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# A Theory for Nyström Methods

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*Summary.* For the numerical solution of differential equations of the *second* order (and systems of ...) there are two possibilities: 1. To transform it into a system of the first order (of doubled dimension) and to integrate by a standard routine. 2. To apply a "direct" method as those invented by Nyström. The benefit of these direct methods is not generally accepted, a historical reason for them was surely the fact that at that time the theories did not consider systems, but single equations only. In any case the second approach is more general, since the class of methods defined in this paper contains the first approach as a special case. So there is more freedom for extending stability or accuracy.

This paper begins with the development of a theory, which extends our theory for first order equations [1] to equations of the second order, and which is applicable to the study of possibly all numerical methods for problems of this type. As an application, we obtain Butcher-type results for Nyström-methods, we characterize numerical methods as applications of a certain set of trees, give formulas for a group-structure (expressing the composition of methods) etc.

Recently in [2] the equations of conditions for Nyström methods have been tabulated up to order 7 (containing errors). Our approach yields not only the correct equations of conditions in a straight-forward way, but also an insight in the structure of methods that is useful for example in choosing good formulas.

## 1. Introduction

We consider systems of differential equations

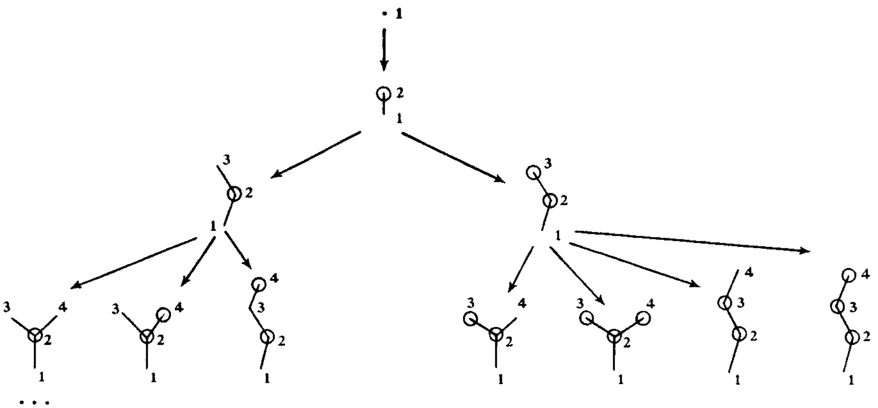
$$y''=f(y,y'), \qquad y(x_0)=y_0, \qquad y'(x_0)=y'_0, \tag{1}$$

where $y$ is in some space $E$ ($\mathbb{R}^n$, say) and $f$ is assumed to be sufficiently differentiable. Since $x$ can be adjusted to the system as $x''=0$, it is of cource no restriction of generality to assume (1) independent of $x$.

We now show that, for differential equations of type (1), it is natural to consider trees with distinguished nodes, $N$(yström)-trees. A continued differentiation of (1) gives using chain rule and $y''=f$:

$$\begin{aligned}
y' &= y' \\
y'' &= f \\
y^{(3)} &= D_1 f\cdot y' + D_2 f\cdot f \\
y^{(4)} &= D_1 D_1 f\cdot (y',y') + D_2 D_1 f\cdot (y',f) + D_1 f\cdot f \\
&\quad + D_1 D_2 f\cdot (f,y') + D_2 D_2 f\cdot (f,f) + D_2 f\cdot (D_1 f\cdot y') + D_2 f\cdot (D_2 f\cdot f)
\end{aligned} \tag{2}$$

These expressions, which very soon become complicated, are now written in terms of monotonically labelled $N$-trees as follows:



(3)

In this representation, each "fat" node represents "$f$" and each branch leaving this node a derivative:

$D_2$ if the sequent node is "fat", and

$D_1$ if the adjacent node is "meagre".

**Proposition 1.** The derivation with respect to $x$ consists of:

1. putting an arc with a meagre node to each fat node (derivative with respect to $y$);

2. putting an arc with a fat node to each fat node (derivative with respect to $y'$);

3. putting an arc with a fat node to each meagre end-node (derivative of $y'$, which is $f$). □

The labels indicate the order of generation of these nodes following this procedure. The set of trees which appear in this way are the monotonically labelled Nyström-trees, denoted by LNT.

## 2. Trees

In this section we give a description of the different sets of trees, which are useful in the theory of Runge-Kutta as well as Nyström methods, namely:

**Definition 2** (Monotonically labelled (rooted) trees (LT)). Let $n \in \mathbb{Z}$, $n \geq 0$. A monotonically labelled tree of order $n$ is a map

$$t: \{2, \ldots, n\} \to \{1, \ldots, n\}$$

such that $t(i) < i$ $(i = 2, \ldots, n)$.

The order is denoted by $\varrho(t)$.

*Example.* The map $2 \mapsto 1$, $3 \mapsto 1$, $4 \mapsto 3$ represents the eighth tree of Figure 1.

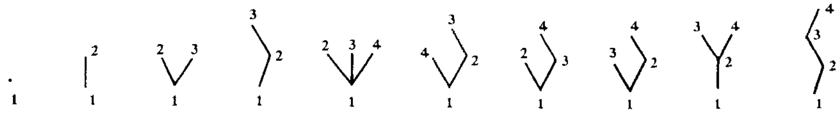


Fig. 1. LT's

The node with number 1 is called the root.

**Definition 3** (Trees (T)). A tree is an equivalence class of LT's which represent the same graph but differ in numeration. This equivalence relation can be defined by

$t \approx u \Leftrightarrow$ 1) $\varrho(t) = \varrho(u)$.

2) There exists a permutation $\sigma$ of $\{1, \ldots, \varrho(t)\}$ such that $\sigma(1) = 1$ and $t(i) = \sigma u \sigma^{-1}(i)$ $(i = 2, \ldots, \varrho(t))$.

*Example.* The 6-th, 7-th, and 8-th LT of Figure 1 are equivalent. Thus in the geometric representation, the labels can be left away.

**Definition 4** (Monotonically labelled Nyström-trees (LNT)). A m.l.$N$-tree of order $n$ is a map $t \in \mathrm{LT}$ together with a specification of its nodes into fat ones and meagre ones, i.e. a second map

$$q: \{1, \ldots, n\} \to \{0, 1\}$$

such that

a) the root is meagre, i.e. $q(1) = 0$;

b) a meagre node has no ramifications and each adjacent node must be fat, i.e.:

$$q(i) = 0 \Rightarrow \operatorname{card}(t^{-1}(i)) \leqq 1 \quad \text{and} \quad q(t^{-1}(i)) = 1 \quad \text{if} \quad t^{-1}(i) \neq \emptyset.$$

Examples are given in Figure 2.

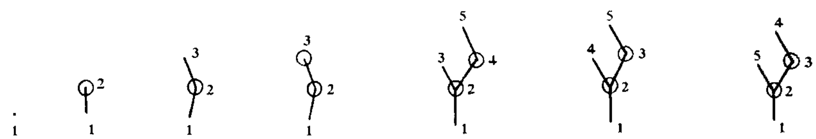


Fig. 2. LNT's

**Definition 5** ($N$(yström)-trees (NT)). A $N$-tree is an equivalence class of LNT's with respect to the equivalence relation

$$(t, q) \sim (u, r) \Leftrightarrow \left.\begin{matrix} 1) \\ 2) \end{matrix}\right\} \text{same as in Definition 3,}$$
$$3) \quad q(i) = r\,\sigma(i).$$

Examples are given in Figure 3.

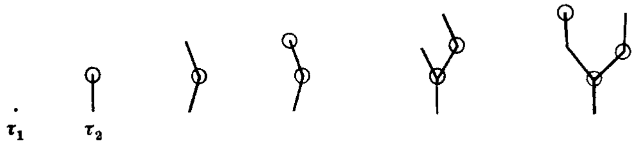



Fig. 3. NT's

In both cases we have the projections LT $\to$ T, LNT $\to$ NT which forget the labelling.

We now come to a construction, which will be fundamental in the next section and with the help of which every $N$-tree can be constructed from NT's of lower order:

**Definition 6.** Let $t_1, \ldots, t_m \in \mathrm{NT}$ and $k \in \mathbb{Z}$ with $0 \leqq k \leqq m$. Then we denote by

$$t = [t_1, \ldots, t_k; t_{k+1}, \ldots, t_m] \tag{4}$$

a new NT which is obtained by:

1. The roots of $t_{k+1}, \ldots, t_m$ are identified to a new fat node "charlie" say;
2. The roots of $t_1, \ldots, t_k$ are connected by a new branch to charlie;
3. Finally a new root is affixed underneath of charlie.

This has sense only if the order is $\geqq 1$ for $t_1, \ldots, t_k$ and $\geqq 2$ for $t_{k+1}, \ldots, t_m$.

*Examples* are given in Figure 4.

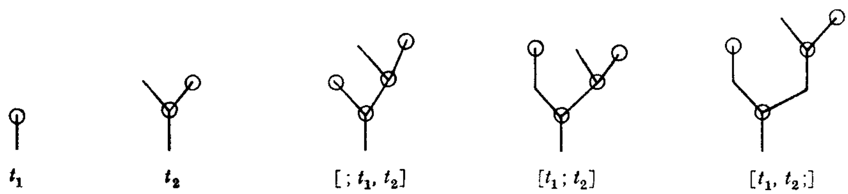



Fig. 4

**Proposition 7.** $\varrho([t_1, \ldots, t_k; t_{k+1}, \ldots, t_m]) = \sum_{i=1}^{m} \varrho(t_i) - m + k + 2$. $\square$

**Proposition 8.** Every $t \in \mathrm{NT}$ with $\varrho(t) \geqq 3$ can be represented in the form (4) with trees of lower order. Except of permutations among $t_1, \ldots, t_k$ and $t_{k+1}, \ldots, t_m$ this representation is unique.

*Proof.* Take away the lowest two nodes (and the adjacent branches) and collect from what results those with meagre roots as $t_1, \ldots, t_k$. The rest, where now the lowest node is fat, will lead to $t_{k+1}, \ldots, t_m$. $\square$

Thus, functions on NT can be defined by recursion on the order.

### 3. The Expansion of the Solution

We next give a recursive definition of the terms, which have appeared in the Taylor-expansion of the solution in (2) and which are in one-to-one correspondence with the NT's.

**Definition 9** (Elementary Differentials). For every $t \in \mathrm{NT}$ we define a function $F(t): E \times E \to E$ recursively by

$$F(\emptyset)(y,y') = y$$
$$F(\tau_1)(y,y') = y'$$
$$F(\tau_2)(y,y') = f(y,y')$$
$$F(t)(y,y') = D_1^k D_2^{m-k} f \cdot (F(t_1), \ldots, F(t_k), F(t_{k+1}), \ldots, F(t_m))$$
$$\text{where} \quad t = [t_1, \ldots, t_k; t_{k+1}, \ldots, t_m].$$

(For the definition of $\tau_1$ and $\tau_2$ see Fig. 3.)

Because of the symmetry of partial derivatives this definition does not depend on permutations among $t_1, \ldots, t_k$ as well as $t_{k+1}, \ldots, t_m$, and is therefore well-defined. In the development of (3), as can be seen from Proposition 1, every LNT of order $p$ appears exactly once in the $p$-th derivative. We thus have:

**Theorem 10.** For the solution of the Equation (1) we have

$$y^{(p)}(x_0) = \sum_{\substack{t \in \mathrm{LNT} \\ \varrho(t) = p}} F(t)(y_0, y_0')$$

and

$$y(x_0 + h) = \sum_{t \in \mathrm{LNT}} F(t)(y_0, y_0') \frac{h^{\varrho(t)}}{\varrho(t)!}. \quad \square$$

In these expressions we use the same symbol $t$ once for an element of LNT and once for the equivalence class of $t$.

## 4. Nyström-Series

Extending the concept of Butcher-series, which was fundamental in [1], we now define (taking regard of Theorem 10)

**Definition 11.** With a mapping $a: \mathrm{NT} \to \mathbb{R}$ we combine the series

$$N(a, y_0, y_0') = \sum_{t \in \mathrm{LNT}} a(t)\, F(t)\, (y_0, y_0') \frac{h^{\varrho(t)}}{\varrho(t)!}$$

and call it $N$(yström)-Series. Its derivative is

$$N'(a, y_0, y_0') = \sum_{\substack{t \in \mathrm{LNT} \\ t \neq \emptyset}} a(t)\, F(t)\, (y_0, y_0') \frac{h^{\varrho(t)-1}}{(\varrho(t)-1)!}.$$

Observe that the exact solution of (1) is a $N$-series $N(p, y_0, y_0')$ with

$$p(t) = 1 \qquad \text{for all } t \in \mathrm{NT} \quad \text{(Theorem 10).} \tag{5}$$

Similarly, $y(x_0 + \varkappa h)$ can be written as a $N$-series $N(p_\varkappa, y_0, y_0')$ with

$$p_\varkappa(t) = \varkappa^{\varrho(t)}. \tag{6}$$

We treat the infinite expansions over LNT in a formal fashion. This is all right as long as one is concerned with coefficient matching. For analytic differential equations, however, the convergence (as power series in $h$) of the actually occurring $N$-series can be deduced from the (complex) Implicit-Function-Theorem.

The coefficients $a(t)$ in the Nyström series are uniquely determined, if the identity should hold for all $f$. This follows from

**Proposition 12.** For every $t \in \mathrm{NT}$ there exists an initial value problem (1) such that for the first component of $F(u)(y_0, y_0')$

$$F(u)(y_0, y_0')_1 \begin{cases} \neq 0 & \text{for } u = t \\ = 0 & \text{for } u \neq t. \end{cases}$$

*Proof.* For $\varrho(t) \leqq 1$ take $f=0$. Otherwise we put $E = \mathbb{R}^{\varrho(t)-1}$ and construct for $f$ a polynomial as follows: Take any representative of $t$ and denote this LNT by $(t, q)$.

Let then for an index $i$

$$M'(i) = \{k \mid i = t(k),\ q(k) = 1\}$$

be the set of the indices of the fat nodes directly above the node labelled $i$ and

$$M(i) = \{k \mid t(k) = l,\ q(l) = 0,\ t(l) = i\} \cup \{k \mid t(k) = i,\ q(k) = 0,\ t^{-1}(k) = \emptyset\}$$

the set of the indices of the fat nodes which are connected with "$i$" via a meagre node and of the meagre end-nodes which are directly above "$i$".

The components of $f$ are then defined by $(i = 2, \ldots, \varrho(t))$

$$f_i((y_2, \ldots, y_{\varrho(t)}), (y_2', \ldots, y_{\varrho(t)}')) = \begin{cases} \prod_{k \in M(i)} y_k \cdot \prod_{k \in M'(i)} y_k' & \text{if } q(i) = 1 \\ 0 & \text{if } q(i) = 0. \end{cases}$$

With the initial values $y_0 = (0, \ldots, 0)$ and $y_0' = (y_{20}', \ldots, y_{\varrho(t),0}')$, where

$$y_{i,0}' = \begin{cases} 0 & \text{if } q(i) = 1 \\ 1 & \text{if } q(i) = 0, \end{cases}$$

this function fullfills all requirements, what is best seen at an example. $\square$

*Example.* Consider the NT of Fig. 5 and take as its representative the LNT which is sketched beside it.


Fig. 5

Then the function $f$ is given by

$$f_2 = y_5 y_4', \quad f_3 = 0, \quad f_4 = y_6, \quad f_5 = 1, \quad f_6 = 0.$$

The corresponding initial values are $y_0 = (0, 0, 0, 0, 0,)$ and $y_0' = (0, 1, 0, 0, 1)$. By definition of the elementary differentials

$$F(t)(y_0, y_0')_1 = \sum_{i,j} \frac{\partial^2 f_2}{\partial y_i\, \partial y_j'} f_i \sum_k \frac{\partial f_j}{\partial y_k} y_k' = 1$$

if $t$ is the considered NT. For all other NT's $u$ $F(u)(y_0, y'_0)_1$ is zero, since the only derivative of $f_2$ that does not vanish is the second ... etc.

**Theorem 13.** Let $a\colon \mathrm{NT} \to \mathbb{R}$, $a'\colon \mathrm{NT} \to \mathbb{R}$ be mappings. If $a(\emptyset)=1$, $a'(\emptyset)=0$ and $a'(\tau_1)=1$, we have

$$\mathrm{f}(N(a,y_0,y'_0), N'(a',y_0,y'_0)) = \sum_{t\in \mathrm{LNT}} a''(t)\, F(t)\,(y_0, y'_0)\, \frac{h^{\varrho(t)-2}}{(\varrho(t)-2)!}$$

where $a''\colon \mathrm{NT} \to \mathbb{R}$ is defined by

$$\begin{aligned} &a''(\emptyset)=a''(\tau_1)=0\\ &a''(\tau_2)=1\\ &a''(t)=a(t_1)\cdot\dots\cdot a(t_k)\, a'(t_{k+1})\cdot\dots\cdot a'(t_m) \quad \text{for} \quad t=[t_1,\dots,t_k;t_{k+1},\dots,t_m]. \end{aligned} \tag{7}$$

*Proof.* Several proofs are possible, for example one could proceed similarly to the proof given in [1] for "Theorem 6". Here we give a different approach using expansions in power series (as far as they exist; if necessary error terms are to be added).

$$\begin{aligned} &f(N(a,y_0,y'_0), N'(a',y_0,y'_0))\\ &\quad = f(y_0,y'_0) + \sum_{m\ge 1}\sum_{k=0}^{m} \frac{1}{k!\,(m-k)!}\, D_1^k D_2^{m-k} f(y_0,y'_0)\\ &\qquad \cdot ((N(a,y_0,y'_0)-y_0)^k (N'(a',y_0,y'_0)-y'_0)^{m-k})\\ &\quad = f(y_0,y'_0) + \sum_{m\ge 1}\sum_{k=0}^{m} \frac{1}{k!\,(m-k)!} \underbrace{\sum_{t_1\in \mathrm{LNT}}\cdots\sum_{t_k\in \mathrm{LNT}}}_{\varrho(t_i)\ge 1}\ \underbrace{\sum_{t_{k+1}\in \mathrm{LNT}}\cdots\sum_{t_m\in \mathrm{LNT}}}_{\varrho(t_i)\ge 2}\\ &\qquad \cdot a(t_1)\dots a(t_k)\, a'(t_{k+1})\dots a'(t_m)\, F([t_1,\dots,t_k;\dots,t_m])\,(y_0,y'_0)\\ &\qquad \cdot \frac{h^{\varrho(t_1)+\dots+\varrho(t_m)-m+k}}{\varrho(t_1)!\dots\varrho(t_k)!\,(\varrho(t_{k+1})-1)!\dots(\varrho(t_m)-1)!} = \cdots. \end{aligned}$$

Let $\mu_1, \mu_2, \dots$ be the numbers of mutually equal LNT's among $t_1, \dots, t_k$ and $\nu_1, \nu_2, \dots$ the numbers of mutually equal LNT's among $t_{k+1}, \dots, t_m$. For a fixed set of trees there are thus $\frac{k!}{\mu_1!\,\mu_2!\dots}\cdot\frac{(m-k)!}{\nu_1!\,\nu_2!\dots}$ different permutations of these trees, which do not change the value of the above summand. We assume now that LNT is an ordered set ($\le$), so, the above sum can be written as follows:

$$\begin{aligned} &= f(y_0,y'_0) + \sum_{m\ge 1}\sum_{k=0}^{m} \underbrace{\sum_{t_1\in \mathrm{LNT}}\cdots\sum_{t_k\in \mathrm{LNT}}}_{t_1\le\dots\le t_k\ \varrho(t_i)\ge 1}\ \underbrace{\sum_{t_{k+1}\in \mathrm{LNT}}\cdots\sum_{t_m\in \mathrm{LNT}}}_{t_{k+1}\le\dots\le t_m\ \varrho(t_i)\ge 2}\\ &\quad \cdot a''([t_1,\dots,t_k;t_{k+1},\dots,t_m])\, F([t_1,\dots,t_k;t_{k+1},\dots,t_m])\,(y_0,y'_0)\\ &\quad \cdot \frac{1}{\mu_1!\,\mu_2!\dots\nu_1!\,\nu_2!\dots}\cdot \binom{\varrho([t_1,\dots,t_k;t_{k+1}\dots,t_m])-2}{\varrho(t_1),\dots,\varrho(t_k),\varrho(t_{k+1})-1,\dots,\varrho(t_m)-1}\\ &\quad \cdot \frac{h^{\varrho([t_1,\dots,t_k;t_{k+1},\dots,t_m])-2}}{(\varrho([t_1,\dots,t_k;t_{k+1},\dots,t_m])-2)!}\,. \end{aligned}$$

To one element of this summation set, e.g. the tupel $(m, k, t_1, \dots, t_k, t_{k+1}, \dots, t_m)$, there correspond in a natural way exactly

$$\frac{1}{\mu_1!\,\mu_2!\dots\nu_1!\,\nu_2!\dots}\cdot\binom{\varrho(t)-2}{\varrho(t_1),\dots,\varrho(t_k),\,\varrho(t_{k+1})-1,\dots,\varrho(t_m)-1}$$

LNT'S $t$, such that

$$t=[t_1,\dots,t_k;\,t_{k+1},\dots,t_m]$$

(equality in the sense of $N$-trees (Definition 5)).

Namely, the labels 1 and 2 are fixed for every LNT. The distribution of the remaining $\varrho(t)-2$ labels gives the multinomial coefficient. Finally we have to devide by $\mu_1!\,\mu_2!\dots$ and $\nu_1!\,\nu_2!\dots$, because an exchange of equal LNT's $t_1,\dots,t_k$ or $t_{k+1},\dots,t_m$ does not change the LNT $t$. Thus we arrive at

$$=f(y_0,y_0')+\sum_{\substack{t\in \mathrm{LNT}\\ \varrho(t)\geq 3}} a''(t)\,F(t)\,(y_0,y_0')\,\frac{h^{\varrho(t)-2}}{(\varrho(t)-2)!}.\quad\square$$

*Remarks.* 1. The notation $a''(t)$ is selected, because $f(N(a,y_0,y_0'),\,N'(a',y_0,y_0'))$ represents a kind of second derivative.

2. If $f$ is not analytic at $(y_0,y_0')$, but its derivatives exist up to a certain order, then Theorem 13 is valid for the truncated series with a remainder term $O(h^{m+1})$.

## 5. Nyström—Methods for Differential Equations

A Nyström method for solving (1) can be defined by:

$$\begin{aligned}Y&=\mathbf{1}y_0+h\,\alpha\,y_0'+h^2A\,f(Y,\overline{Y})\\ \overline{Y}&=\mathbf{1}y_0'+h\overline{A}\,f(Y,\overline{Y}).\end{aligned}\tag{8}$$

Here $Y=(Y_1,\dots,Y_s)$ and $\overline{Y}=(\overline{Y}_1,\dots,\overline{Y}_s)$ are vectors, whose components are elements of $E$. $f(Y,\overline{Y})$ denotes the vector with the components $f(Y_j,\overline{Y}_j)$, $h$ the step-size and $\mathbf{1}=(1,\dots,1)^T$. The $s$-vector $\alpha=(\alpha_1,\dots,\alpha_s)^T$ and the real $(s,s)$-matrices $A=(a_{ij})$ and $\overline{A}=(\bar a_{ij})$ determine the method. They must be fitted to equalize $Y_s=y_1$ with the solution at $x_0+h$ up to a certain order, and $\overline{Y}_s=y_1'$ with $y'(x_0+h)$.

The method is called explicit ($Y$ and $\overline{Y}$ can be computed explicitly from (8)) if the matrices $A$ and $\overline{A}$ have zeros in and above the diagonal.

Usually in literature only explicit Nyström methods are considered, the theory of this paper, however, applies to implicit methods as well.

For a nonautonomuous system

$$y''=f(x,y,y')$$

we add $x''=0$ and formula (8) becomes (if explicit)

$$\begin{aligned}k_i&=f\Big(x_0+\alpha_i h,\,y_0+\alpha_i h\,y_0'+h^2\sum_{j=1}^{i-1}a_{ij}k_j,\,y_0'+h\sum_{j=1}^{i-1}\bar a_{ij}k_j\Big)\\ y_1&=y_0+\alpha_s h\,y_0'+h^2\sum_{j=1}^{s-1}a_{sj}k_j\\ y_1'&=y_0'+h\sum_{j=1}^{s-1}\bar a_{sj}k_j.\end{aligned}$$

Here we have introduced the values $k_i = f(x_0+\alpha_i h, Y_i, \bar{Y}_i)$, what makes the formulas better adjusted to numerical computations.

It is of course also possible to define multi-step methods, hybrid methods or general multi-value methods, etc, in a similar way.

## 6. Conditions for the Parameters

We now use Theorem 13 to derive the order conditions for $\alpha_i$, $a_{ij}$, $\bar{a}_{ij}$ by equalizing the $N$-series of $y(x_0+h)$ and $Y_s$ (resp. $y'(x_0+h)$ and $\bar{Y}_s$) up to a certain order.

Assume for $Y_i$ a $N$-series

$$Y_i = N(a_i, y_0, y_0')$$

and for $\bar{Y}_i$ the derivative of a $N$-series

$$\bar{Y}_i = N'(a_i', y_0, y_0').$$

With $a(t) = (a_1(t), \ldots, a_s(t))^T$ and $a'(t) = (a_1'(t), \ldots, a_s'(t))^T$ we have

$$Y = \sum_{t \in \mathrm{LNT}} a(t)\, F(t)\,(y_0, y_0')\,\frac{h^{\varrho(t)}}{\varrho(t)!} = N(a, y_0, y_0')$$

and

$$\bar{Y} = \sum_{t \in \mathrm{LNT}} a'(t)\, F(t)\,(y_0, y_0')\,\frac{h^{\varrho(t)-1}}{(\varrho(t)-1)!} = N'(a', y_0 y_0').$$

We further use the notation $a''(t) = (a_1''(t), \ldots, a_s''(t))^T$.

**Theorem 14.** For the Nyström method (8) we have

$$Y = N(a, y_0, y_0') \quad \text{and} \quad \bar{Y} = N'(a', y_0, y_0'),$$

where

$$\begin{aligned} a(\emptyset) &= \mathbf{1}, & a'(\emptyset) &= 0, \\ a(\tau_1) &= \alpha, & a'(\tau_1) &= \mathbf{1}, \\ a(t) &= \varrho(t) \cdot (\varrho(t)-1)\, A\, a''(t), \\ a'(t) &= (\varrho(t)-1)\, \bar{A}\, a''(t). & & \varrho(t) \geqq 2 \end{aligned} \tag{9}$$

*Proof.* By inserting Theorem 13 into (8). □

Comparing this theorem with Theorem 10 we see that

$$Y_s - y(x_0+h) = O(h^{p+1}) \quad \text{iff} \quad a_s(t) = 1 \quad \text{for } \varrho(t) \leqq p$$

and

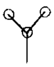
$$\bar{Y}_s - y'(x_0+h) = O(h^{p+1}) \quad \text{iff} \quad a_s'(t) = 1 \quad \text{for } \varrho(t) \leqq p+1.$$

In Table 1 we present the above conditions for $N$-trees with $\varrho(t) \leqq 4$.

The following theorem shows how the final shape of these conditions, which results from the recurrence process of Theorem 14, can be directly obtained from the $N$-tree:

**Theorem 15.** Attach to every fat node of a NT $t$ a summation letter ($k, l, m, n, \ldots$ etc.).

Table 1

| $t$ | $\varrho(t)$ | $a_s(t)=1$ | $a'_s(t)=1$ |
|---|---|---|---|
| . | 1 | $\alpha_s=1$ | $1=1$ |
|  | 2 | $2\sum_k a_{sk}=1$ | $\sum_k \bar{a}_{sk}=1$ |
|  | 3 | $6\sum_k a_{sk}\alpha_k=1$ | $2\sum_k \bar{a}_{sk}\alpha_k=1$ |
|  | 3 | $6\sum_{kl} a_{sk}\bar{a}_{kl}=1$ | $2\sum_{kl} \bar{a}_{sk}\bar{a}_{kl}=1$ |
|  | 4 | $12\sum_k a_{sk}\alpha_k^2=1$ | $3\sum_k \bar{a}_{sk}\alpha_k^2=1$ |
|  | 4 | $12\sum_{kl} a_{sk}\alpha_k\bar{a}_{kl}=1$ | $3\sum_{kl} \bar{a}_{sk}\alpha_k\bar{a}_{kl}=1$ |
|  | 4 | $12\sum_{klm} a_{sk}\bar{a}_{kl}\bar{a}_{km}=1$ | $3\sum_{klm} \bar{a}_{sk}\bar{a}_{kl}\bar{a}_{km}=1$ |
|  | 4 | $24\sum_{kl} a_{sk}a_{kl}=1$ | $6\sum_{kl} \bar{a}_{sk}a_{kl}=1$ |
|  | 4 | $24\sum_{kl} a_{sk}\bar{a}_{kl}\alpha_l=1$ | $6\sum_{kl} \bar{a}_{sk}\bar{a}_{kl}\alpha_l=1$ |
|  | 4 | $24\sum_{klm} a_{sk}\bar{a}_{kl}\bar{a}_{lm}=1$ | $6\sum_{klm} \bar{a}_{sk}\bar{a}_{kl}\bar{a}_{lm}=1$ |

Then the order condition for $t$ has the form

$$\gamma(t)\sum_{k,l,m,\ldots} a_{sk}\,\Psi=1,\qquad \frac{\gamma(t)}{\varrho(t)}\sum_{k,l,m,\ldots}\bar{a}_{sk}\Psi=1$$

where $\Psi$ is a product which contains the factors

$\bar{a}_{kl}$ whenever a lower node "$k$" is directly connected with a higher node "$l$",
$a_{kl}$ whenever a lower node "$k$" is connected via a meagre node with "$l$" and
$\alpha_k^q$ whenever the lower node "$k$" is connected with $q$ meagre end-nodes.

$\gamma(t)$ is the classical coefficient introduced by John Butcher (for trees). It is the product of all $\varrho(u)$, where $u$ runs over all trees which are got, if one root after the other is left away. □

*Example.* For the $N$-tree sketched in Figure 6 one has the equations

$$15\cdot 14\cdot 4\cdot 7\cdot 2\cdot 4\cdot 2\sum_{klmnpr} a_{sk}\,\bar{a}_{kl}\,\bar{a}_{km}\,\alpha_k^2\,a_{lp}\,\alpha_l\,\bar{a}_{mn}\,\alpha_n^3\,a_{mr}=1$$

$$14\cdot 4\cdot 7\cdot 2\cdot 4\cdot 2\sum_{klmnpr} \bar{a}_{sk}\,\bar{a}_{kl}\,\bar{a}_{km}\,\alpha_k^2\,a_{lp}\,\alpha_l\,\bar{a}_{mn}\,\alpha_n^3\,a_{mr}=1.$$

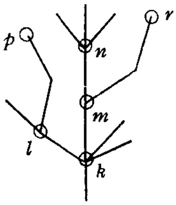



Fig. 6

## 7. Simplifying Assumptions

The equations of condition are nonlinear equations in the parameters $\alpha_i$, $a_{ij}$, $\bar{a}_{ij}$. In this section we give conditions to be satisfied in order to reduce the large number of conditions.

**Proposition 16.** Let $u_1$ and $u_2$ be two $N$-trees as sketched in Figure 7, where the encircled parts are assumed to be identical. Then the condition

$$p \sum_l a_{kl} \alpha_l^{p-1} = \alpha_k^p \qquad (k=1, \ldots, s) \tag{10}$$

implies, that for $a$, $a'$ defined by Theorem 14 $a(u_1)=a(u_2)$ and $a'(u_1)=a'(u_2)$. Similarly,

$$p(p-1) \sum_l a_{kl} \alpha_l^{p-2} = \alpha_k^p \qquad (k=1, \ldots, s) \tag{11}$$

implies that $a(v_1)=a(v_2)$ and $a'(v_1)=a'(v_2)$ (Fig. 7).

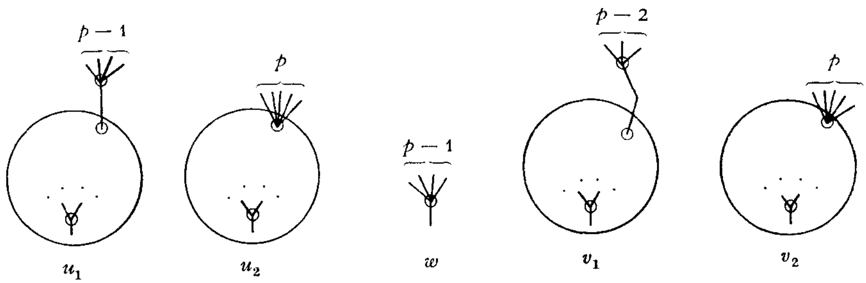



Fig. 7

*Proof.* In the representation of $u_1$ and $u_2$ all $N$-trees are equal with one exception. But this can be written as

$$\bar{u}_1 = [t_1, \ldots, t_k; t_{k+1}, \ldots, t_m, w] \quad \text{with} \quad w = [\underbrace{\tau_1, \ldots, \tau_1}_{p-1};]$$

resp.

$$\bar{u}_2 = [t_1, \ldots, t_k, \overbrace{\tau_1, \ldots, \tau_1}^{p}; t_{k+1}, \ldots, t_m].$$

$\varrho(\bar{u}_1) = \varrho(\bar{u}_2)$ is evident and (10) implies $a''(\bar{u}_1) = a''(\bar{u}_2)$. Thus we obtain the result by the formulas (9).

The second part of this proposition is proved in the same way. □

Already the conditions (10) with $p=1$ and (11) with $p=2$ reduce the number of equations considerably. The remaining ones are seen in Table 2 for $\varrho(t) \leq 5$. (This table corresponds to that of [2].)

If in addition $f(y, y')$ does not depend on $y'$, many equations can be left away, since the corresponding elementary differentials vanish (Table 3).

Table 2

| $t$ | $\varrho(t)$ | $a_s(t) = 1$ | $a'_s(t) = 1$ |
|---|---|---|---|
| · | 1 | $\alpha_s = 1$ | $1 = 1$ |
|  | 2 | $2\sum a_{sk} = 1$ | $\sum \bar{a}_{sk} = 1$ |
|  | 3 | $6\sum a_{sk}\alpha_k = 1$ | $2\sum \bar{a}_{sk}\alpha_k = 1$ |
|  | 4 | $12\sum a_{sk}\alpha_k^2 = 1$ | $3\sum \bar{a}_{sk}\alpha_k^2 = 1$ |
|  | 4 | $24\sum a_{sk}\bar{a}_{kl}\alpha_l = 1$ | $6\sum \bar{a}_{sk}\bar{a}_{kl}\alpha_l = 1$ |
|  | 5 | $20\sum a_{sk}\alpha_k^3 = 1$ | $4\sum \bar{a}_{sk}\alpha_k^3 = 1$ |
|  | 5 | $40\sum a_{sk}\alpha_k\bar{a}_{kl}\alpha_l = 1$ | $8\sum \bar{a}_{sk}\alpha_k\bar{a}_{kl}\alpha_l = 1$ |
|  | 5 | $60\sum a_{sk}\bar{a}_{kl}\alpha_l^2 = 1$ | $12\sum \bar{a}_{sk}\bar{a}_{kl}\alpha_l^2 = 1$ |
|  | 5 | $120\sum a_{sk}\bar{a}_{kl}\bar{a}_{lm}\alpha_m = 1$ | $24\sum \bar{a}_{sk}\bar{a}_{kl}\bar{a}_{lm}\alpha_m = 1$ |
|  | 5 | $120\sum a_{sk}a_{kl}\alpha_l = 1$ | $24\sum \bar{a}_{sk}a_{kl}\alpha_l = 1$ |

Table 3

| $t$ | $\varrho(t)$ | $a_s(t) = 1$ | $a'_s(t) = 1$ |
|---|---|---|---|
| · | 1 | $\alpha_s = 1$ | $1 = 1$ |
|  | 2 | $2\sum a_{sk} = 1$ | $\sum \bar{a}_{sk} = 1$ |
|  | 3 | $6\sum a_{sk}\alpha_k = 1$ | $2\sum \bar{a}_{sk}\alpha_k = 1$ |
|  | 4 | $12\sum a_{sk}\alpha_k^2 = 1$ | $3\sum \bar{a}_{sk}\alpha_k^2 = 1$ |
|  | 5 | $20\sum a_{sk}\alpha_k^3 = 1$ | $4\sum \bar{a}_{sk}\alpha_k^3 = 1$ |
|  | 5 | $120\sum a_{sk}a_{kl}\alpha_l = 1$ | $24\sum \bar{a}_{sk}a_{kl}\alpha_l = 1$ |
|  | 6 | $30\sum a_{sk}\alpha_k^4 = 1$ | $5\sum \bar{a}_{sk}\alpha_k^4 = 1$ |
|  | 6 | $180\sum a_{sk}\alpha_k a_{kl}\alpha_l = 1$ | $30\sum \bar{a}_{sk}\alpha_k a_{kl}\alpha_l = 1$ |
|  | 6 | $360\sum a_{sk}a_{kl}\alpha_l^2 = 1$ | $60\sum \bar{a}_{sk}a_{kl}\alpha_l^2 = 1$ |

## 8. Pairs of $N$-Trees

In order to extend this theory (group operation, composition of methods, global error, asymptotic expansion, ...) we need the concept of "Pairs of $N$-trees".

**Definition 17.** A LNT $u = (u, r)$ is a *LN-subtree* of the LNT $t = (t, q)$ if

a) $\varrho(u) \leqq \varrho(t)$,

b) $t|_{\{2,\ldots,\varrho(u)\}} = u$ and $q|_{\{1,\ldots,\varrho(u)\}} = r$.

For a fixed $k$ $(0 \leqq k \leqq \varrho(t))$ there exists exactly one LN-subtree $u$ of $t$ with $\varrho(u) = k$.

**Definition 18.** A *monotonically labelled pair of N-trees* (LPNT) $u \subset t$ is a LNT together with a LN-subtree $u$.

In the geometric representation we distinguish the LN-subtree by doubled lines. Examples are given in Figure 8.

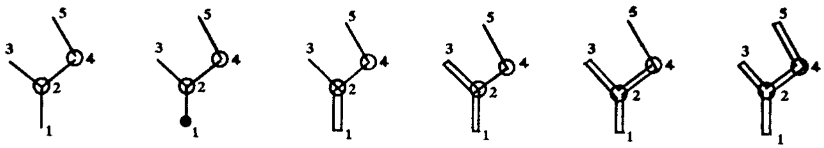



Fig. 8

**Definition 19** (Pairs of N-trees (PNT)). A pair of $N$-trees is an equivalence class of LPNT's with respect to the equivalence relation

$$(u_1, r_1) \subset (t_1, q_1) \sim (u_2, r_2) \subset (t_2, q_2)$$

1) $\varrho(t_1) = \varrho(t_2)$, $\quad \varrho(u_1) = \varrho(u_2)$;

2) There exists a permutation $\sigma$ of $\{1, \ldots, \varrho(t_1)\}$ such that $\sigma(1) = 1$, $\sigma(\{1, \ldots, \varrho(u_1)\}) = \{1, \ldots, \varrho(u_1)\}$ and $t_1(i) = \sigma t_2 \sigma^{-1}(i)$ for $i = 2, \ldots, \varrho(t_1)$;

3) $q_1(i) = q_2 \sigma(i)$.

In Figure 9 two equivalent LPNT's are sketched $(\sigma = (3, 4))$.

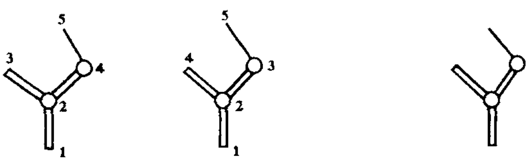



Fig. 9

As can be seen, this equivalence relation is just made to identify trees with different labels, but with the same geometrical structure. Thus, in the graphical representations the labels are omitted.

**Definition 20.** Let $u_1 \subset t_1, \ldots, u_m \subset t_m \in \mathrm{PNT}$ and $k \in \mathbb{Z}$ with $0 \leqq k \leqq m$ ($\varrho(t_i) \geqq 1$ for $i = 1, \ldots, k$; $\varrho(t_i) \geqq 2$, $\varrho(u_i) \geqq 1$ for $i = k+1, \ldots, m$). Then we denote by

$$u \subset t = \langle u_1 \subset t_1, \ldots, u_k \subset t_k;\ u_{k+1} \subset t_{k+1}, \ldots, u_m \subset t_m \rangle \tag{12}$$

a new PNT which is obtained by:

1.
2. same as in Definition 6 with $t_i$ replaced by $u_i \subset t_i$.
3.
4. The branches which connect the root of $u \subset t$ with charlie as well as the branches connecting charlie with the roots of $u_i \subset t_i$ ($i = 1, \ldots, k$), $u_i \neq \emptyset$ are doubled.

Analogous to Proposition 8 we have:

**Proposition 21.** Every $u \subset t \in \mathrm{PNT}$ with $\varrho(t) \geqq 3$ and $\varrho(u) \geqq 2$ can be represented in the form (12) with pairs of $N$-trees of lower order. Except of permutations among $u_1 \subset t_1, \ldots, u_k \subset t_k$ and $u_{k+1} \subset t_{k+1}, \ldots, u_m \subset t_m$ this representation is unique. □

## 9. Composition of *N*-Series

In this section we give the general theorem on the composition of $N$-series which extends "Theorem 6" of [1]. First of all we prove the following generalization of Theorem 13:

**Theorem 22.** Let $a\colon \mathrm{NT} \to \mathbb{R}$, $a'\colon \mathrm{NT} \to \mathbb{R}$ be mappings. If $a(\emptyset) = 1$, $a'(\emptyset) = 0$, $a'(\tau_1) = 1$, we have for any LNT $u$

$$F(u)\,(N(a, y_0, y_0'),\ N'(a', y_0, y_0')) = \sum_{u \subset t \in \mathrm{LPNT}} a(u \subset t)\, F(t)\,(y_0, y_0')\, \frac{h^{\varrho(t) - \varrho(u)}}{(\varrho(t) - \varrho(u))!}$$

where $a\colon \mathrm{PNT} \to \mathbb{R}$ is defined by

$$\begin{aligned} a(\emptyset \subset t) &= a(t) \\ a(\tau_1 \subset t) &= a'(t) \\ a(\tau_2 \subset \tau_2) &= 1 \\ a(u \subset t) &= a(u_1 \subset t_1) \cdot \cdots \cdot a(u_m \subset t_m) \quad \text{for} \\ & u \subset t = \langle u_1 \subset t_1, \ldots, u_k \subset t_k;\ u_{k+1} \subset t_{k+1}, \ldots, u_m \subset t_m \rangle. \end{aligned} \tag{13}$$

The summation is over all LPNT's such that the distinguished subtree is equal to the given LNT $u$.

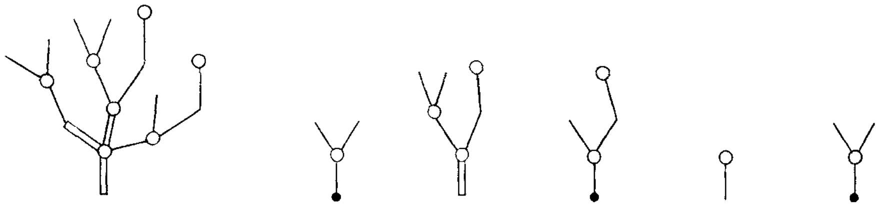
*Remark.* Observe that $u \subset t$ is once used as an element of LPNT and once as an element of PNT. We use the same symbol since there is no possibility of confusion.

*Proof.* The first three relations of (13) are immediately seen from the definition of the elementary differentials. The last one can be proved in the same manner as the proof of Theorem 13 was done. □

*Example.* Let $u \subset t = \langle u_1 \subset t_1;\ u_2 \subset t_2, u_3 \subset t_3 \rangle$ be as in Figure 10. For $u_1 \subset t_1$ and $u_3 \subset t_3$ the function $a$ is already defined, $u_2 \subset t_2$ is again decomposable as $u_2 \subset t_2 =$

$\langle u_4 \subset t_4;\, u_5 \subset t_5 \rangle$. So finally by (13)

$$a(u \subset t) = a(u_1 \subset t_1)\, a(u_4 \subset t_4)\, a(u_5 \subset t_5)\, a(u_3 \subset t_3) = a'(t_1)\, a(t_4)\, a'(t_5)\, a'(t_3).$$



$u \subset t$ | $u_1 \subset t_1$ $(u_1 = \tau_1)$ | $u_2 \subset t_2$ | $u_3 \subset t_3$ $(u_3 = \tau_1)$ | $u_4 \subset t_4$ $(u_4 = \emptyset)$ | $u_5 \subset t_5$ $(u_5 = \tau_1)$

Fig. 10

*Remark.* The situation is similar to that in the proof of Proposition 8: One has to remove $u$ and the adjacent branches and, from what rests, collect the trees with meagre roots as $v_1, \ldots, v_i$. To each of the others one has to affix a new root with one branch to obtain $w_1, \ldots, w_j$. Then

$$a(u \subset t) = a(v_1) \ldots a(v_i)\, a'(w_1) \ldots a'(w_j). \tag{13a}$$

Observe that (7) of Theorem 13 can now be written as

$$a''(t) = a(\tau_2 \subset t).$$

**Definition 23.** For $t \in \mathrm{NT}$, $u \subset t \in \mathrm{PNT}$ we define

$\alpha(t)$ = the number of LNT's in the equivalence class of $t$,

$\alpha(u \subset t)$ = the number of LPNT's in the equivalence class of $u \subset t$.

$\alpha(t)$ and $\alpha(u \subset t)$ give the number of possible monotonic labellings of the nodes of $t$ such that, in the second case, the nodes of $u$ are labelled first.

**Theorem 24** (Composition of $N$-series). Let $a, a', b, b'$ be mappings $\mathrm{NT} \to \mathbb{R}$ such that $a(\emptyset) = 1$, $a'(\emptyset) = 0$, $a'(\tau_1) = 1$, $b'(\emptyset) = 0$. Then

$$N(b, N(a, y_0, y_0'), N'(a', y_0, y_0')) = N(a\, b, y_0, y_0')$$

$$N'(b', N(a, y_0, y_0'), N'(a', y_0, y_0')) = N'((a\, b)', y_0, y_0')$$

where the mappings $a\, b$ and $(a\, b)'$ are given by

$$(a\, b)(t) = \sum_{u \subset t \in \mathrm{PNT}} \binom{\varrho(t)}{\varrho(u)} \frac{\alpha(u \subset t)}{\alpha(t)}\, b(u)\, a(u \subset t)$$

$$(a\, b)'(t) = \sum_{\substack{u \subset t \in \mathrm{PNT} \\ u \neq \emptyset}} \binom{\varrho(t) - 1}{\varrho(u) - 1} \frac{\alpha(u \subset t)}{\alpha(t)}\, b'(u)\, a(u \subset t). \tag{14}$$

$((a\, b)'(\emptyset) = 0)$.

*Remark.* If $t$ is a fixed $N$-tree, $\sum_{u \subset t \in \mathrm{PNT}}$ expresses the summation over all pairs $u \subset w$ such that $w = t$ as $N$-trees. This notation we shall use throughout this paper.

*Proof of Theorem 24.* Using Theorem 22 we have

$$\begin{aligned}
&N(b, N(a, y_0, y_0'), N'(a', y_0, y_0'))\\
&= \sum_{u\in \mathrm{LNT}} b(u)\, F(u)\, (N(a, y_0, y_0'), N'(a', y_0, y_0'))\, \frac{h^{\varrho(u)}}{\varrho(u)!}\\
&= \sum_{u\in \mathrm{LNT}} \sum_{u\subset t\in \mathrm{LPNT}} b(u)\, a(u\subset t)\, F(t)\,(y_0, y_0')\, \frac{h^{\varrho(t)}}{\varrho(u)!\,(\varrho(t)-\varrho(u))!}\\
&= \sum_{t\in \mathrm{NT}} \Bigg(\sum_{u\subset t\in \mathrm{LPNT}} \binom{\varrho(t)}{\varrho(u)} b(u)\, a(u\subset t)\Bigg) F(t)\,(y_0, y_0')\, \frac{h^{\varrho(t)}}{\varrho(t)!}\\
&= \sum_{t\in \mathrm{LNT}} \Bigg(\sum_{u\subset t\in \mathrm{PNT}} \binom{\varrho(t)}{\varrho(u)} \frac{\alpha(u\subset t)}{\alpha(t)}\, b(u)\, a(u\subset t)\Bigg) F(t)\,(y_0, y_0')\, \frac{h^{\varrho(t)}}{\varrho(t)!}\,.
\end{aligned}$$

The second part of Theorem 24 is proved in the same way. □

*Example.* For the first trees, the composition (14) is as follows:

$$\begin{aligned}
&(a\,b)\,(\emptyset) = b\,(\emptyset)\\
&(a\,b)\,(\tau_1) = b\,(\emptyset)\; a\,(\tau_1) + b\,(\tau_1)\\
&(a\,b)\,(\tau_2) = b\,(\emptyset)\; a\,(\tau_2) + \binom{2}{1} b\,(\tau_1)\; a'(\tau_2) + b\,(\tau_2)\\
&\ldots\\
&(a\,b)'\,(\emptyset) = 0\\
&(a\,b)'\,(\tau_1) = b'(\tau_1)\\
&(a\,b)'\,(\tau_2) = b'(\tau_1)\; a'(\tau_2) + b'(\tau_2).
\end{aligned}$$

**Corollary 25.** Suppose that the numerical results $y_1$, $y_1'$ of a method $(s, \alpha, A, \bar{A})$ are taken as initial values for a second method $(r, \beta, B, \bar{B})$. Then the final result can be interpreted as the result of *one* method $(r+s, \gamma, C, \bar{C})$ where

$$\gamma = \begin{pmatrix} \alpha \\ L\alpha + \beta \end{pmatrix}, \quad C = \begin{pmatrix} A & 0 \\ LA + M\bar{A} & B \end{pmatrix}, \quad \bar{C} = \begin{pmatrix} \bar{A} & 0 \\ L\bar{A} & \bar{B} \end{pmatrix}$$

$$L = \begin{pmatrix} 0\cdots 0 & 1 \\ \vdots \quad \vdots & \vdots \\ 0\cdots 0 & 1 \end{pmatrix}, \quad M = \begin{pmatrix} 0\cdots 0 & \beta_1 \\ \vdots \quad \vdots & \vdots \\ 0\cdots 0 & \beta_r \end{pmatrix}.$$

Then for the composed method we have (for the last components) for $t\in \mathrm{NT}$

$$c_{r+s}(t) = (a_s\, b_r)\,(t), \qquad c'_{r+s}(t) = (a_s\, b_r)'\,(t)$$

with the composition of Theorem 24.

*Proof.* The proof is simply by inserting formula (8) into a similar expression for the second method and using $\mathbf{1}\cdot y_1 = LY$, $\mathbf{1}\cdot y_1' = L\bar{Y}$, $\beta\cdot y_1' = M\bar{Y}$. □

Denoting by

$$G = \{(a, a') \,/\, a\colon \mathrm{NT} \to \mathbb{R}, \quad a'\colon \mathrm{NT} \to \mathbb{R}, \quad a(\emptyset) = 1, \quad a'(\emptyset) = 0, \quad a'(\tau_1) = 1\},$$

we see that formulas (14) define a composition on $G$:

$$\begin{aligned}
G \times G &\to G\\
((a, a'), (b, b')) &\mapsto (a\,b, (a\,b)').
\end{aligned}$$

**Proposition 26.** $G$ with the above relation is a group.

*Proof.* The associativity follows from Proposition 12, because of

$$N((a\,b)\,c, y_0, y_0') = \cdots = N(a\,(b\,c), y_0, y_0').$$

As a right-neutral element we have $(o, o')$, where

$$o(t) = \begin{cases} 1 & \text{if } t=\emptyset \\ 0 & \text{else} \end{cases} \qquad o'(t) = \begin{cases} 1 & \text{if } t=\tau_1 \\ 0 & \text{else.} \end{cases}$$

The existence of a right inverse is seen from the formulas (14), because $b(t)$, $b'(t)$ can be computed explicitly in terms of $a$, $a'$ and $b(u)$, $b'(u)$ with $\varrho(u) < \varrho(t)$. □

## 10. Numerical Examples

We now shortly demonstrate how numerical methods could actually be found.

Note first that for the coefficients $\bar{a}_{ij}$ the same conditions are obtained as for classical Runge Kutta methods. Indeed, the condition $a_s'(t)=1$ for $t \in \mathrm{NT}$, where $t$ has only *one* meagre node (the root), is just the same as the order condition for Runge Kutta methods for that tree, when the root has been removed (cf. Theorem 15). Thus one can take the coefficients of any Runge Kutta method (of order $q$) as $\bar{A}$. If one then puts $A = \bar{A}^2$, $\alpha = \bar{A}\,\mathbb{1}$, then all order conditions (up to $q$) are satisfied, since this choice corresponds exactly to the RK method $\bar{A}$ applied to the system

$$\begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \begin{pmatrix} y_2 \\ f(y_1, y_2) \end{pmatrix}.$$

Other solutions, however, are possible. So if we choose for $\bar{A}$ Kuttas classical method

$$\bar{A} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1/6 & 1/3 & 1/3 & 1/6 & 0 \end{pmatrix},$$

the condition (10) with $p=1$ gives $\bar{A}\,\mathbb{1} = \alpha$, thus

$$\alpha = (0, 1/2, 1/2, 1, 1)^T.$$

Then the remaining conditions of Table 1 give

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \lambda & 0 & 0 & 0 & 0 \\ 1/4-\lambda-\nu & \nu & 0 & 0 & 0 \\ 2\nu & 1/2-2\nu-\mu & \mu & 0 & 0 \\ 1/6 & 1/6 & 1/6 & 0 & 0 \end{pmatrix}.$$

The parameters $\lambda, \nu, \mu$ can freely be chosen. In every case we have Nyström methods of order 4. Special values could be determined by (11) with $p=2$ leading to $\lambda = 1/8$. Trying to equalize also some of the conditions of higher order, we are led to $\nu = 1/10$ and $\mu = 1/5$. So we have

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 1/8 & 0 & 0 & 0 & 0 \\ 1/40 & 1/10 & 0 & 0 & 0 \\ 1/5 & 1/10 & 1/5 & 0 & 0 \\ 1/6 & 1/6 & 1/6 & 0 & 0 \end{pmatrix}.$$

Computing the leading error terms — we have made a computer program which generates automatically the $N$-trees and corresponding coefficients up to any order — one sees that the above choice of parameters gives results closer to the solution that the RK method ($\lambda = \nu = \mu = 0$).

Passing from RK to $N$-methods it is impossible (what follows from the remarks at the beginning of this section) to improve the order with the same number of function evaluations. However, if we look for $N$-methods for the special differential equation $y'' = f(x, y)$, where $f$ is independent of $y'$, the number of conditions is reduced and we can gain order. So for example it is possible to obtain order 6 with only 5 function evaluations. Such a method, chosen in order to make round-off errors and the leading error term small, is given by

$$\alpha = (0,\ 1/5,\ 1/2,\ 4/5,\ 1,\ 1)^T,$$

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{50} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{8} & 0 & 0 & 0 & 0 \\ \frac{14}{125} & \frac{2}{25} & \frac{16}{125} & 0 & 0 & 0 \\ -\frac{1}{9} & \frac{14}{27} & 0 & \frac{5}{54} & 0 & 0 \\ \frac{1}{16} & \frac{25}{108} & \frac{4}{27} & \frac{25}{432} & 0 & 0 \end{pmatrix}.$$

The last row of $\bar{A}$ (the other elements of $\bar{A}$ are not used with this special type of equations) is given by

$$\left(\frac{1}{16} \quad \frac{125}{432} \quad \frac{8}{27} \quad \frac{125}{432} \quad \frac{1}{16} \quad 0\right).$$

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