end{aligned} \tag{31}$$

introduced by Coleman in [10] (also compare [21,18,19,14]), which are denoted as two-step hybrid methods. Such methods (31) can be regarded as GLN methods corresponding to the reduced tableau

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cc} A & e + c & -c \\ \hline b^{\intercal} & 2 & -1 \\ 0 & 1 & 0 \end{array}\right]$$

obtained by assuming the remaining coefficient matrices in (3) equal to the zero matrix. Such methods are characterized by the the input vector $y^{[n-1]} = [y_{n-1} \quad y_{n-2}]^{\intercal}$. The corresponding set of order and stage order conditions (18)-(19) takes the form

$$\begin{cases} E\eta = A\overline{\eta} + e + c\xi_1 - c\xi_2, \\ E\xi_1 = b^{\intercal}\overline{\eta} + 2\xi_1 - \xi_2, \\ E\xi_2 = \xi_1. \end{cases} \tag{32}$$

The coefficients for ξ_1, ξ_2 can be found in Table 3. We observe that the third equation in (32) is trivial by the definition of ξ_1.

tree	$E\xi_1(t)$	$\xi_1(t)$	$\xi_2(t)$
$\emptyset$	1	1	1
	1	0	-1
	1	0	1
	1	0	-1
$\vdots$	$\vdots$	$\vdots$	$\vdots$
t	1	0	$(-1)^{\rho(t)}$

Table 3 Values of $E\xi_1$, ξ_1 and ξ_2 for Coleman hybrid methods regarded as GLNs

Two-step Runge-Kutta-Nyström methods
Two-step Runge-Kutta-Nyström methods (TSRKN)

$$\begin{aligned}
Y_i^{[n-1]} &= y_{n-2} + hc_i y'_{n-2} + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j^{[n-1]}), \quad i = 1, \ldots, s, \\
Y_i^{[n]} &= y_{n-1} + hc_i y'_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}), \quad i = 1, \ldots, s, \\
hy'_n &= (1-\theta)hy'_{n-1} + \theta hy'_{n-2} + h^2 v'_j f(Y_j^{[n-1]}) + h^2 w'_j f(Y_j^{[n]}), \qquad (33) \\
y_n &= (1-\theta)y_{n-1} + \theta y_{n-2} + h\sum_{j=1}^{s} v'_j y'_{n-2} + h\sum_{j=1}^{s} w'_j y'_{n-1} \\
&\quad + h^2 \sum_{j=1}^{s} v_j f(Y_j^{[n-1]}) + h^2 \sum_{j=1}^{s} w_j f(Y_j^{[n]}),
\end{aligned}$$

have been introduced and analyzed by Paternoster in [28–31]. Such methods depend on two consecutive approximations to the solution and its first derivative in the grid points, but also on two consecutive approximations to the stage values, in line with the idea employed by Jackiewicz et al. (compare [2,11,13, 22,17,15,16,24,26]) in the context of two-step Runge–Kutta methods for first order ODEs. TSRKN methods can be represented as GLNs (2) with $r = s+2$ and $r' = 2$ through the tableau (3)

$$\left[\begin{array}{c|c|c} \mathbf{A} & \mathbf{P} & \mathbf{U} \\ \hline \mathbf{C} & \mathbf{R} & \mathbf{W} \\ \hline \mathbf{B} & \mathbf{Q} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cc|ccc} A & c & 0 & e & 0 & 0 \\ \hline w'^{\intercal} & 1-\theta & \theta & 0 & 0 & v'^{\intercal} \\ 0 & 1 & 0 & 0 & 0 & 0 \\ \hline w^{\intercal} & w'^{\intercal}e & v'^{\intercal}e & 1-\theta & \theta & v^{\intercal} \\ 0 & 0 & 0 & 1 & 0 & 0 \\ I & 0 & 0 & 0 & 0 & 0 \end{array}\right],$$

in correspondence of the input vectors $y^{[n-1]} = [y_{n-1} \quad y_{n-2} \quad h^2 f(Y^{[n-1]})]^{\intercal}$, $y'^{[n-1]} = [y'_{n-1} \quad y'_{n-2}]^{\intercal}$. The set of order conditions for these methods has the form

$$\begin{cases} E\eta_i = \displaystyle\sum_{j=1}^{s} a_{ij}\overline{\eta}_j + c_i\delta_1 + \xi_1, \quad i = 1, \ldots, s, \\ E\delta_1 = \displaystyle\sum_{j=1}^{s} w'_j\overline{\eta}_j + (1-\theta)\delta_1 + \theta\delta_2 + \sum_{j=1}^{s} v'_j\xi_{3j}, \\ E\delta_2 = \delta_1, \\ E\xi_1 = \displaystyle\sum_{j=1}^{s} w_j\overline{\eta}_j + \sum_{j=1}^{s} w'_j\delta_1 + \sum_{j=1}^{s} v'_j\delta_2 + (1-\theta)\xi_1 + \theta\xi_2 + \sum_{j=1}^{s} v_j\xi_{3j}, \\ E\xi_2 = \xi_1, \\ E\xi_{3i} = \overline{\eta}_i \quad i = 1, \ldots, s, \end{cases} \tag{34}$$

whose coefficients $E\xi_1$, $E\delta_1$, ξ_1, ξ_2, δ_1 and δ_2 can be found in Table 4. We also observe that in the system (34) there are automatically satisfied conditions, i.e. the third, the fifth and the sixth.

tree	$E\xi_1(t)$	$E\delta_1(t)$	$\xi_1(t)$	$\xi_2(t)$	$\delta_1(t)$	$\delta_2(t)$
$\emptyset$	1	0	1	1	0	0
	1	1	0	-1	1	1
	1	2	0	1	0	-1
	1	3	0	-1	0	1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
t	1	$\rho(t)$	0	$(-1)^{\rho(t)}$	0	$(-1)^{\rho(t)-1}$

Table 4 Values of $E\xi_1$, $E\delta_1$, ξ_1, ξ_2, δ_1 and δ_2 for TSRKN methods regarded as GLNs

4 Construction of a family of methods of order 4

We now employ the order results provided in Section 3, to derive a new method of order 4. We focus our attention on GLN methods (2) whose vectors of external approximations satisfy

$$y^{[n]} \approx \begin{bmatrix} y(x_n) \\ h^2 y''(x_n) \\ h^3 y'''(x_n) \\ h^4 y^{(4)}(x_n) \end{bmatrix}, \qquad hy'^{[n]} \approx hy'(x_n). \tag{35}$$

For GLN methods (2) depending on input vectors of the form (35), exact starting values can be obtained by differentiation from the initial condition: in fact

$$\xi'(t) = \delta_{\rho(t),1}, \qquad \xi_i(t) = \rho(t)\delta_{\rho(t),i},$$

$i = 1, \dots, 4$, being $t \in SNT$ and $\delta_{i,j}$ the usual Kronecker delta. In the remainder of the section, we denote by e_i the vectors of the canonical basis of $\mathbb{R}^4$. The second and third equations in (20) and (21) lead to the so-called preconsistency conditions [20], which assume the form

$$\mathbf{U}e_1 = e, \quad \mathbf{V}e_1 = e_1, \quad \mathbf{W}e_1 = 0, \quad \mathbf{P}e = \mathbf{c}, \quad \mathbf{Q}e = e_1, \quad \mathbf{R}e = e.$$

Similarly, the second and third equalities in (22) provide the consistency conditions [20]

$$\begin{aligned} e_1 + 2e_2 &= 2\mathbf{B}e + 2\mathbf{V}e_2, \\ 1 &= \mathbf{C}e + \mathbf{W}e_2. \end{aligned} \tag{36}$$

Conditions of order 2 are

$$\begin{aligned} e_1 + 6e_2 + 6e_3 &= 6\mathbf{B}\mathbf{c} + 6\mathbf{V}e_3, \\ 1 &= 2\mathbf{C}\mathbf{c} + 2\mathbf{W}e_3, \end{aligned} \tag{37}$$

and leads to (23). Order 3 is achieved by imposing

$$\begin{aligned} e_1 + 12e_2 + 24e_3 + 24e_4 &= 12\mathbf{B}\mathbf{c}^{\mathbf{2}} + 24\mathbf{V}e_4, \\ 4 &= 12\mathbf{C}\mathbf{c}^{\mathbf{2}} + 24\mathbf{W}e_4. \end{aligned} \tag{38}$$

and

$$\begin{aligned} e_1 + 12e_2 + 24e_3 + 24e_4 &= 12\mathbf{B}\eta(\circ) + 24\mathbf{V}e_4, \\ 4 &= 12\mathbf{C}\eta(\circ) + 24\mathbf{W}e_4, \end{aligned} \tag{39}$$

where $\eta(\circ) = 2\mathbf{A}e + 2\mathbf{U}e_2$. We finally report the conditions for order 4,

$$\begin{aligned} e_1 + 20e_2 + 60e_3 + 120e_4 &= 20\mathbf{B}\mathbf{c}^{\mathbf{3}}, \\ 5 &= 20\mathbf{C}\mathbf{c}^{\mathbf{3}}, \end{aligned} \tag{40}$$

$$\begin{aligned} e_1 + 20e_2 + 60e_3 + 120e_4 &= 20\mathbf{B}\mathbf{c}\eta(\circ), \\ 5 &= 20\mathbf{C}\mathbf{c}\eta(\circ), \end{aligned} \tag{41}$$

and

$$\begin{aligned} e_1 + 20e_2 + 60e_3 + 120e_4 &= 20\mathbf{B}\eta(\begin{smallmatrix}\bullet\\ |\\ \circ\end{smallmatrix}), \\ 5 &= 20\mathbf{C}\eta(\begin{smallmatrix}\bullet\\ |\\ \circ\end{smallmatrix}), \end{aligned} \tag{42}$$

where $\eta(\begin{smallmatrix}\bullet\\ |\\ \circ\end{smallmatrix}) = 6\mathbf{A}\mathbf{c} + 6\mathbf{U}e_3$. Solving the above order conditions lead to the following four-parameter family of one stage order 4 GLN methods (2)

$$\left[\begin{array}{c|c|c} \mathbf{A} & \mathbf{P} & \mathbf{U} \\ \hline \mathbf{C} & \mathbf{R} & \mathbf{W} \\ \hline \mathbf{B} & \mathbf{Q} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|c|ccccc} \frac{1}{2}\left(c^2 - 2u_2\right) & c & 1 & u_2 & u_3 & u_4 \\ \hline \frac{1}{4c^3} & 1 & 0 & \frac{4c^3-1}{4c^3} & \frac{2c^2-1}{4c^2} & \frac{4c-3}{24c} \\ \hline \frac{1}{20c^3} & 1 & 1 & \frac{10c^3-1}{20c^3} & \frac{10c^2-3}{60c^2} & \frac{5c-3}{120c} \\ \frac{1}{c^3} & 0 & 0 & \frac{c^3-1}{c^3} & \frac{c^2-1}{c^2} & \frac{c-1}{2c} \\ \frac{3}{c^3} & 0 & 0 & -\frac{3}{c^3} & \frac{c^2-3}{c^2} & \frac{2c-3}{2c} \\ \frac{6}{c^3} & 0 & 0 & -\frac{6}{c^3} & -\frac{6}{c^2} & \frac{c-3}{c} \end{array}\right],$$

in correspondence of the input vectors (35). According to [20], we estimate that these methods are obviously zero-stable and, therefore, convergent since they are also consistent (see [20]) if $c > 41/30$. An example, for $c = 3/2$ and $u_2 = 1/2$, $u_3 = u_4 = 1$, is given by

$$\left[\begin{array}{c|c|c} \mathbf{A} & \mathbf{P} & \mathbf{U} \\ \hline \mathbf{C} & \mathbf{R} & \mathbf{W} \\ \hline \mathbf{B} & \mathbf{Q} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|c|cccc} \frac{5}{8} & \frac{3}{2} & 1 & \frac{1}{2} & 1 & 1 \\ \hline \frac{2}{27} & 1 & 0 & \frac{25}{27} & \frac{7}{18} & \frac{1}{12} \\ \hline \frac{2}{135} & 1 & 1 & \frac{131}{270} & \frac{13}{90} & \frac{1}{40} \\ \frac{8}{27} & 0 & 0 & \frac{19}{27} & \frac{5}{9} & \frac{1}{6} \\ \frac{8}{9} & 0 & 0 & -\frac{8}{9} & -\frac{1}{3} & 0 \\ \frac{16}{9} & 0 & 0 & -\frac{16}{9} & -\frac{8}{3} & -1 \end{array}\right].$$

This is GLN method (2) depending one stage and of order 4, which is higher than that attainable by one stage RKN methods [23,25], equal to 2.

5 Conclusions

We have focused our attention on the algebraic theory of order for the family of GLN methods (2) for second order ODEs (1). By suitably adapting the theory of SN-series to the case of GLN methods, we have derived general order conditions, which also properly contain those of other numerical methods already known in the literature, as explained in Section 3, and constructed a family of one-stage methods of order 4. The general approach provided here can be used to finally derive new irreducible GLN methods, which are not Runge-Kutta nor linear multistep methods, more efficient than existing classical methods.

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