General Nyström methods in Nordsieck form: error analysis

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Abstract

The paper is concerned with the analysis of the error associated to a family of multi-value numerical methods for the solution of initial value problems based on special second order ordinary differential equations. Such methods, denoted as General Nyström methods, provide at each step point an approximation to the Nordsieck vector associated to the solution of the problem. Order issues for such methods based on the theory of rooted trees are here provided, as well as an accuracy analysis is carried out, leading to a representation of the local truncation error.

Key words: Second order ordinary differential equations, multi-value numerical methods, general Nyström methods, error analysis, order conditions

1. Introduction

We focus our attention on the numerical solution of special second order Ordinary Differential Equations (ODEs)

$$\begin{cases} y''(x) = f(y(x)), \quad x \in [x_0, X], \\ y(x_0) = y_0 \in \mathbb{R}^d, \\ y'(x_0) = y'_0 \in \mathbb{R}^d, \end{cases} \tag{1.1}$$

with $f : \mathbb{R}^d \to \mathbb{R}^d$ smooth enough to ensure the well-posedness of the problem. The specific purpose is that of analyzing the accuracy properties of the family of General Linear Nyström (GLN) methods

$$\begin{aligned} Y_i^{[n]} &= h^2 \sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} u_{ij} y_j^{[n-1]}, \quad i = 1, ..., s, \\ y_i^{[n]} &= h^2 \sum_{j=1}^{s} b_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} v_{ij} y_j^{[n-1]}, \quad i = 1, ..., r, \end{aligned} \tag{1.2}$$

introduced in [8] and furtherly investigated in [9, 10, 11], as extension of the family of General Linear Methods for first order ODEs [1, 5, 6, 18]. The procedures involved in

(1.2) essentially updates the vector of approximations

$$y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix} \in \mathbb{R}^{rd},$$

from the point x_{n-1} to x_n of the discretization. The supervector $y^{[n-1]}$ is usually denoted as vector of the *external* stages. It is worth observing that every subvector $y_i^{[n-1]} \in \mathbb{R}^d$ approximates some solution related quantities (such as the solution itself, linear combinations of its derivatives, past evaluations of the f function and so on). The supervector

$$Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ Y_2^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix} \in \mathbb{R}^{sd}, \tag{1.3}$$

whose components appear in (1.2), is the so-called vector of *internal* stages, providing approximations to the solution in a set of internal points $x_{n-1} + c_j h$, $j = 1, 2, \dots, s$, where $\mathbf{c} = [c_1, c_2, \dots, c_s]^\intercal$ is the vector of the *abscissae* of the method.

We observe that a more specialized formulation of (1.2) can be given (see [8]) by splitting the vector $y^{[n-1]}$ in two complementary parts, one of which containing all the approximations related to the first derivative of the solution. Such a splitted formulation, widely employed in [8], is not considered in this manuscript, which is mainly focused on the more general formulation (1.2).

A more compact representation of (1.2) is obtained by regarding it in tensor form, i.e.

$$\begin{aligned} Y^{[n]} &= h^2(\mathbf{A} \otimes \mathbf{I})F^{[n]} + (\mathbf{U} \otimes \mathbf{I})y^{[n-1]}, \\ y^{[n]} &= h^2(\mathbf{B} \otimes \mathbf{I})F^{[n]} + (\mathbf{V} \otimes \mathbf{I})y^{[n-1]}, \end{aligned} \tag{1.4}$$

where $\otimes$ denotes the usual Kronecker tensor product of matrices. This representation involves the coefficient matrices $\mathbf{A} \in \mathbb{R}^{s\times s}$, $\mathbf{U} \in \mathbb{R}^{s\times r}$, $\mathbf{B} \in \mathbb{R}^{r\times s}$, $\mathbf{V} \in \mathbb{R}^{r\times r}$, which can be collected in the following partitioned $(s + r) \times (s + r)$ matrix

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right], \tag{1.5}$$

denoted as the Butcher tableau of the method.

The treatise is focused on the family of GLN methods (1.4) in Nordsieck form, i.e. such that the vector of external approximations satisfies

$$y^{[n]} \approx \begin{bmatrix} y(x_n) \\ hy'(x_n) \\ h^2 y''(x_n) \\ \vdots \\ h^r y^{(r)}(x_n) \end{bmatrix}, \tag{1.6}$$

that is an approximation to the Nordsieck vector [2, 17, 18, 20]. In particular, we aim to carry out an error analysis, which allows to introduce initial building blocks for implementation issues, such as the development of error estimators.

More specifically, the paper is organized as follows: Section 2 summarizes the main tool needed along the treatise, i.e. the theory of rooted trees for (1.4), introduced in [11]; Section 3 provides a theory of order conditions for Nordsieck methods which exploits the special structure of the method; Section 4 contains an error analysis for Nordsieck methods, while issues for error estimation are presented in Section 5; some conclusions are given in Section 6.

2. Order Conditions for GLNs

In [11], the authors have introduced a theory of rooted trees for (1.2), generalizing the results in [7, 16, 17]. In particular, the set of Special Nyström-trees (SNT)

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

is the domain where the basic operators involved in the formulation of order conditions are defined. Such operators are now recalled.

Let us consider $t_1, \ldots, t_k \in SNT$ and the tree $t = [t_1, \ldots, t_k]$ obtained according to the composition rules described in [11]. Correspondingly, we define elementary differentials by recursion, as follows

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

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 [7, 16])

$$\begin{aligned} &\rho(\bullet) = 1, \quad \rho(\circ) = 2, \quad \rho(t) = 2 + \sum_{i=1}^{k} \mu_i \rho(t_i), \\ &\alpha(\bullet) = \alpha(\circ) = 1, \quad \alpha(t) = (\rho(t) - 2)! \prod_{i=1}^{k} \frac{1}{\mu_i!} \left(\frac{\alpha(t_i)}{\rho(t_i)}\right)^{\mu_i}. \end{aligned} \tag{2.1}$$

In correspondence to the introduced theory of rooted trees, a general set of order conditions for (1.2) has been derived in [11]. To this purpose, the main tool is given by SN-series

$$SN(a, y, y') = \sum_{t \in SNT} \frac{h^{\rho(t)}}{\rho(t)!} \alpha(t) a(t) F(t)(y, y') \tag{2.2}$$

related to the problem (1.1). By denoting η and ξ the coefficients of the SN-series expansions of the internal and external stages respectively, we obtain by (1.2) that

$$\begin{cases} \eta(t) = \mathbf{A}\overline{\eta}(t) + \mathbf{U}\xi(t), \\ \widehat{\xi}(t) = \mathbf{B}\overline{\eta}(t) + \mathbf{V}\xi(t). \end{cases} \tag{2.3}$$

where $\overline{\eta}(t) = \rho(t)\,(\rho(t)-1)\,\eta''(t)$, being

$$\eta''(t) = \begin{cases} 0, & \text{if } t = \emptyset, \bullet \\ 1, & \text{if } t = \circ \\ \eta(t_1)\cdots\eta(t_k), & \text{if } t = [t_1,\ldots,t_k]. \end{cases}$$

The following result holds, compare [11].

Theorem 2.1. *If the operator $\widehat{\xi}$ in (2.3) of a given GLN (1.2) is such that $\widehat{\xi}_i(t)$ coincide with the corresponding coefficients $E\xi_i(t)$ in the Taylor series expansions of the exact values approximated by $y_i^{[n]}$ for any $t \in SNT$ of order $\rho(t) \le p$, then the method has order p, i.e.*

$$E\xi(t) = \mathbf{B}\overline{\eta}(t) + \mathbf{V}\xi(t), \qquad t \in SNT, \quad \rho(t) \le p. \tag{2.4}$$

Moreover, the method has stage order q if the operators $\eta_i(t)$, $i = 1,\ldots,s$, in (2.3) 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 less or equal to q.

3. Nordsieck methods

For GLN methods (1.2) depending on input vectors of the form (1.6), the values of the entries of $\xi(t)$ can be easily computed as follows

$$\xi_i(t) = \rho(t)!\,\delta_{\rho(t),i-1}, \quad i = 1,\ldots,r, \tag{3.1}$$

being $t \in SNT$ and $\delta_{i,j}$ the usual Kronecker delta. This formula can be obtained by SN-series arguments: indeed, looking for a SN-representation of the input vector

$$y_i^{[n-1]} = SN(\xi_i, y, y'),$$

and taking into account that $y_i^{[n-1]} \approx h^{i-1}y^{(i-1)}(x_{n-1})$, we have

$$\begin{aligned} h^{i-1}y^{(i-1)}(x_{n-1}) &= SN(\xi_i, y, y') \\ &= 0\cdot y(x_{n-1}) + 0\cdot hy'(x_{n-1}) + \ldots + \frac{h^{i-1}}{(i-1)!}\xi_i y^{(i-1)}(x_{n-1}) + \ldots \end{aligned}$$

Thus, by comparison of the left and right-hand sides, we get (3.1).

The corresponding values of $E\xi(t)$ can be again computed by means of Taylor series expansion and are reported in Table 1. We are able to provide order conditions specialized to the Nordsieck case [2, 17, 18, 20], i.e.

$$\mathbf{e_1} + 3\mathbf{e_2} + 6\mathbf{e_3} + 6\mathbf{e_4} = 6(\mathbf{Bc} + \mathbf{Ve_4})$$

for order 2,

$$\mathbf{e_1} + 4\mathbf{e_2} + 12\mathbf{e_3} + 24\mathbf{e_4} + 24\mathbf{e_5} = 12(\mathbf{B}\eta(\circ) + 2\mathbf{Ve_5})$$

for order 3,

$$\mathbf{e_1} + 5\mathbf{e_2} + 20\mathbf{e_3} + 60\mathbf{e_4} + 120\mathbf{e_5} + 120\mathbf{e_6} = 20(\mathbf{B}\eta(\overset{\bullet}{\circ}) + 6\mathbf{Ve_6})$$

$E\xi(\emptyset)$	$E\xi(\bullet)$	$E\xi(\circ)$	$\dots$	$E\xi(t)$
1	1	1	$\dots$	1
0	1	2	$\dots$	$\rho(t)$
0	0	2	$\dots$	$\rho(t)(\rho(t)-1)$
0	0	0	$\dots$	$\rho(t)(\rho(t)-1)(\rho(t)-2)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
0	0	0	$\dots$	$\rho(t)!$

Table 1: Values of $E\xi(t)$ in (2.4) for Nordsieck methods

for order 4, with

$$\eta(\circ) = 2(\mathbf{Ae} + \mathbf{Ue}_3),$$
$$\eta(\overset{\bullet}{\circ}) = 6(\mathbf{Ac} + \mathbf{Ue_4}),$$

being $\mathbf{e}$ the vector of ones in $\mathbb{R}^s$ and $\mathbf{e}_i$ the $i-th$ vector of the canonical basis of $\mathbb{R}^r$ if $i <= r$ and the zero-vector otwerwise.

3.1. A remark on convergence analysis

The results reported in Section 2 are now employed to provide an alternative proof of convergence for GLN methods (1.4) in Nordsieck form. To this purpose, we recall the following classical results, adapted to GLN methods in [8].

Theorem 3.1. *A GLN method* (1.4) *is convergent if and only if it is consistent and zero-stable.*

The notions of consistency for GLN methods (1.4) is now given in terms of operators of rooted trees.

Definition 3.1. *A GLN method (1.2) is consistent if*

$$\begin{aligned} &\mathbf{U}\xi(\emptyset) = \mathbf{e}, \quad \mathbf{V}\xi(\emptyset) = E\xi(\emptyset),\\ &\mathbf{U}\xi(\bullet) = \mathbf{c}, \quad \mathbf{V}\xi(\bullet) = E\xi(\bullet),\\ &2\mathbf{B}e + \mathbf{V}\xi(\circ) = E\xi(\circ). \end{aligned} \tag{3.2}$$

We also recall the definition of zero-stability given in [8].

Definition 3.2. *A GLN method (1.2) is zero-stable if the roots of the minimal polynomial of the* $\mathbf{V}$ *matrix lie on or within the unit circle and the multiplicity of the zeros on the unit circle is at most two.*

Thus, the following convergence result holds.

Theorem 3.2. *A GLN method* (1.2) *with input vector* $y^{[n]}$ *defined as in* (1.6) *is convergent if its Butcher tableau* (1.5) *has the form*

$$\left[\begin{array}{c|ccccc} \mathbf{A} & \mathbf{e} & \mathbf{c} & \frac{\mathbf{c}^2}{2} - \mathbf{A}\mathbf{e} & \widetilde{U} \\ \hline \mathbf{B} & \mathbf{e_1} & \mathbf{e_1} + \mathbf{e_2} & \frac{\mathbf{e_1}}{2} + \mathbf{e_2} + \mathbf{e_3} - \mathbf{B}e & \widetilde{V} \end{array}\right] \tag{3.3}$$

with $\widetilde{U} \in \mathbb{R}^{s\times(r-3)}$, $\widetilde{V} \in \mathbb{R}^{r\times(r-3)}$ *and all the eigenvalues of* $\overline{V}$ *have modulus strictly less than 1, where* $\overline{V}$ *is obtained by the matrix* $\mathbf{V}$ *removing its first two rows and columns.*

Proof: In force of the criterion provided by Theorem 3.1, we are allowed to study the convergence of GLN methods (1.4) by consistency and zero-stability analysis. Due to the nature (1.6) of the input vectors, we have

$$\xi(\emptyset) = \mathbf{e_1}, \quad \xi(\bullet) = \mathbf{e_2}, \quad \xi(\circ) = 2\mathbf{e_3}.$$

The vectors $E\xi(\emptyset)$, $E\xi(\bullet)$ and $E\xi(\circ)$ respectively assume the form $\mathbf{e_1}, \mathbf{e_1} + \mathbf{e_2}, \mathbf{e_1} + 2\mathbf{e_2} + 2\mathbf{e_3}$ (see Table 1). Taking into account these expressions of the mentioned vectors, conditions (3.2) give the expression (3.3) of the Butcher tableau. Correspondingly, the matrix $\mathbf{V}$ assumes the form

$$\mathbf{V} = \left[\begin{array}{cc|cc} 1 & 1 & \frac{1}{2} - \sum_{i=1}^{s} b_{1i} & \widetilde{v}_1 \\ 0 & 1 & 1 - \sum_{i=1}^{s} b_{2i} & \widetilde{v}_2 \\ \hline 0 & 0 & & \\ \vdots & \vdots & \overline{V} & \\ 0 & 0 & & \end{array}\right],$$

where $\widetilde{v}_1$ and $\widetilde{v}_2$ are the first two rows of the matrix $\widetilde{V}$. Hence, the matrix $\mathbf{V}$ is block upper triangular, with a 2×2 block having eigenvalues 1 with multiplicity 2. As a consequence, the method is zero-stable if the eigenvalues of $\overline{V}$ have moduli strictly less than 1, which completes the proof. □

4. Error analysis

Following the lines drawn in [3, 4, 6, 18] for the first order case, we now analyze the local discretization error associated to GLN methods (1.2), whose vector of external stages is given by the Nordsieck vector (1.6). Since we are approximating the Nordsieck vector at each step, we define the vectors $\tilde{y}^{[n-1]}, \tilde{y}^{[n]} \in \mathbb{R}^{rd}$ of the local solutions by

$$\begin{aligned} \tilde{y}_i^{[n-1]} &= \delta_{i0} y(x_{n-1}) + \delta_{i1} h y'(x_{n-1}) + \ldots + \delta_{ip} h^p y^{(p)}(x_{n-1}), \\ \tilde{y}_i^{[n]} &= \delta_{i0} y(x_n) + \delta_{i1} h y'(x_n) + \ldots + \delta_{ip} h^p y^{(p)}(x_n), \end{aligned}$$

where δ_{ij} is again the usual Kronecker delta. Thus, the local discretization error associated to the $i-th$ external stage of (1.2) is given by

$$le_i(x_n) = \tilde{y}_i^{[n]} - h^2 \sum_{j=1}^{s} b_{ij} f(\tilde{Y}_j^{[n]}) - \sum_{j=1}^{r} v_{ij} \tilde{y}_j^{[n-1]}, i = 1, 2, \ldots, r, \tag{4.1}$$

being

$$\tilde{Y}_i^{[n]} = h^2 \sum_{j=1}^{s} a_{ij} f(\tilde{Y}_j^{[n]}) - \sum_{j=1}^{r} u_{ij} \tilde{y}_j^{[n-1]}, i = 1, 2, \ldots, s. \tag{4.2}$$

The following result holds.

Theorem 4.1. *For the numerical solution of the* (1.1)*, with f globally Lipschitz, consider a GLN method* (1.2) *of order p and stage order q. Denoted by $\mathbf{I}$ the identity matrix in $\mathbb{R}^{r\times r}$, the local truncation error associated to the grid point x_n is given by*

$$le(x_n) = (\phi_p \otimes \mathbf{I}) h^{p+1} y^{(p+1)}(x_{n-1}) + O(h^{p+2}), \tag{4.3}$$

if $q = p$ or $q = p-1$, where

$$\phi_p = \sum_{k=1}^{p+1} \frac{\mathbf{e}_{p+1-k}}{k!} - \frac{\mathbf{B}\mathbf{c}^{p-1}}{(p-1)!}.$$

Proof: We observe that, due to the fact that the method (1.2) has stage order q,

$$y(x_{n-1} + c_i h) = h^2 \sum_{j=1}^{s} a_{ij} f(y(x_{n-1} + c_j h)) + \sum_{j=1}^{r} u_{ij} \tilde{y}_j^{[n-1]} + \zeta_i(h), \tag{4.4}$$

where

$$\zeta_i(h) = \begin{cases} O(h^{p+1}), & \text{if } q = p, \\ O(h^p), & \text{if } q = p-1. \end{cases} \tag{4.5}$$

Subtracting (4.4) from (4.2), we obtain

$$\tilde{Y}_i^{[n]} - y(x_{n-1} + c_i h) = h^2 \sum_{j=1}^{s} a_{ij} \left(f\left(\tilde{Y}_i^{[n]}\right) - f\left(y(x_{n-1} + c_i h)\right)\right) - \zeta_i(h), \quad i = 1, \ldots, s.$$

Supposing that $L > 0$ is the Lipschitz constant of f, we have

$$\left\|\tilde{Y}^{[n]} - y(x_{n-1} + \mathbf{c}h)\right\| \leq h^2 L \, \|\mathbf{A}\| \, \left\|\tilde{Y}^{[n]} - y(x_{n-1} + \mathbf{c}h)\right\| + \|\zeta(h)\|,$$

i.e.

$$(1 - h^2 L \, \|\mathbf{A}\|) \, \left\|\tilde{Y}^{[n]} - y(x_{n-1} + \mathbf{c}h)\right\| \leq \|\zeta(h)\|,$$

where $y(x_{n-1} + \mathbf{c}h) = [y(x_{n-1} + c_i h)]_{i=1}^{s}$. We assume that h_0 is a real number such that

$$h_0 L \|\mathbf{A}\| < 1.$$

Hence, for any $h^2 \leq h_0$,

$$\left\|\tilde{Y}^{[n]} - y(x_{n-1} + \mathbf{c}h)\right\| \leq \frac{\|\zeta(h)\|}{1 - h_0 L \|\mathbf{A}\|}.$$

Consequently, for (4.5),

$$\left\|\tilde{Y}^{[n]} - y(x_{n-1} + \mathbf{c}h)\right\| = \begin{cases} O(h^{p+1}), & \text{if } q = p, \\ O(h^p), & \text{if } q = p - 1. \end{cases}$$

In the case $q = p$, inserting $\tilde{Y}^{[n]} = y(x_{n-1} + c_i h) + O(h^{p+1})$ into (4.1), we obtain

$$\sum_{k=0}^{p} \delta_{ik} h^k y^{(k)}(x_n) = h^2 \sum_{j=1}^{s} b_{ij} y''(x_{n-1} + c_j h) + \sum_{j=1}^{r} \sum_{k=0}^{p} v_{ij} \delta_{jk} h^k y^{(k)}(x_{n-1}) - le_i(x_n).$$

Expanding $y^{(k)}(x_n)$ and $y''(x_{n-1} + c_j h)$ in Taylor series around x_{n-1} and collecting in powers of h, we get

$$\sum_{k=0}^{p} \left(\sum_{l=0}^{k} \frac{k!}{l!} \delta_{i,k-l} - \sum_{j=1}^{s} (k(k-1)) b_{ij} c_j^{k-2} - \sum_{j=1}^{r} k! v_{ij} \delta_{jk} \right) \frac{h^k}{k!} y^{(k)}(x_{n-1}) +$$
$$+ \left(\sum_{l=1}^{p+1} \frac{\delta_{i,p+1-l}}{l!} - \sum_{j=1}^{s} \frac{b_{ij} c_j^{p-1}}{(p-1)!} \right) h^{p+1} y^{(p+1)}(x_{n-1}) = le_i(x_n) + O(h^{p+2}).$$

If $q = p$ or $q = p - 1$, all the terms up to order $O(h^p)$ vanish (compare [9]), and the local truncation error takes the form

$$le_i(x_n) = \left(\sum_{l=1}^{p+1} \frac{\delta_{i,p+1-l}}{l!} - \sum_{j=1}^{s} \frac{b_{ij} c_j^{p-1}}{(p-1)!} \right) h^{p+1} y^{(p+1)}(x_{n-1}) + O(h^{p+2}),$$

that is equivalent to (4.3). □

An alternative proof of Theorem 4.1 can be given using SN series (2.2), as follows. The expression of $le(x_n)$ given in (4.1) is equivalent to (compare Theorem 2.1)

$$le(x_n) = \tilde{y}(x_n) - y^{[n]} = SN(E\xi, y, y') - SN(\mathbf{B}\overline{\eta} + \mathbf{V}\xi, y, y') = SN(E\xi - \mathbf{B}\overline{\eta} - \mathbf{V}\xi, y, y'),$$

i.e.

$$le(x_n) = \sum_{t \in SNT} \frac{h^{\rho(t)}}{\rho(t)!} \alpha(t) \left(E\xi(t) - \mathbf{B}\overline{\eta}(t) - \mathbf{V}\xi(t) \right) F(t)(y, y')$$

and, since the method has order p, all the terms corresponding to the trees of order less or equal to p disappear, providing

$$le(x_n) = \sum_{\rho(t)=p+1} \frac{h^{\rho(t)}}{\rho(t)!} \alpha(t) \left(E\xi(t) - \mathbf{B}\overline{\eta}(t) - \mathbf{V}\xi(t) \right) F(t)(y, y') + O(h^{p+2}). \qquad (4.6)$$

The coefficients $E(\xi)(t)$ and $\xi(t)$ depend only on $\rho(t) = p + 1$ and not on the specific considered tree (compare (3.1) and Table 1). We observe that, if $t = [t_1, t_2, \ldots, t_k]$, we have (see [11])

$$\overline{\eta}(t) = \rho(t)(\rho(t) - 1)\eta(t_1)\eta(t_2) \ldots, \eta(t_k) = p(p + 1)\mathbf{c}^{p-1}.$$

Substituting this expression in (4.6) gives the thesis.

5. A remark on error estimation

As an application of the result proved in Section 4, we derive a computable error estimate for given a GLN method (1.4) of order p and stage-order $q = p - 1$. In order to achieve this purpose, we propose a formula to approximate the $(p+1)$-st derivative appearing in (4.3), of the form

$$h^{p+1}y^{(p+1)}(x_{n-1}) = h^2(\alpha \otimes \mathbf{I})F^{[n]} + (\beta \otimes \mathbf{I})y^{[n-1]} + O(h^{p+2}), \tag{5.7}$$

with $\alpha \in \mathbb{R}^s$ and $\beta \in \mathbb{R}^r$. Such a choice, similarly as in [18], is carried out in order to provide a formula only depending on quantities already computed in a prescribed step, i.e. the vector of stage derivatives $F^{[n]}$ and the vector of the external stages $y^{[n-1]}$, thus avoiding to increase the computational cost of the numerical scheme.

First, we replace in (5.7) the SN-series expansion of $F^{[n]}$ and $y^{[n-1]}$

$$h^{p+1}y^{(p+1)}(t_{n-1}) = (\alpha \otimes \mathbf{I})SN(\overline{\eta}, y, y') + (\beta \otimes \mathbf{I})SN(\xi, y, y')$$

and we determine α and β by comparing the corresponding powers of h appearing in the left and right-hand sides. We compute these values for the one-stage GLN method of order 4 and stage order 3 introduced in [9], with $\mathbf{A} = \left[\frac{1}{4}\right]$,

$$\mathbf{U} = \begin{bmatrix} 1 & c & \frac{-1+2c^2}{4} & \frac{1}{12}\left(\frac{3c}{2} + c^3\right) & \frac{c\left(-3+c^3\right)}{24} \end{bmatrix},$$

$$\mathbf{B} = \begin{bmatrix} \frac{42-64c+37c^2-10c^3+c^4}{24} \\ \frac{67-76c+30c^2-4c^3}{24} \\ \frac{(-3+c)(-2+c)}{2} \\ \frac{5}{2} - c \\ 1 \end{bmatrix},$$

$$\mathbf{V} = \begin{bmatrix} 1 & 1 & \frac{-30+64c-37c^2+10c^3-c^4}{24} & \frac{4-42c+64c^2-37c^3+10c^4-c^5}{24} & \frac{2-42c^2+64c^3-37c^4+10c^5-c^6}{48} \\ 0 & 1 & \frac{-43+76c-30c^2+4c^3}{24} & \frac{12-67c+76c^2-30c^3+4c^4}{24} & \frac{16-67c^2+76c^3-30c^4+4c^5}{48} \\ 0 & 0 & \frac{-4+5c-c^2}{2} & \frac{2-6c+5c^2-c^3}{2} & \frac{2-6c^2+5c^3-c^4}{4} \\ 0 & 0 & c - \frac{5}{2} & 1 - \frac{5c}{2} + c^2 & \frac{4-5c^2+2c^3}{4} \\ 0 & 0 & -1 & -c & 1 - \frac{c^2}{2} \end{bmatrix},$$

where $c \approx 0.3754243604533405$ is the only root in $(0, 1)$ of the polynomial

$$a(x) = 6 - 210x^3 + 320x^4 - 185x^5 + 50x^6 - 5x^7.$$

As regards the coefficients $\alpha \in \mathbb{R}$ and $\beta \in \mathbb{R}^5$ in (5.7) for this method, they result as solution of the linear system

$$\begin{aligned} \beta \mathbf{e}_1 &= 0 \\ \beta \mathbf{e}_2 &= 0 \\ 2\alpha \mathbf{e} + 2\beta \mathbf{e}_3 &= 0 \\ 6\alpha \mathbf{c} + 6\beta \mathbf{e}_4 &= 0 \\ 12\alpha \mathbf{c^2} + 24\beta \mathbf{e}_5 &= 0 \\ 20\alpha \mathbf{c^3} &= 120 \end{aligned}$$

providing

$$\alpha = \frac{6}{c^3}, \qquad \beta = \begin{bmatrix} 0 \\ 0 \\ -\frac{6}{c^3} \\ -\frac{6}{c^2} \\ -\frac{3}{c} \end{bmatrix}.$$

We test the effectiveness of the approach on the periodic stiff problem introduced by Kramarz in [19]

$$y''(t) = \begin{bmatrix} \mu - 2 & 2\mu - 2 \\ 1 - \mu & 1 - 2\mu \end{bmatrix} y(x), \quad t \in [0, 20]$$

with initial conditions

$$y(0) = [2, -1]^T, \quad y'(0) = [0, 0]^T.$$

The exact solution is $y(t) = [2\cos(x), -\cos(x)]^T$ and does not depend on μ (the dependence on this particular solution is eliminated by the initial conditions). Assuming that $\mu = 2500$, Fig. 1 depicts the error

$$\begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \end{bmatrix} - \begin{bmatrix} 2\cos(x_n) \\ -\cos(x_n) \end{bmatrix}, \quad n \geq 1 \tag{5.8}$$

and the principal error term in (4.3), where the vector of error costants ϕ_p is equal to

$$\begin{bmatrix} \frac{3-c^3(42-64c+37c^2-10c^3+c^4)}{72} \\ \frac{12-67c^3+76c^4-30c^5+4c^6}{72} \\ \frac{1}{2} - \frac{(-3+c)(-2+c)c^3}{6} \\ \frac{6-5c^3+2c^4}{6} \\ 1 - \frac{c^3}{3} \end{bmatrix}.$$

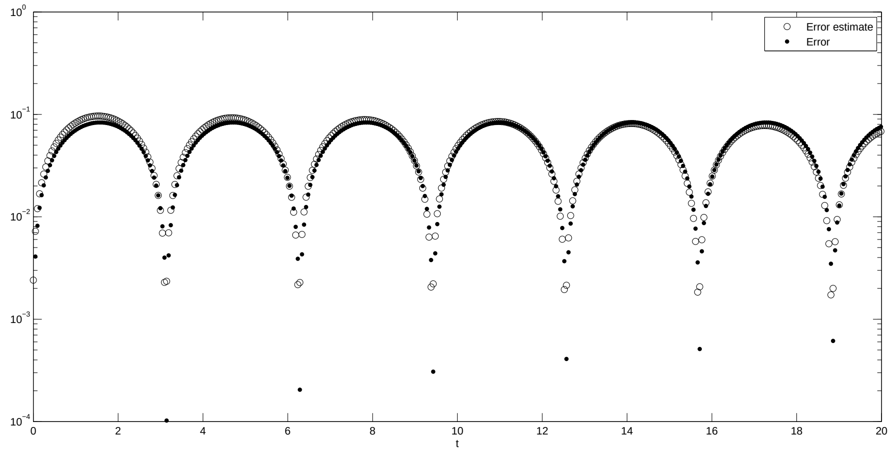

Figure 1: Pointwise comparison of the error (5.8) and the principal error term in (4.3)

6. Conclusions

We have analyzed some accuracy issues related to the numerical solution of second order ODEs (1.1) by means of GLN methods (1.2). In particular, we have assumed that the methods provide approximations to the Nordsieck vector (1.6) at each step point. For such methods, some issues regarding order conditions and convergence have been given by employing the theory of rooted trees, leading to general order conditions up to order 4 that are satisfied in a more general setting than that described in [9]: indeed, the order conditions provided in [9] hold true only for high stage order methods; this hypothesis is here neglected. In addition, an accuracy analysis has been provided, in order to obtain a possible representation of the local truncation error associated to (1.2) and its estimate, as discussed in Section 5.

Future developments of this research will be devoted to explore, within the family of GLN methods, near-conservation properties arising from symmetry or a generalization of G-symplecticity, defined for multi-value methods solving first order ODEs (compare [12, 14, 15] and references therein), in order to appoach conservative problems such as second order Hamiltonian systems, and the analysis of their long-term properties [13, 15]. In addition, in order to exploit the generality of the approach and the large number of degrees of freedom involved in the formulation of the methods, we will also aim to treat constructive issues, even by means of optimization techniques, in order to derive new examples of methods which improve existing ones. Up to now, the author have derived a first example in [9] of methods which results more accurate and efficient than the analog Runge-Kutta-Nyström.

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References

[1] K. Burrage, J.C. Butcher, Non-linear stability of a general class of differential equation methods, BIT 20, 185–203 (1980).

[2] J.C. Butcher, P. Chartier, Z. Jackiewicz, Nordsieck representation of DIMSIMs, Numer. Algorithms 16, 209–230 (1997).

[3] J.C. Butcher, Z. Jackiewicz, W.M. Wright, Error propagation for general linear methods for ordinary differential equations, J . Complezity 23, 560–580 (2007).

[4] J.C. Butcher, H. Podhaisky, On error estimation in General Linear Methods for stiff ODEs, Appl. Numer. Math. 56(3–4), 345–357 (2006).

[5] J. C. Butcher, General linear methods, Acta Numerica 15, 157–256 (2006).

[6] J. C. Butcher, Numerical methods for Ordinary Differential Equations, Second Edition, Wiley, Chichester, 2008.

[7] J. P. Coleman, Order conditions for a class of two-step methods for $y'' = f(x, y)$, IMA Journal of Numerical Analysis (2003) 23, 197–220.

[8] R. D'Ambrosio, E. Esposito, B. Paternoster, General Linear Methods for $y'' = f(y(t))$, Numer. Algor. 61 (2), 331–349 (2012) .

[9] R. D'Ambrosio, B. Paternoster, P-Stable general Nyström methods for $y'' = f(y(t))$, . J. Comput. Appl. Math. 262, 271–280 (2014).

[10] R. D'Ambrosio, B. Paternoster, A general framework for numerical methods solving second order differential problems, Math. Comput. Simul, doi: 10.1016/j.matcom.2014.04.007, to appear.

[11] R. D'Ambrosio, G. De Martino, B. Paternoster, Order Conditions for General Linear Nyström methods, Numer Algor 65, 579595 (2014).

[12] R. D'Ambrosio, G. De Martino, B. Paternoster, Numerical integration of Hamiltonian problems by G-symplectic methods, Adv. Comput. Math. 40(2), 553–575 (2014).

[13] R. D'Ambrosio, E. Hairer, Long-term stability of multi-value methods for ordinary differential equations, J. Sci. Comput. 60(3), 627–640 (2014).

[14] R. D'Ambrosio, E. Hairer, C.J. Zbinden, G-symplecticity implies conjugate-symplecticity of the underlying one-step method, BIT 53, 867–872 (2013).

[15] E. Hairer, C. Lubich and G. Wanner, Geometric numerical integration. Structure-preserving algorithms for ordinary differential equations, Second edition, Springer Series in Computational Mathematics 31, Springer-Verlag, Berlin, 2006.

[16] E. Hairer, G. Wanner, A theory for Nyström Methods, Numer. Math. 25, 383–400 (1976).

[17] E. Hairer, S.P.Nørsett and G. Wanner, Solving Ordinary Differential Equations, Second edition, Springer Series in Computational Mathematics 8, Springer-Verlag, Berlin, 2008.

[18] Z. Jackiewicz, General Linear Methods for Ordinary Differential Equations, John Wiley & Sons, Hoboken, New Jersey (2009).

[19] L. Kramarz, Stability of collocation methods for the numerical solution of $y'' = f(t, y)$, BIT 20, (1980) 215–222.

[20] A. Nordsieck, On Numerical Integration of Ordinary Differential Equations, Math. Comput. 16, 22–49 (1962).