Continuous Extensions to Nyström Methods for the Explicit Solution of Second Order Initial Value Problems

September 26, 1994

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Abstract. In this work, we consider interpolants for Nyström methods, i.e., second order initial value problems. We give a short introduction to the theory behind the discrete methods, and extend some of the work to continuous, explicit Nyström methods. Interpolants for continuous, explicit Runge-Kutta methods have been intensively studied by several authors, but there has not been much effort devoted to continuous Nyström methods. We therefore extend some of the work by Owren [31].

Hamiltonian problems and symplectic integrators have been thoroughly studied the past few years. We derive the conditions for continuous Nyström methods to be symplectic, and discuss whether or not we really need symplectic dense output.

Keywords: Interpolants, Dense Output, Nyström Methods, Runge-Kutta Methods, Second Order Initial Value Problems, Symplectic Methods, Symplectic Interpolants

AMS subject classification: 65L05

1 Introduction

Conventional explicit Nyström methods are generally designed to approximate the solution of a system of second order ordinary differential equations on a mesh. The size of the mesh will typically be determined by some step size selection algorithm, and the steps will in general be chosen as large as possible constrained by some tolerances to stability and accuracy. Sometimes, however, the solution is required in points not covered by the mesh. The obvious thing to do in this case, would be to take a smaller step to hit the desired point. But what should we do if we do not know the additional points in advance? An effective method for output of results at randomly chosen points within an interval should be provided.

And, indeed, such methods are available for some of the most well known numerical one-step (Runge-Kutta) schemes today. We call the methods *interpolants* or *continuous extensions.*

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Among the applications for interpolants are handling of discontinuities/singularities, delay differential equations, and the need for the numerical solution at a dense set of output points (graphical representation of the solution).

The field of interpolation in Runge-Kutta methods is not very old. The early work by Horn [25, 26] represent some of the first written papers on the subject. Among others, Shampine [39, 38], Enright et al. [13], Gladwell et al. [22], Dormand and Prince [9], Owren [31], Owren and Zennaro [32, 33], Verner [44] and Verner and Zennaro [45] have considered dense output for Runge-Kutta methods. A paper by Enright et al. [12] (to appear) contains a survey of the explicit Runge-Kutta method. In that paper, the present state of continuous approximations for explicit Runge-Kutta methods are discussed. The classical paper by Enright et al. [13] contains a general procedure for the construction of interpolants for Runge-Kutta formulas. A "boot-strapping" process for the increasing of the order of the interpolant until the maximum order of $p+1$ is attained, is described. The main concern is Hermite and Hermite-Birkhoff interpolation. A general discussion on applications of interpolants is also given.

We see that quite a lot of work has been spent on working out a theory on interpolants for first order explicit Runge-Kutta methods. Many authors have contributed to this field of numerical analysis. But not much has been published when it comes to methods for the continuous solution of second order problems. Continuous extensions for some Nyström methods have been presented, but the theory on the subject is not very well discussed.

In this work, continuous extensions to Nyström methods will be considered. We show that it is possible to extend the theory for explicit Runge-Kutta methods to explicit Nyström methods. The interpolants presented are designed to be used in conjunction with the corresponding discrete methods. The function evaluations of the discrete methods constitutes the core of the new system, and thus, at a small increase of cost, the solution and the derivative may be generated within a successful step. This will improve the efficiency of existing discrete methods.

We emphasize that when we talk about Nyström methods in this work, we implicitly mean *explicit* Nyström methods. It should be clear that the results obtained are only valid in that case.

Discrete Runge-Kutta-Nyström methods of various order have been developed by several authors, among them are Bettis [3], Fehlberg [15, 14, 17], Fehlberg, Filippi and Gräf [11], Filippi and Gräf [18], and Dormand, El-Mikkawy and Prince [6]. Fine [19] has derived five-stage $(3,4)$ and six-stage $(4,5)$ pairs, while Sharp and Fine [40, 42] have derived eight-stage $(5,6)$ pairs. Fehlberg [16] derived $(4,5)$ through $(7,8)$ pairs, and Filippi and Gräf [18] have made Runge-Kutta-Nyström formula-pairs of order 8(7), 9(8), 10(9) and 11(10) for the special Nyström method. Numerical experiments have shown that the construction of high order Runge-Kutta-Nyström methods really is worthwhile, since the computational results are much better than for lower order methods. The step-size strategy by Bettis [3], and Dormand and Prince [8] is used with great success.

Existing Runge-Kutta-Nyström pairs offer two advantages compared with Runge-Kutta pairs of the same order applied to the equivalent first order initial value problem. The numerical testing of Fine [19], and Sharp and Fine [40, 41] shows that $(3,4)$, $(4,5)$ and $(5,6)$ Runge-Kutta-Nyström pairs generally are more efficient than Runge-Kutta pairs. In addition, since

Runge-Kutta-Nyström pairs use the same number of stages as Runge-Kutta pairs, and since the stage evaluation consists of the second derivative components only, Runge-Kutta-Nyström pairs require only half the storage for their stages.

There are two kinds of interpolants for Nyström methods. The classical interpolation theory, e.g. Hermite and Hermite-Birkhoff, may be extended to these methods. In this work, we have not studied this approach. We have instead considered so called *dense output*-interpolation. In this case, we equip the methods with continuous weights. These weights depend on an interpolation parameter, θ, usually between 0 and 1. When a successful step has been performed, we are able to find, with minimum cost, the solution and the derivative with given order of approximation at every point θh, $\theta \in [0,1]$, with none or just a few new function evaluations.

Continuous Runge-Kutta-Nyström methods of various orders have been developed by a few authors, and among them are Papageorgiou and Tsitouras [35, 43, 34], Dormand and Prince [10], Horn [25] and Fine [20]. Dormand and Prince [10] have considered both the classical way of writing interpolants and the more recent dense output. They have derived the conditions to be satisfied for the two implementations to be equal, and also the conditions of continuity for the interpolants. Some of the methods in [6] have been equipped with continuous extensions. Papageorgiou and Tsitouras [34] have derived dense formulas for Runge-Kutta-(Nyström) methods with reduced phase-errors, and in [35], they present a general theory of the so called *scaled* Runge-Kutta-Nyström methods. They also show some scaled extensions for selected methods, in particular, sixth and fifth order interpolants for the RKNF6(7) and RKNB4(5) methods by Fehlberg and Bettis, respectively. In [43] they present high order Hermite type interpolants. These interpolants correspond to the $(9,8(6))$ Runge-Kutta-Nyström method of the FSAL mode presented by Dormand et al. [7]. The interpolants which approximate the solution is of $\mathcal{O}(h^9)$ and C^2, while the interpolant which approximate the corresponding derivative is of $\mathcal{O}(h^8)$ and C^1. In addition, a general algorithm for computer calculation of the coefficients of interpolants is described.

In Section 2 we describe the general form of the Nyström methods. We discuss the order of such methods, and compare autonomous methods with non-autonomous methods. In Section 3 we consider continuous Nyström methods. The order conditions are derived, and continuity and error estimation is discussed.

Sections 3.1 and 4 are devoted to the study of the maximum order attainable with a method using a given number of stages. The barriers we study are similar to the Butcher barriers EN(p) for the discrete case of Runge-Kutta methods, and also similar to the numbers CEN(p) presented by Owren [31] for the continuous case of explicit Runge-Kutta methods.

In Section 6 we discuss the stage reuse feature, and discuss differentiability of the methods.

Symplectic methods have gained much attention the last few years, and the conditions for Nyström methods to be symplectic is well known. In Section 7 we derive the condition for a continuous Nyström method to be symplectic, but we conclude with the rather depressing result that such methods can be of order at most one.

2 Nyström Methods for Second Order Differential Equations

Many differential equations appearing in practical problems are of second order, i.e., they can be written in the form

$$y''(x) = f(x, y(x), y'(x)) \tag{1}$$

with the initial conditions

$$y(x_0) = y_0 \qquad \text{and} \qquad y'(x_0) = y_0' \tag{2}$$

This is because acceleration (the second derivative) often plays an important role in physical systems. Consider for example

- a vibrating mass on a spring: $my'' + ky = 0$,
- the current in an RLC-circuit: $LI'' + RI' + 1/C \cdot I = E'$,
- a pendulum: $\ell\theta'' + g\sin\theta = 0$, or
- Duffing's equation: $\ddot{x} + \delta\dot{x} - x + x^3 = \gamma\cos\omega t$

In this work, we consider the solution of second order differential equations of the form (1). The main concern will be how to construct methods that allow the user to find the solution and the derivative of the solution at randomly chosen points within a step. We want to provide methods, for doing this, which require a minimum amount of work. We start by defining the discrete versions of the methods.

Definition 2.1 (Runge-Kutta-Nyström Method) *The Runge-Kutta-Nyström method is defined by*

$$\begin{aligned} k_i &= f(x_n + c_i h, y_n + c_i h y_n' + h^2 \sum_j \overline{a}_{ij} k_j, y_n' + h \sum_j a_{ij} k_j) && (3) \\ y_{n+1} &= y_n + h y_n' + h^2 \sum_i \overline{b}_i k_i && (4) \\ y_{n+1}' &= y_n' + h \sum_i b_i k_i && (5) \end{aligned}$$

where

$$\overline{a}_{ij} = \sum_k a_{ik} a_{kj}, \qquad \overline{b}_i = \sum_j b_j a_{ji} \tag{6}$$

In the following, we will use the term *Nyström method* to denote a general method of the form (3) – (5), regardless of whether or not the conditions (6) are satisfied. We will use *Runge-Kutta-Nyström* if we want to emphasize that the method is derived from/or has a corresponding Runge-Kutta method. We therefore define:

Definition 2.2 (General Nyström (GN) Method, [23]) *We denote by a Nyström method a method of the form (3) – (5) without requiring the conditions (6) to be satisfied.*

If the system is independent of $y'(x)$, the Nyström method simplifies, and we call it a *special Nyström* method:

Definition 2.3 (Special Nyström (SN) Method, [23]) *We call the method*

$$\begin{aligned} k_i &= f(x_n + c_i h, y_n + c_i h y'_n + h^2 \sum_j \overline{a}_{ij} k_j) && (7) \\ y_{n+1} &= y_n + h y'_n + h^2 \sum_i \overline{b}_i k_i && (8) \\ y'_{n+1} &= y'_n + h \sum_i b_i k_i && (9) \end{aligned}$$

for the problem $y''(x) = f(x, y)$, a special Nyström method.

We see that for SN methods, the coefficients a_{ij} are no longer needed. So, in the case of these methods, we write a_{ij} instead of $\overline{a}_{ij}$ in order to simplify the notation.

In order to write down the order conditions for Nyström methods, we have to define what we mean by the order of a method. The intuitive definition would be to require the difference between the approximation and the true solution to be of $\mathcal{O}(h^{p+1})$, where p is the order of approximation. In the same way, we would require the difference between the approximation to the derivative of the solution and the true derivative of the solution to be of $\mathcal{O}(h^p)$. This is the intuitive definition, since we loose one order by differentiation.

But, as noted by Gear [21], since the approximation to the derivative enters the approximation to the solution itself, if the first approximation is of order $p-1$ and the second is of order p, the overall approximation to the solution will be of order $p-1$, i.e., the lower order of the first approximation destroys the overall order of approximation. On the other hand, if both approximations is of the same order, p, the approximation to the solution will also be of order p. That the argument works is easily seen by applying methods based on these two cases to a simple test problem, e.g. $y'' = y'$, with $y(0) = 1$ and $y'(0) = 1$. This leads to the definition given in e.g. [23].

Definition 2.4 (Order, [23]) *A Nyström method is of order p if, for sufficiently smooth problems (1),*

$$y(x_n + h) - y_{n+1} = \mathcal{O}(h^{p+1}) \qquad (10)$$

and

$$y'(x_n + h) - y'_{n+1} = \mathcal{O}(h^{p+1}) \qquad (11)$$

We consider what will happen when we apply a Nyström method to an autonomous system, and what restrictions we must put on the coefficients in order to retain the same order as in the case of non-autonomous systems. In the case of Runge-Kutta methods, the requirement turns out to be

$$\sum_{j=1}^{s} a_{ij} = c_i$$

We first consider an SN-method applied to the initial value problem

$$\begin{aligned} y'' &= f(v, y) \\ v'' &= 0 \end{aligned} \quad \text{with} \quad \begin{aligned} y(x_0) &= y_0 \\ v(x_0) &= x_0 \end{aligned} \quad \text{and} \quad \begin{aligned} y'(x_0) &= y'_0 \\ v'(x_0) &= x'_0 = 1 \end{aligned}$$

With $z(x) = [y(x)^T, v(x)]^T$ and $F(z) = [f(v,y)^T, 0]^T$, we get

$$z'' = F(z), \qquad \text{with} \qquad \begin{array}{rcl} z(x_0) & = & [y_0^T, x_0]^T \\ z'(x_0) & = & [y_0'^T, 1]^T \end{array}$$

When applying an SN-method to this system, we get

$$\begin{aligned} k_i &= F(z_0 + c_i h z_0' + h^2 \sum_j \overline{a}_{ij} k_j) \\ z_1 &= z_0 + h z_0' + h^2 \sum_i \overline{b}_i k_i \\ z_1' &= z_0' + h \sum_i b_i k_i \end{aligned}$$

With the splitting $k_i = [\overline{k}_i^T, \ell_i]^T$, $i = 1, \ldots, s$, we find that

$$\begin{aligned} \ell_i &= 0 \\ \overline{k}_i &= f(v(x_0) + c_i h v'(x_0) + h^2 \sum_j \overline{a}_{ij} \ell_j, y_0 + c_i h y_0' + h^2 \sum_j \overline{a}_{ij} k_j) \\ &= f(x_0 + c_i h, y_0 + c_i h y_0' + h^2 \sum_j \overline{a}_{ij} k_j) \end{aligned}$$

We see that in the case of SN-methods, we do not have to require any relationship between the $\overline{a}_{ij}$'s and the c_i's.

In the case of GN-methods, we get a similar result. We do not have to require any relationship between the coefficients.

3 Continuous Nyström Methods

Consider the continuous, explicit, s-stage Nyström method for the computation of the numerical solution of problem (1) with initial conditions (2) on the interval $I = [x_n, x_{n+1}]$,

$$k_i = f\Big(x_n + c_i h, y_n + c_i h y_n' + h^2 \sum_{j=1}^{i-1} \overline{a}_{ij} k_j, y_n' + h \sum_{j=1}^{i-1} a_{ij} k_j\Big), \qquad i = 2, \ldots, s, \tag{12}$$

$$u(x_n + \theta h) = y_n + \theta h y_n' + h^2 \sum_{i=1}^{s} \overline{b}_i(\theta) k_i \tag{13}$$

$$v(x_n + \theta h) = y_n' + h \sum_{i=1}^{s} b_i(\theta) k_i \tag{14}$$

where $h = x_{n+1} - x_n$. The vectors y_n and y_n' approximate $y(x_n)$ and $y'(x_n)$, respectively, and θ is the interpolation variable. $u(x_n + \theta h)$ is a continuous approximation to $y(x)$ on the interval $[x_n, x_n + h]$ and $v(x_n + \theta h)$ is the approximation to the derivative $y'(x)$ on the same interval. The $b_i(\theta)$'s, $i = 1, \ldots, s$, and the $\overline{b}_i(\theta)$'s, $i = 1, \ldots, s$, are polynomials in θ of degree less or equal to a number d, where d is a positive integer. The other parameters can be found in the Butcher tableau corresponding to a specific method. We require $b_i(0) = 0$ and $\overline{b}_i(0) = 0$ for $i = 1, \ldots, s$, so that

$$u(x_n) = y_n \qquad \text{and} \qquad v(x_n) = y'_n \tag{15}$$

Since we work with an explicit scheme, the coefficients a_{ij} and $\overline{a}_{ij}$ define strictly lower triangular $s \times s$ matrices, which in turn gives $c_1 = 0$ and reduces the first stage to $k_1 = f(x_n, y_n, y'_n)$. Observe that we get a conventional discrete Nyström method by setting $\theta = 1$ in the scheme, i.e.,

$$y(x_{n+1}) := u(x_n + h) \qquad \text{and} \qquad y'(x_{n+1}) := v(x_n + h) \tag{16}$$

if we require $b_i(1) = b_i$ and $\overline{b}_i(1) = b_i$, $i = 1, \ldots, s$. This also takes care of the continuity. The order of accuracy to which Nyström interpolants approximate the local solution and its first derivative, is given by the following definition (see comment to Definition 2.4):

Definition 3.1 (Order) *The uniform order of a continuous Nyström scheme is defined as the greatest integer p for which*

$$\max_{0 \le \theta \le 1} |y(x_n + \theta h) - u(x_n + \theta h)| = \mathcal{O}(h^{p+1}) \tag{17}$$

and

$$\max_{0 \le \theta \le 1} |y'(x_n + \theta h) - v(x_n + \theta h)| = \mathcal{O}(h^{p+1}) \tag{18}$$

where $|\cdot|$ stands for any norm on $\mathbb{R}^m$.

We consider the continuous version of the order conditions.

Theorem 3.1 (Continuous Order Conditions, GN-trees) *The error of the approximation (12) – (14) is of order p (i.e., the local error satisfies Definition 3.1), if and only if*

$$\begin{aligned} \textstyle\sum_{i=1}^s \overline{b}_i(\theta)\Phi_i(t) &= \tfrac{\theta^{\rho(t)+1}}{(\rho(t)+1)\,\gamma(t)} && \text{for all N-trees } t \text{ with } \rho(t) \le p-1, \\ \textstyle\sum_{i=1}^s b_i(\theta)\Phi_i(t) &= \tfrac{\theta^{\rho(t)}}{\gamma(t)} && \text{for all N-trees } t \text{ with } \rho(t) \le p \end{aligned} \tag{19}$$

where the functions are defined in the usual way, i.e.,

$\rho(t)$**:** *is the order of t, i.e., the number of nodes in t.*

$\alpha(t)$**:** *denotes the number of possible monotone labeling of t.*

$\gamma(t)$**:** *$\gamma(t)$ is defined recursively by*

$$\gamma(t) = \rho(t)\gamma(t_1)\cdots\gamma(t_r)$$

if $t = [t_1, \cdots, t_r]$.

$\Phi_j(t)$**:** *is a sum over the indices of all fat nodes of a labeled N-tree t, without the index of the root.*

Proof: The qth derivative of the numerical approximation with respect to h and the $(q-1)$th derivative of the numerical approximation to the derivative of the solution is given in Theorem 14.9 in [24], with b_i and $\overline{b}_i$ replaced by $b_i(\theta)$ and $\overline{b}_i(\theta)$, respectively. The qth derivative of the exact solution $y(x_n+\theta h)$ is given by $\theta^q y^{(q)}(x_n+\theta h)$. If we look at the condition for the $\overline{b}_i$'s, we have that $\rho(t) = q-1$, i.e. $q = \rho(t)+1$, and the order condition follows directly after noticing that it has to be fulfilled for all $\rho(t) \le p-1$. The condition for the b_i's follow in the same way, but in this case the condition has to be fulfilled for all $\rho(t) \le p$.
The *if* part follows directly from the above discussion, and the *only if* part follows from the fact that the elementary differentials for different trees are independent (see [23]). □

In the same way, we find the continuous order conditions for the SN-trees.

Theorem 3.2 (Continuous Order Conditions, SN-trees) *A Nyström method (12) — (14) for the special differential equation $y'' = f(x,y)$ is of order p, iff*

$$\begin{aligned} \sum_{j=1}^{s} \overline{b}_j(\theta)\Phi_j(t) &= \frac{\theta^{\rho(t)+1}}{(\rho(t)+1)\gamma(t)} \quad \text{for all SN-trees } t \text{ with } \rho(t) \le p-1, \\ \sum_{j=1}^{s} b_i(\theta)\Phi_j(t) &= \frac{\theta^{\rho(t)}}{\gamma(t)} \quad \text{for all SN-trees } t \text{ with } \rho(t) \le p \end{aligned} \tag{20}$$

where the functions are defined in Theorem 3.1.

Proof: The proof follows in the same way as for Theorem 3.1. □

3.1 On the Construction of Continuous Nyström methods

There are in general two ways to obtain a continuous extension to Nyström methods.

1. The first way is to construct a new pair of Nyström formulas, which integrate from x_n with a step of size θh_n, where normally $\theta \in [0,1]$. These new pairs use the function evaluations of one existing Nyström method as a core of the new system. This method has been named *dense output.*

2. The other way is to construct an interpolant based on a sufficient number of approximations y_m to $y(x_m)$, $m \in \mathbb{R}$ and $m \in [n, n+1]$, and the corresponding derivatives, y'_m. This is the classical interpolants, e.g. Hermite and Hermite-Birkhoff.

Dormand and Prince [10] have shown the equivalence of these two ways of making continuous Runge-Kutta-Nyström methods.

In this work, only dense output will be considered.

A question that might be risen is why we need two interpolants, one for y and one for y'. One could argue that we only need the interpolant for y, since we can find the other one by differentiating. And this is indeed true. But, by definition, we have required the two approximations to be of the same order. If we differentiate $u(x_n+\theta h)$, we loose order, i.e., $v(x_n+\theta h)$ is a better approximation to $y'(x_n+\theta h)$ than $u'(x_n+\theta h)$ is.

Throughout this work, we stick to our definition, and require the same order of approximation for both $u(x_n+\theta h)$ and $v(x_n+\theta h)$ (see also the discussion of Definition 2.4).

3.2 On the Order of the Continuous Approximation

It should be noted that in the case of treating dense output, it has been argued that it is sufficient to have $q = p-1$, where q is the uniform order of the continuous extension (see [12]). To see this, consider the error produced by the interpolant,

$$u(x_n + \theta h) - y(x_n + \theta h),$$

where $u(x_n + \theta h)$ is the continuous approximation and $y(x_n + \theta h)$ is the exact solution at $x_n + \theta h$. We denote by $y_n(x_n + \theta h)$ the exact solution after a step of size θh when starting at y_n, and rewrite the expression to get

$$u(x_n + \theta h) - y(x_n + \theta h) = [u(x_n + \theta h) - y_n(x_n + \theta h)] + [y_n(x_n + \theta h) - y(x_n + \theta h)],$$

with $y_n(x_n) = u(x_n) = y_n$. Here, the first part constitutes the local error in the interpolant and the last part is the global error at a point $x_n + \theta h$, when the discrete method takes a step of size θh. The first part is of order $\mathcal{O}(h^{q+1})$ while the second part is of order $\mathcal{O}(h^p)$. If we require them to be of the same order, we get $q = p - 1$. In the same way,

$$v(x_n + \theta h) - y'(x_n + \theta h) = [v(x_n + \theta h) - y'_n(x_n + \theta h)] + [y'_n(x_n + \theta h) - y'(x_n + \theta h)],$$

with $y'_n(x_n) = v(x_n) = y'_n$. Here also, the first part constitutes the local error in the interpolant and the last part is the global error at a point $x_n + \theta h$, when the discrete method takes a step of size θh. We emphasize that we are not supposed to continue the integration from a point supplied by the dense formula, we only want to use the interpolant for possible output at points within the interval $(x_n, x_n + h)$. If we, however, impose $q = p$, then the interpolation error will, in general, be small compared to the global error of the discrete formula (see [12]).

3.3 On Continuity

We want our methods to be globally continuous, i.e., we want the value of the interpolant at $\theta = 1$ to be equal to the discrete approximation. The requirement to be satisfied is then

$$\sum_{i=1}^{s} b_i k_i = \sum_{i=1}^{\widehat{s}} b_i(1) k_i, \tag{21}$$

where $\widehat{s} \geq s$ is the total number of stages for the continuous method, $b_i(1)$, $i = 1, \ldots, \widehat{s}$, are the weights of the interpolant evaluated at $\theta = 1$, and b_i, $i = 1, \ldots, s$, are the weights of the discrete method. Since k_i, $i = 1, \ldots, \widehat{s}$, are function evaluations, the only way to satisfy the requirement (21) in general, is to require that

$$b_i(1) = b_i, \qquad i = 1, \ldots, s \tag{22}$$

and

$$b_i(1) = 0, \qquad i = s + 1, \ldots, \widehat{s} \tag{23}$$

To the end of this work, we will assume that (22) and (23) are fulfilled.

3.4 Error Estimation

When constructing methods, the error estimation process must be taken into account. Usually, a (continuous) method of order p is equipped with a discrete formula of order q to obtain an error estimate at the end point of each step. q normally equals either $p+1$ or $p-1$. Often we try to find a pair satisfying $q = p+1$, and use local extrapolation. But, as in the case of explicit Runge-Kutta methods, we get the following theorem (see also Owren and Zennaro [33]).

Theorem 3.3 *There exists no special Nyström SN($p, p+1$) pairs with $s = \mathrm{CSNEN}(p)$ stages, where $\mathrm{CSNEN}(p)$ is the minimum number of stages needed to obtain order p.*

Proof: See [33]. Assume that $s = \mathrm{CSNEN}(p)$ for a method given by the $s \times s$ matrix A. We have, by definition[2], $\mathrm{rank}\,(F_p(A)) = s$, and hence, it is not possible to find two distinct sets of weights satisfying the first N_p' discrete order conditions. □

3.5 Minimizing the Error Constant

For a continuous Nyström method of order p, the error polynomials are given by

$$\overline{e}_i(\theta) = \theta^{\rho(t_i)+1} - (\rho(t_i)+1)\gamma(t_i)\sum_{j=1}^{s}\overline{b}_j(\theta)\Phi_j(t_i), \qquad i = N_{p-1}+1, \ldots, N_p,$$

and

$$e_i(\theta) = \theta^{\rho(t_i)} - \gamma(t_i)\sum_{j=1}^{s} b_i(\theta)\Phi_j(t_i), \qquad i = N_p+1, \ldots, N_{p+1},$$

where N_q is the number of N-trees of order less or equal to q. We see that $\overline{e}_i(0) = 0$ and that $e_i(0) = 0$.

The local truncation error is then given by

$$|y(x_n+\theta h) - u(x_n+\theta h)| = \frac{h^{p+1}}{(p+1)!}\left|\sum_{i=N_{p-1}+1}^{N_p} \overline{e}_i(\theta)\alpha(t_i)F(t_i)(x_n,y_n)\right| + \mathcal{O}(h^{p+2})$$

and

$$|y'(x_n+\theta h) - v(x_n+\theta h)| = \frac{h^{p+1}}{(p+1)!}\left|\sum_{i=N_p+1}^{N_{p+1}} e_i(\theta)\alpha(t_i)F(t_i)(x_n,y_n)\right| + \mathcal{O}(h^{p+2})$$

We want to minimize the error in our approximation, but it is not obvious which norm to use. Calvo et al. [4] minimize the quantity

$$g^* = \int_0^1 g(\theta)d\theta$$

[2] We use nomenclature from Section 5.

over the free parameters, where

$$g(\theta) = \sqrt{\frac{\sum_{i=N_p+1}^{N_{p+1}}[e_i(\theta)\alpha(t_i)]^2}{\sum_{i=N_p+1}^{N_{p+1}}[e_i(1)\alpha(t_i)]^2}}$$

in the case of continuous, explicit Runge-Kutta methods. In the same way, we could then minimize $G = g^* + \overline{g}^*$, where

$$g^* = \int_0^1 g(\theta)d\theta$$

and

$$\overline{g}^* = \int_0^1 \overline{g}(\theta)d\theta$$

and where

$$g(\theta) = \sqrt{\frac{\sum_{i=N_p+1}^{N_{p+1}}[e_i(\theta)\alpha(t_i)]^2}{\sum_{i=N_p+1}^{N_{p+1}}[e_i(1)\alpha(t_i)]^2}}$$

and

$$\overline{g}(\theta) = \sqrt{\frac{\sum_{i=N_{p-1}+1}^{N_p}[\overline{e}_i(\theta)\alpha(t_i)]^2}{\sum_{i=N_{p-1}+1}^{N_p}[\overline{e}_i(1)\alpha(t_i)]^2}}$$

Enright et al. [13] use the norm

$$\max_{N_p+1\leq i\leq N_{p+1}} \{\max_{\theta\in[0,\theta_e]} |e_i(\theta)|\}$$

where $\theta_e = 1$ or $\theta_e = 2$ in the case of CERK methods. We extend this idea, and use the norm

$$\max_{N_p+1\leq i\leq N_{p+1}} \{\max_{\theta\in[0,\theta_e]} |e_i(\theta)|\} + \max_{N_{p-1}+1\leq i\leq N_p} \{\max_{\theta\in[0,\theta_e]} |\overline{e}_i(\theta)|\}$$

where again $\theta_e = 1$ or $\theta_e = 2$.

Since we are dealing with polynomials, we warn against using the continuous extension outside the domain $\theta \in [0,1]$. Almost all interpolants introduce large errors in $\theta \in [1,2]$. However, Enright et al. [13] point out that in some applications (e.g. problems with discontinuities or delay differential equations) we might need to consider the error in the interval $\theta \in [0,2]$.

Owren and Zennaro [33] have pointed out that several numerical investigations have indicated that the vector of error polynomials tends to have one dominating component. This is the polynomial corresponding to the tree $[_p\tau]_p$. We have not found out if this also is the case for Nyström methods, but it is very likely that it is. In addition, Owren and Zennaro [33] point out that these polynomials turn out to be independent or only weakly dependent on some of the free parameters.

3.6 General Runge-Kutta-Nyström Methods

Before we start the work on finding the maximum order attainable for a method with a given number of stages, we have at least an upper bound on the order in the case of Runge-Kutta-Nyström methods.

Remark 3.1 *A general Runge-Kutta-Nyström method cannot attain order greater than $p = s$, the number of stages.*

Verification: An explicit Runge-Kutta method attains at most order $p = s$, and a general Runge-Kutta-Nyström method can be derived from a corresponding Runge-Kutta method. The order can not be higher if the Runge-Kutta method is rewritten in another way, and the remark follows.

□

4 On the Addition of new Stages

In this section, we follow the work by Owren [31]. The purpose is to extend the theory to continuous Nyström methods. A handy way of determining the minimum number of stages needed to obtain a given order for CERK methods is known (see [31]), but the corresponding theory for continuous Nyström methods has not been developed before.

Definition 4.1 (s^*) *We define s^* as the number of distinct values of the numerical coefficients c_i, $i = 1, \ldots, s$.*

We obviously have that $s^* \leq s$.

Theorem 4.1 *The polynomials $b_i'(\theta)$, $i = 1, \ldots, s$, span the whole space Π_{d-1} of polynomials of degree less or equal to $d-1$. At least $d-1$ polynomials among the $\overline{b}_i'(\theta)$, $i = 1, \ldots, s$, are linearly independent, but they can not be characterized in the same way as the $b_i'(\theta)$'s since they do not involve the zeroth degree polynomial.*

Proof: For every $r \geq 1$, there exists an elementary weight of the form (we define that if $c_{i^*} = 0$, then $c_{i^*}^0 := 1$)

$$\sum_{i=1}^{s} b_i'(\theta) c_i^{r-1} \qquad \text{and} \qquad \sum_{i=1}^{s} \overline{b}_i'(\theta) c_i^{r-1}$$

such that

$$\sum_{i=1}^{s} b_i'(\theta) c_i^{r-1} = \theta^{r-1}, \qquad 1 \leq r \leq d, \tag{24}$$

and

$$\sum_{i=1}^{s} \overline{b}_i'(\theta) c_i^{r-1} = \frac{\theta^r}{r}, \qquad 1 \leq r \leq d-1 \tag{25}$$

It is clear that the matrix $C := [c_i^{r-1}]_{i=1,r=1}^{s,d}$ satisfies

$$\operatorname{rank}(C) = \min\{s^*, d\}$$

and that $\overline{C} := [c_i^{r-1}]_{i=1,r=1}^{s,d-1}$ satisfies

$$\operatorname{rank}(\overline{C}) = \min\{s^*, d-1\}$$

We consider the matrices $B := [[b_i'(\theta_j)]^T]_{i=1,j=1}^{d,s}$ and $\Theta := [\theta_j^{r-1}]_{r=1,j=1}^{d,d}$ built up from d distinct values $\theta_j,\ 0 \leq \theta_j \leq 1$ $(0^0 := 1)$, and the matrices $\overline{B} := [[\overline{b}_i'(\theta_j)]^T]_{i=1,j=1}^{d-1,s}$ and $\overline{\Theta} := [\overline{\theta}_j^r/r]_{r=1,j=1}^{d-1,d-1}$ built up from $d-1$ distinct values $\overline{\theta}_j,\ 0 \leq \overline{\theta}_j \leq 1$ $(0^0 := 1)$, so that $\overline{\Theta}$ has full rank.

We have

$$\operatorname{rank}(B) \leq d, \qquad \operatorname{rank}(\Theta) = d$$

and

$$\operatorname{rank}(\overline{B}) \leq d-1, \qquad \operatorname{rank}(\overline{\Theta}) = d-1$$

From (24) and (25), we get

$$BC = \Theta \qquad \text{and} \qquad \overline{B}\,\overline{C} = \overline{\Theta}$$

and it follows that

$$\begin{aligned} d &\leq \min\{\operatorname{rank}(C), \operatorname{rank}(B)\} \\ &= \min\{\min\{s^*, d\}, \operatorname{rank}(B)\} \end{aligned}$$

and we obviously have that

$$d \leq s^* \qquad \text{and} \qquad \operatorname{rank}(B) = d$$

In the same way,

$$\begin{aligned} d-1 &\leq \min\{\operatorname{rank}(\overline{C}), \operatorname{rank}(\overline{B})\} \\ &= \min\{\min\{s^*, d-1\}, \operatorname{rank}(\overline{B})\} \end{aligned}$$

and hence

$$d \leq s^* \ \text{(again)} \qquad \text{and} \qquad \operatorname{rank}(\overline{B}) = d-1$$

$\operatorname{rank}(B) = d$ states that at least d polynomials among the $b_i'(\theta)$'s are linearly independent. Since they all have degree less or equal to $d-1$, they span the whole space Π_{d-1}. In the same way, $\operatorname{rank}(\overline{B}) = d-1$ implies that at least $d-1$ polynomials among the $\overline{b}_i'(\theta)$'s are linearly independent. But since they do not involve the constant polynomial, we can not characterize these polynomials as we did for the $b_i(\theta)$'s. $\square$

In order to fulfill Definition 3.1, it is necessary that the degree d of the polynomials $b_i(\theta)$ satisfy $d \geq p$ (just look at the Taylor expansion). However, if $d > p$, approximate solutions can be obtained whose derivatives are unbounded as $h \to 0$ (we may get to zero or negative order and still have polynomials left, see [28]). In accordance with Owren [31], we always choose $d = p$, so that the polynomials $b_i(\theta)$ span the space Π_{p-1} of polynomials of degree $p-1$.

We now put

$$z_j(\theta) := b_j'(\theta) \qquad \text{and} \qquad \overline{z}_j(\theta) := \overline{b}_j'(\theta), \qquad j = 1, \ldots, s \tag{26}$$

This is because of the requirements $b_i(0) = \overline{b}_i(0) = 0$, $i = 1, \ldots, s$. If we did not work with the derivatives, we would have to impose these restrictions explicitly. In this case, we integrate afterwards with suitable bounds.

By differentiating (19) we get

$$\sum_{j=1}^{s} \overline{z}_j(\theta)\Phi_j(t) = \frac{\theta^{\rho(t)}}{\gamma(t)} \quad \text{for all N-trees, } t, \text{ with } \rho(t) \le p-1, \tag{27}$$

and

$$\sum_{j=1}^{s} z_j(\theta)\Phi_j(t) = \frac{\rho(t)\theta^{\rho(t)-1}}{\gamma(t)} \quad \text{for all N-trees, } t, \text{ with } \rho(t) \le p, \tag{28}$$

For each $r \ge 1$, let n_r be the number of trees such that $\rho(t) = r$. In the rest of this section, we will not impose this restriction. We also use the abbreviation

$$N'_k = \sum_{r=1}^{k} n_r$$

A continuous Nyström method of order p must then satisfy N_p conditions (27) and (28), where

$$\begin{aligned} N_p &= N'_p + N'_{p-1} \\ &= n_p + 2\sum_{r=1}^{p-1} n_r \end{aligned}$$

Table 1 shows the N_p's, $p = 1, \ldots, 6$, for general and special Nyström trees. However, if we apply some simplifying assumptions, e.g.

$$c_i = \sum_{j=1}^{s} a_{ij}, \qquad i = 1, \ldots, s, \tag{29}$$

and

$$\frac{c_i^2}{2} = \sum_{j=1}^{s} \overline{a}_{ij}, \qquad i = 1, \ldots, s, \tag{30}$$

the number of conditions to be satisfied are significantly reduced, as shown in the same table.

In general, we can number the N'_k trees t increasingly in terms of $\rho(t)$, such that $\rho(t_i) > \rho(t_j)$ only if $i > j$. We now rewrite the conditions (27) and (28) as

$$\sum_{j=1}^{s} \phi_{ij}\overline{z}_j(\theta) = \frac{\theta^{\rho(t_i)}}{\gamma(t_i)}, \qquad i = 1, \ldots, N'_{p-1}, \tag{31}$$

and

$$\sum_{j=1}^{s} \phi_{ij} z_j(\theta) = \frac{\rho(t_i)\theta^{\rho(t_i)-1}}{\gamma(t_i)}, \qquad i = 1, \ldots, N'_p, \tag{32}$$

where $\phi_{ij} = \Phi_j(t_i)$. By writing

$$\overline{z}_j(\theta) = \sum_{k=1}^{p-1} \overline{z}_{jk}\theta^k \qquad \text{and} \qquad z_j(\theta) = \sum_{k=0}^{p-1} z_{jk}\theta^k, \tag{33}$$

	No simplifying assumptions applied						Simplifying assumptions applied: (29) and (30)					
Order	GN-trees			SN-trees			GN-trees			SN-trees		
p	n_p	N'_p	N_p	n_p	N'_p	N_p	n_p	N'_p	N_p	n_p	N'_p	N_p
1	1	1	1	1	1	1	1	1	1	1	1	1
2	2	3	4	1	2	3	1	2	3	1	2	3
3	6	9	12	2	4	6	2	4	6	1	3	5
4	18	27	36	3	7	11	5	9	13	2	5	8
5	60	87	114	6	13	20	13	22	31	3	8	13
6	204	291	378	10	23	36	34	56	78	5	13	21

Table 1: The N_p's, $p = 1, \ldots, 6$, for general and special Nyström trees, with and without simplifying assumptions applied.

and

$$\frac{\theta^{\rho(t_i)}}{\gamma(t_i)} = \sum_{\ell=1}^{p-1} \overline{q}_{i\ell}\theta^{\ell} \qquad \text{and} \qquad \frac{\rho(t_i)\theta^{\rho(t_i)-1}}{\gamma(t_i)} = \sum_{\ell=0}^{p-1} q_{i\ell}\theta^{\ell}, \tag{34}$$

and by defining

- the $N'_p \times s$ matrix $\Phi_Z := ((\phi_{ij}))$,
- the $N'_{p-1} \times s$ matrix $\Phi_{\overline{Z}} := ((\phi_{ij}))$,
- the $s \times p$ matrix $Z := ((z_{jk}))$,
- the $s \times (p-1)$ matrix $\overline{Z} := ((\overline{z}_{jk}))$,
- the $N'_p \times p$ matrix $Q := ((q_{i\ell}))$, and
- the $N'_{p-1} \times (p-1)$ matrix $\overline{Q} := ((\overline{q}_{i\ell}))$,

we get

$$\Phi_Z Z = Q, \qquad \text{and} \qquad \Phi_{\overline{Z}}\overline{Z} = \overline{Q} \tag{35}$$

Corollary 4.1 *The parameters $q_{i\ell}$ and $\overline{q}_{i\ell}$ satisfy*

$$\begin{aligned} q_{i,\rho(t_i)-1} &= \frac{\rho(t_i)}{\gamma(t_i)}, \qquad q_{i\ell} = 0 \ \forall \ \ell \neq \rho(t_i) - 1 \\ \overline{q}_{i,\rho(t_i)} &= \frac{1}{\gamma(t_i)}, \qquad \overline{q}_{i\ell} = 0 \ \forall \ \ell \neq \rho(t_i) \end{aligned}$$

Proof: The corollary follows trivially from (34). □

Following Owren [31], we introduce the following applications.

Definition 4.2 (Applications to GN-methods) *In the case of GN-methods, we define*

$$F_p : \bigcup_{s\geq 1}[\mathcal{L}(R^s,R^s)\times\mathcal{L}(R^s,R^s)] \to \bigcup_{s\geq 1}\mathcal{L}(R^s,R^{N'_p}) \quad \textit{such that} \quad F_p(A,\overline{A}) := \Phi_Z,$$

$$\overline{F}_p : \bigcup_{s\geq 1}[\mathcal{L}(R^s,R^s)\times\mathcal{L}(R^s,R^s)] \to \bigcup_{s\geq 1}\mathcal{L}(R^s,R^{N'_{p-1}}) \quad \textit{such that} \quad \overline{F}_p(A,\overline{A}) := \Phi_{\overline{Z}},$$

and

$$G_p : \bigcup_{s\geq 1}[\mathcal{L}(R^s,R^s)\times\mathcal{L}(R^s,R^s)] \to \bigcup_{s\geq 1}\mathcal{L}(R^{s+p},R^{N'_p})$$
$$\textit{such that} \qquad G_p(A,\overline{A}) := \Phi_Z \mid Q,$$

$$\overline{G}_p : \bigcup_{s\geq 1}[\mathcal{L}(R^s,R^s)\times\mathcal{L}(R^s,R^s)] \to \bigcup_{s\geq 1}\mathcal{L}(R^{s+p-1},R^{N'_{p-1}})$$
$$\textit{such that} \qquad \overline{G}_p(A,\overline{A}) := \Phi_{\overline{Z}} \mid \overline{Q}$$

where $\Phi_Z \mid Q$ *is the* $N'_p \times (s+p)$ *matrix obtained by attaching the rows of* Q *to the rows of* Φ_Z*, and* $\Phi_{\overline{Z}} \mid \overline{Q}$ *is the* $N'_{p-1}\times(s+p-1)$ *matrix obtained by attaching the rows of* $\overline{Q}$ *to the rows of* $\Phi_{\overline{Z}}$*.*

Definition 4.3 (Applications to SN-methods) *In the case of SN-methods, we define*

$$F_p : \bigcup_{s\geq 1}\mathcal{L}(R^s,R^s) \to \bigcup_{s\geq 1}\mathcal{L}(R^s,R^{N'_p}) \quad \textit{such that} \quad F_p(A) := \Phi_Z,$$

$$\overline{F}_p : \bigcup_{s\geq 1}\mathcal{L}(R^s,R^s) \to \bigcup_{s\geq 1}\mathcal{L}(R^s,R^{N'_{p-1}}) \quad \textit{such that} \quad \overline{F}_p(A) := \Phi_{\overline{Z}},$$

and

$$G_p : \bigcup_{s\geq 1}\mathcal{L}(R^s,R^s) \to \bigcup_{s\geq 1}\mathcal{L}(R^{s+p},R^{N'_p}) \qquad \textit{such that} \qquad G_p(A) := \Phi_Z \mid Q,$$

$$\overline{G}_p : \bigcup_{s\geq 1}\mathcal{L}(R^s,R^s) \to \bigcup_{s\geq 1}\mathcal{L}(R^{s+p-1},R^{N'_{p-1}}) \qquad \textit{such that} \qquad \overline{G}_p(A) := \Phi_{\overline{Z}} \mid \overline{Q}$$

where $\Phi_Z \mid Q$ *is the* $N'_p \times (s+p)$ *matrix obtained by attaching the rows of* Q *to the rows of* Φ_Z*, and* $\Phi_{\overline{Z}} \mid \overline{Q}$ *is the* $N'_{p-1}\times(s+p-1)$ *matrix obtained by attaching the rows of* $\overline{Q}$ *to the rows of* $\Phi_{\overline{Z}}$*.*

We will not distinguish more between these applications than using different numbers of arguments. It should be clear from the context whether we are talking about GN- or SN-methods.

Theorem 4.2 (GN) *Strictly lower triangular* $s\times s$ *matrices* A *and* $\overline{A}$ *define an* s*-stage continuous Nyström method of order* p *if and only if*

$$rank(F_p(A,\overline{A})) = rank(G_p(A,\overline{A}))$$

and

$$rank(\overline{F}_p(A,\overline{A})) = rank(\overline{G}_p(A,\overline{A}))$$

Proof: Any continuous Nyström method of order p, (35), satisfies

$$\text{rank}\,(F_p(A,\overline{A})) = \text{rank}\,(G_p(A,\overline{A})) \qquad \text{and} \qquad \text{rank}\,(\overline{F}_p(A,\overline{A})) = \text{rank}\,(\overline{G}_p(A,\overline{A})) \tag{36}$$

On the other hand, if $s \times s$ matrices A and $\overline{A}$ are such that (36) is satisfied, then the systems

$$F_p(A,\overline{A})Z = Q \qquad \text{and} \qquad F_p(A,\overline{A})\overline{Z} = \overline{Q}$$

have at least one solution Z and one solution $\overline{Z}$. By (26) and (33), the two matrices Z and $\overline{Z}$ uniquely define s polynomials $b_i(\theta)$, $i = 1, \ldots, s$, and s polynomials $\overline{b}_i(\theta)$, $i = 1, \ldots, s$, of degree less or equal to p such that $b_i(0) = \overline{b}_i(0) = 0$, and hence, the matrices A and $\overline{A}$ define the stages of some continuous Nyström method of order p. □

Theorem 4.3 (SN) *A strictly lower triangular $s \times s$ matrix A defines an s-stage continuous Nyström method of order p if and only if*

$$rank(F_p(A)) = rank(G_p(A))$$

and

$$rank(\overline{F}_p(A)) = rank(\overline{G}_p(A))$$

Proof: The proof follows in the same way as for Theorem 4.2. □

A question arising from this is how many new stages one has to implement into the continuous extension in order to retain the same order as in the discrete case.

Theorem 4.4 (GN) *Let the $s \times s$ matrices A and $\overline{A}$ define a discrete explicit Nyström method of order p. Consider a continuous extension of this method with $\widehat{s}$ stages and uniform order p. Then*

$$\widehat{s} - s \geq max\{\delta_1, \delta_2\}$$

where $\delta_1 = rank(G_p(A,\overline{A})) - rank(F_p(A,\overline{A}))$ and $\delta_2 = rank(\overline{G}_p(A,\overline{A})) - rank(\overline{F}_p(A,\overline{A}))$.

Proof: Let the $\widehat{s} \times \widehat{s}$ matrices $\widehat{A}$ and $\widehat{\overline{A}}$ define the extended method. We have that

$$\text{rank}(F_p(\widehat{A},\widehat{\overline{A}})) - \text{rank}(F_p(A,\overline{A})) \leq \widehat{s} - s,$$

since the first s columns of $F_p(\widehat{A},\widehat{\overline{A}})$ and $F_p(A,\overline{A})$ are identical. In the same way,

$$\text{rank}(\overline{F}_p(\widehat{A},\widehat{\overline{A}})) - \text{rank}(\overline{F}_p(A,\overline{A})) \leq \widehat{s} - s.$$

On the other hand, the $\widehat{s} - s$ additional stages can not decrease the rank of $G_p(A,\overline{A})$ or $\overline{G}_p(A,\overline{A})$. This implies that we must have

$$\text{rank}(G_p(\widehat{A},\widehat{\overline{A}})) \geq \text{rank}(G_p(A,\overline{A})) \qquad \text{and} \qquad \text{rank}(\overline{G}_p(\widehat{A},\widehat{\overline{A}})) \geq \text{rank}(\overline{G}_p(A,\overline{A})).$$

Using Theorem 4.2, we have that

$$\begin{aligned}
\delta_1 &= \text{rank}(G_p(A,\overline{A})) - \text{rank}(F_p(A,\overline{A})) \\
&\leq \text{rank}(G_p(\widehat{A},\widehat{\overline{A}})) - \text{rank}(F_p(A,\overline{A})) \\
&= \text{rank}(F_p(\widehat{A},\widehat{\overline{A}})) - \text{rank}(F_p(A,\overline{A})) \\
&\leq \widehat{s} - s
\end{aligned}$$

and

$$
\begin{aligned}
\delta_2 &= \operatorname{rank}(\overline{G}_p(A,\overline{A})) - \operatorname{rank}(\overline{F}_p(A,\overline{A})) \\
&\leq \operatorname{rank}(\overline{G}_p(\widehat{A},\widehat{\overline{A}})) - \operatorname{rank}(\overline{F}_p(A,\overline{A})) \\
&= \operatorname{rank}(\overline{F}_p(\widehat{A},\widehat{\overline{A}})) - \operatorname{rank}(\overline{F}_p(A,\overline{A})) \\
&\leq \widehat{s} - s
\end{aligned}
$$

□

Theorem 4.5 (SN) *Let the $s \times s$ matrix A define a discrete explicit Nyström method of order p. Consider a continuous extension of this method with $\widehat{s}$ stages and uniform order p. Then*

$$\widehat{s} - s \geq max\{\delta_1, \delta_2\}$$

where $\delta_1 = rank(G_p(A)) - rank(F_p(A))$ and $\delta_2 = rank(\overline{G}_p(A)) - rank(\overline{F}_p(A))$.

Proof: The proof follows in the same way as for Theorem 4.4. □

In the following discussion, we will only be interested in matrices belonging to the set $\mathcal{M}^p$, i.e., matrices A that fulfills Theorem 4.2 or Theorem 4.3 (see Owren [31]):

Definition 4.4 ($\mathcal{M}^p$) *In the case of GN-methods, we define $\mathcal{M}^p$ to be the set*

$$\mathcal{M}^p := \{(A,\overline{A}\,) \in \textstyle\bigcup_{s\geq 1}[\mathcal{L}(R^s,R^s)\times\mathcal{L}(R^s,R^s)] \;\;|\;\; \begin{array}{l} A \text{ and } \overline{A} \text{ are strictly lower triangular,} \\ rank(F_p(A,\overline{A})) = rank(G_p(A,\overline{A})) \text{ and} \\ rank(\overline{F}_p(A,\overline{A})) = rank(\overline{G}_p(A,\overline{A}))\ \}, \end{array}$$

and in the case of SN-methods, we define $\mathcal{M}^p$ to be the set

$$\mathcal{M}^p := \{A \in \textstyle\bigcup_{s\geq 1}\mathcal{L}(R^s,R^s) \;\;|\;\; \begin{array}{l} A \text{ is strictly lower triangular,} \\ rank(F_p(A)) = rank(G_p(A)) \text{ and} \\ rank(\overline{F}_p(A)) = rank(\overline{G}_p(A))\ \} \end{array}$$

Definition 4.5 (Dimension of L) *We say that s is the dimension of L if L is an $s \times s$ matrix, and we write*

$$\dim(L) = s$$

In general, we have

$$\dim(\overline{A}) = \dim(A) \geq \operatorname{rank}(F_p(A,\overline{A}))$$

and

$$\dim(\overline{A}) = \dim(A) \geq \operatorname{rank}(\overline{F}_p(A,\overline{A}))$$

Following Owren [31], we define the set of p-minimal matrices.

Definition 4.6 (p-minimal matrices, [31]) *In the case of GN-methods, we define $A, \overline{A} \in \mathcal{M}^p$ to be p-minimal if*

$$\dim(\overline{A}) = \dim(A) = rank(F_p(A, \overline{A}))$$

and in the case of SN-methods, we define $A \in \mathcal{M}^p$ to be p-minimal if

$$\dim(A) = rank(F_p(A))$$

Definition 4.7 *In the case of GN-methods, we define $\mathcal{M}_*^p$ to be the set*

$$\mathcal{M}_*^p := \{A, \overline{A} \in \mathcal{M}^p \mid A \textit{ and } \overline{A} \textit{ are p-minimal}\},$$

and in the case of SN-methods,

$$\mathcal{M}_*^p := \{A \in \mathcal{M}^p \mid A \textit{ is p-minimal}\}$$

Theorem 4.6 (GN) *If $A, \overline{A} \in \mathcal{M}_*^p$, then none of them can have two identical rows. In addition,*

$$\dim(\overline{A}) = \dim(A) \leq N_p'$$

Proof: Two identical rows in A or $\overline{A}$ would imply two identical columns in $F_p(A, \overline{A})$ and $\overline{F}_p(A, \overline{A})$. This would decrease the rank. Part two follows from the fact that $\text{rank}(F_p(A, \overline{A})) \leq N_p'$. □

Theorem 4.7 (SN) *If $A \in \mathcal{M}_*^p$, then it cannot have two identical rows. In addition,*

$$dim(A) \leq N_p'$$

Proof: The proof follows in the same way as for Theorem 4.6. □

Corollary 4.2 *If $A, \overline{A} \in \mathcal{M}_*^p$ and we assume that the simplifying conditions (29) and (30) have been imposed, we must have $c_2 \neq 0$. With assumption (30), the same is true for SN-methods.*

Proof: The corollary follows directly from Theorem 4.6, since $c_2 = 0$ would make the first two rows in both A and $\overline{A}$ identical. □

When working with SN-methods, the following theorem allows us to restrict ourselves to p-minimal matrices, as in the case of CERK methods.

Theorem 4.8 (SN) *Let $A \in \mathcal{M}^p$ be such that*

$$\rho := rank(F_p(A)) < \dim(A)$$

Then there exists a matrix $A^* \in \mathcal{M}_*^p$ such that $\dim(A^*) = \rho$.

Proof: See Owren [31]. We prove that there exists a matrix $A' \in \mathcal{M}^p$ such that $\dim(A') = \dim(A) - 1$ and $\text{rank}\,(F_p(A)) = \rho$. If this matrix A' is not the one we are seeking, we can apply the same procedure $(\dim(A) - \rho)$ times in order to prove the theorem.

We put $\Phi = F_p(A)$ and say that Φ is of dimension $N_p \times s$. We also put $s := \dim(A)$.

The rest of the proof follows in the same way as the proof of Theorem 2.5 in Owren [31].

□

5 Order Barriers

In this section, we shall take a closer look at the order conditions associated with continuous special Nyström methods.

We want to determine lower bounds for the numbers

$$\mathrm{CSNEN}\,(p) := \min_{m(s)\in M_p} s$$

where $m(s)$ is a continuous special Nyström method with s stages, and M_p is the set of all continuous special Nyström methods of order p. The numbers CSNEN(p) are similar to the Butcher barriers EN(p) for the discrete case for Runge-Kutta methods, and also similar to the numbers CEN(p) presented by Owren [31] for the continuous case of explicit Runge-Kutta methods.

Corollary 5.1 *The set $\mathcal{M}_*^p$ is non-empty for all $p > 1$, and the minimum number of stages CSNEN(p) required for a continuous Nyström method of order p is*

$$CSNEN(p) = \min_{A\in\mathcal{M}_*^p} \dim(A)$$

Proof: The set $\mathcal{M}_*^p$ is obviously non-empty by Theorem 4.8, and the lower bound on the numbers CSNEN(p) is a direct consequence of the same theorem. □

Corollary 5.2 *If $A \in \mathcal{M}^p$ and $A \notin \mathcal{M}_*^p$, then $\dim(A) > CSNEN(p)$.* □

Definition 5.1 (Primary conditions) *We call*

(a) $\sum_{j=1}^{s} z_j(\theta)c_j^{r-1} = \theta^{r-1}, \qquad r = 1, \ldots, p,$

(b) $\sum_{j=1}^{s} \overline{z}_j(\theta)c_j^{r-1} = \frac{\theta^r}{r}, \qquad r = 1, \ldots, p-1,$

the primary order conditions.

The right hand side of **(a)** is independent of $\rho(t_r)$ and $\gamma(t_r)$ since

$$\rho(t_r) = \gamma(t_r), \qquad r = 1, \ldots, p,$$

corresponding to the trees shown in Figure 1. The trees corresponding to all the primary conditions are defined recursively by

$$\tau^r := [\tau, \tau^{r-2}],$$

where $\tau := [\ ]$ and $\tau^2 := [\tau]$.

The *secondary conditions* follows as the rest of the order conditions:

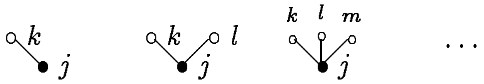

Figure 1: The trees corresponding to the primary conditions

Definition 5.2 (Secondary conditions) *The order conditions remaining when removing the primary conditions from the total order conditions, are called the secondary order conditions.*

Throughout the rest of this section, we assume $c_1 = 0$, and since the matrices A are strictly lower triangular, the secondary conditions do not explicitly contain the polynomials $z_1(\theta)$, $z_2(\theta)$, $\overline{z}_1(\theta)$ or $\overline{z}_2(\theta)$, since they all satisfy $\phi_{i1} = \phi_{i2} = \overline{\phi}_{i1} = \overline{\phi}_{i2} = 0$.

Corollary 5.3 *All the secondary conditions correspond to trees of order $r \geq 3$, and this implies that $q_{i0} = q_{i1} = \overline{q}_{i1} = \overline{q}_{i2} = 0$ in (34).*

Proof: By equating powers of θ and recognizing which powers have to vanish, the result follows.

□

We follow Owren [31], and define the following equivalence relation on the set of indices $\{1, \ldots, s\}$ for an $s \times s$ matrix $A \in \mathcal{M}_*^p$ with $p \geq 3$:

Definition 5.3 (Owren [31]) *We define, for an $s \times s$ matrix $A \in \mathcal{M}_*^p$ with $p \geq 3$, the equivalence relation on the set of indices $\{1, \ldots, s\}$*

$$i \equiv j \qquad \text{if and only if} \qquad c_i = c_j.$$

There are s^* equivalence classes $S_1, \ldots, S_{s^*}$, and we assume that $1 \in S_1$, that is, $c_i = 0 \Leftrightarrow i \in S_1$. We also assume that $2 \in S_2$ (see Corollary 4.2).

Definition 5.4 (Good index set, [31]) *For an $s \times s$ matrix $A \in \mathcal{M}_*^p$ with $p \geq 3$ we shall call a* **good index set** *either the empty set $\emptyset$ or any non-empty subset of $\{3, \ldots, s\}$ which elements do not belong to more than $p - 3$ equivalence classes among $S_3, \ldots, S_{s^*}$.*

From this definition, we get the following result.

Corollary 5.4 ([31]) *If $p = 3$, then $S \subset S_1 \cup S_2$ for any good index set S.* □

Corollary 5.5 *The equivalence classes $S_1, \ldots, S_{s^*}$ are all non-empty.*

Proof: Since there are exactly s^* different c_i's, the indices of these will have to go into distinct equivalence classes. Hence, there will be at least one element in each set. □

Example 5.1 (Good index sets) *Assume $p = 6$ and $s = s^* = 7$. This implies that elements can not belong to more than 3 equivalence classes among $S_3, \dots, S_7$ and still constitute a good index set. Each equivalence class must include exactly one element, i.e.,*

$$S_3 = \{3\}, \qquad S_4 = \{4\}, \qquad S_5 = \{5\}, \qquad S_6 = \{6\}, \qquad S_7 = \{7\}$$

Then

$$S = \{3, 4, 7\} \qquad \text{or} \qquad S = \{\emptyset\}$$

are examples of good index sets while

$$S = \{3, 4, 5, 7\}$$

is an example of a not good index set.

In the case of SN-methods, we do not consider the $\overline{z}_j(\theta)$'s in the rest of this section. This is because we are interested in the minimum number of stages necessary for a method of a given order, and since there are most conditions to be satisfied for the $z_j(\theta)$'s, $N'_p > N'_{p-1}$, these conditions will be the limiting ones.

Lemma 5.1 ([31]) *Let $A \in \mathcal{M}_*^p$ with $p \geq 3$ and let S be a good index set for A. Then, in the set of polynomials*

$$\{z_j(\theta) \mid j \geq 3,\, j \notin S\}$$

there exists at least one, say $z_J(\theta)$, such that $z_{J1} \neq 0$.

Proof: By (12) to (14), it is necessary that the number s^* of distinct c_i's satisfies

$$s^* \geq p,$$

so $s^* - (p - 3 + 2)$ equivalence classes have to stay outside S. If $s^* = p$, at least $s^* - (p-1) = 1$ non-empty equivalence class has to be left, i.e., the two sets of polynomials are non-empty.

We choose an index $j_k \in S_k$ for any $k = 3, \dots, s^*$, and assume, without restrictions, that $S \subset S_1 \cup S_2 \cup \dots \cup S_r$ for some $r \leq p - 1 \leq s^* - 1$. The polynomials $z_j(\theta)$, $j = 1, \dots, s$, satisfy the primary conditions for any polynomial $\pi(\theta) \in \Pi_{p-1}$. We put

$$\pi(\theta) = \sum_{i=1}^{p-1} \alpha_i \theta^i$$

Inserting the expression for θ^i, we obtain

$$\begin{aligned}
\pi(\theta) &= \sum_{i=1}^{p-1} \alpha_i \sum_{j=1}^{s} z_j(\theta) c_j^i \\
&= \sum_{j=1}^{s} z_j(\theta) \sum_{i=1}^{p-1} \alpha_i c_j^i \\
&= \sum_{j=1}^{s} z_j(\theta) \pi(c_j) \\
&= \sum_{k=1}^{s^*} \pi(c_{j_k}) \sum_{j \in S_k} z_j(\theta) \qquad (37)
\end{aligned}$$

We define $\pi(\theta) := \theta(\theta - c_2)(\theta - c_{j_3}) \cdots (\theta - c_{j_r})$, and get $\pi(c_j) = 0$ for all $j \in S_1 \cup S_2 \cup \cdots \cup S_r$, so that (37) becomes

$$\pi(\theta) = \sum_{k=r+1}^{s^*} \pi(c_{j_k}) \sum_{j \in S_k} z_j(\theta)$$

The coefficient of θ in $\pi(\theta)$ is now $(-1)^{r-1} c_2 c_{j_3} \cdots c_{j_r} \neq 0$. We know that $\pi(c_{j_k}) \neq 0$ for all $k = r+1, \ldots, s^*$, and hence, the proof is complete. □

Definition 5.5 *We say that N (≥ 1) conditions (31) or (32) are linearly independent iff the corresponding N rows of the matrix $G_p(A)$ or $\overline{G}_p(A)$, respectively, are linearly independent.*

The next lemma follows immediately.

Lemma 5.2 ([31]) *Let $A \in \mathcal{M}^p$ and let N conditions (32) be linearly independent. Then they explicitly involve N polynomials $z_j(\theta)$.*

Proof: Since rank $(F_p(A))$ = rank $(G_p(A))$, if N rows of the matrix $G_p(A)$ are linearly independent then the same N rows of the matrix $F_p(A)$ must be linearly independent too. This is a sufficient observation in order to verify the lemma. □

The next theorem gives a lower bound on the numbers $CSNEN(p)$, and take the same form the bound for CEN(p) for the CERK methods.

Theorem 5.1 (CSNEN(p),[31]) *Let $A \in \mathcal{M}^p_*$ with $p \geq 3$, and let N secondary conditions for $z_j(\theta)$ be linearly independent. Let S be the set formed by the indices $j \geq 3$ of the polynomials $z_j(\theta)$ which are not explicitly involved by these N conditions (possibly $S = \emptyset$). Then*

$$\dim(A) \geq N + \mu + 2,$$

where μ is the cardinality of S. Moreover, if S is a good index set for A, then

$$\dim(A) \geq N + \mu + 3.$$

Proof: The N conditions are secondary, i.e., by the comment to Definition 5.2, they do not involve $z_1(\theta)$ or $z_2(\theta)$. By Lemma 5.2 we have that

$$\dim(A) \geq N + \mu + 2$$

Now, assume that S is a good index set for A and that $\dim(A) = N + \mu + 2$. Then there are exactly N polynomials $z_j(\theta)$, the only existing ones with $j \geq 3$ and $j \notin S$, which are involved by these N conditions. Consider the $N \times N$ matrix Φ^*, obtained by removing the $\mu + 2$ elements corresponding to the missing polynomials $z_j(\theta)$ in each of these N rows of $F_p(A)$. This matrix is non-singular, since we, from the original matrix, picked out N linearly independent conditions. By removing columns from this matrix Φ^*, we can not make it singular. Solving the new system

$$\Phi^* Z^* = Q^*$$

where Z^* and Q^* are defined by the N conditions, yields $z_{j1} = 0$ (and also $z_{j0} = 0$) for all $j \geq 3$, $j \notin S$, which contradicts Lemma 5.1. □

This result is the same as the one obtained in the case of CERK methods. The reason is the similarity between the CERK methods and the SN-methods.

6 Continuous Nyström Methods with the Stage Reuse Property

In this section, we consider the FSAL property. The reason why we want to implement this property in our methods is that we want to save some function evaluations.

In the case of GN-methods, the formula for computing the stage values takes the following form:

$$k_i = f(x_n + c_i h, y_n + c_i h y'_n + h^2 \sum_{j=1}^{s} \overline{a}_{ij} k_j, y'_n + h \sum_{j=1}^{s} a_{ij} k_j)$$

In order to implement stage reuse, we require that

$$k_s = f(x_{n+1}, y_{n+1}, y'_{n+1}),$$

i.e., that $c_s = 1$, $\overline{b}_j(1) = \overline{a}_{sj}$, $j = 1, \ldots, s$, and $b_j(1) = a_{sj}$, $j = 1, \ldots, s$.

In the same way, when considering SN-methods, the formula for computing the stage values takes the form:

$$k_i = f(x_n + c_i h, y_n + c_i h y'_n + h^2 \sum_{j=1}^{s} \overline{a}_{ij} k_j)$$

We require that

$$k_s = f(x_{n+1}, y_{n+1}),$$

i.e., that $c_s = 1$ and $\overline{b}_j(1) = \overline{a}_{sj}$, $j = 1, \ldots, s$.

We thus end up with the following definitions.

Definition 6.1 (Stage Reuse, GN methods) *We say that a general Nyström method implements stage reuse iff*

$$c_s = 1, \qquad \textit{and} \qquad \left.\begin{array}{rcl} \overline{a}_{sj} & = & \overline{b}_j(1), \\ a_{sj} & = & b_j(1), \end{array}\right\} \qquad j = 1, \ldots s$$

Definition 6.2 (Stage Reuse, SN methods) *We say that a special Nyström method implements stage reuse iff*

$$c_s = 1, \qquad \textit{and} \qquad \overline{a}_{sj} = \overline{b}_j(1), \qquad j = 1, \ldots s$$

As far as possible, we should try to implement FSAL in our methods. A method with s stages effectively use only $s - 1$ function evaluations (except for the first step).

7 Symplectic Nyström Methods

In this chapter, we are concerned with Nyström methods for Hamiltonian systems of the form

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \qquad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \qquad 1 \le i \le d, \tag{38}$$

where the integer d is the number of degrees of freedom and the Hamiltonian $H = H(\mathbf{p}, \mathbf{q}) = H(p_1, \ldots, p_d, q_1, \ldots, q_d)$ is a smooth, real function defined in $\mathbb{R}^{2d}$. We say that a numerical method is symplectic if, when applied to Hamiltonian problems, it generates numerical solutions which inherit the property of symplecticness.

We recommend the book by Sanz-Serna and Calvo [37] both as an introduction and as advanced reading on symplectical numerical methods. The classical book by Arnold [2] gives a mathematical treatment of the property.

Integration methods for (38) are often based on the fact that the flow $\phi_{t,H}$ of a Hamiltonian system is a symplectic transformation (see [2]). $\phi_{t,H}$ being symplectic means that it preserves the differential 2-form

$$\omega_2(dp_0, dq_0) = dp \wedge dq = \sum_{i=1}^{d} dp_i \wedge dq_i \tag{39}$$

where $\wedge$ denotes the exterior product between two differential 1-forms. If $d = 1$, the 2-form ω_2 can be interpreted as an area in $\mathbb{R}^2$ so that a transformation being symplectic can be viewed as preservation of area (see [5]).

The next theorem by Okunbor and Skeel [30] gives the general form of a discrete, symplectic Nyström method.

Theorem 7.1 (Canonical Nyström Methods, [36]) *Assume that the coefficients of a Nyström method*

$$\begin{array}{c|cccc} 0 & & & & \\ c_2 & a_{21} & & & \\ \vdots & \vdots & \ddots & & \\ 1 & a_{s1} & \cdots & a_{s,s-1} & \\ \hline & \overline{b}_1 & \cdots & \overline{b}_{s-1} & \overline{b}_s \\ \hline & b_1 & \cdots & b_{s-1} & b_s \end{array} \tag{40}$$

satisfy the conditions

$$\begin{aligned} \overline{b}_i &= b_i(1 - c_i), \qquad & 1 \le i \le s, \\ b_i(\overline{b}_j - a_{ij}) &= b_j(\overline{b}_i - a_{ji}), \qquad & 1 \le i, j \le s \end{aligned}$$

Then the method is symplectic when applied to Hamiltonian problems (38).

Proof: See Okunbor and Skeel [30]. □

7.1 Canonical Continuous Nyström Methods

In this section we consider a Hamiltonian dynamical system

$$\dot{q} = M^{-1}p, \qquad \dot{p} = -\frac{\partial V(q)}{\partial q} = F(q), \tag{41}$$

with Hamiltonian $H(q,p) = \frac{1}{2}p^T M^{-1} p + V(q)$. If we differentiate $\dot{q}$ in (41) and substitute the expression for $\dot{p}$, we obtain

$$\ddot{q} = -M^{-1}\frac{\partial V(q)}{\partial q} = f(q) \tag{42}$$

An s-stage continuous Nyström method for (42) is given by

$$\begin{aligned} Y_i &= q_n + c_i h \dot{q}_n + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j), \qquad i = 1,\ldots,s, \\ q_{n+1} &= q_n + \theta h \dot{q}_n + h^2 \sum_{i=1}^{s} b_i(\theta) f(Y_i), \\ \dot{q}_{n+1} &= \dot{q}_n + h \sum_{i=1}^{s} \overline{b}_i(\theta) f(Y_i) \end{aligned} \tag{43}$$

We now write the continuous Nyström method for (41) as

$$\begin{aligned} Y_i^J &= q_n^J + c_i h M_{JJ}^{-1} p_n^J + h^2 \sum_{j=1}^{s} a_{ij} M_{JJ}^{-1} F^J(Y_j), \qquad i = 1,\ldots,s \\ q_{n+1}^J &= q_n^J + \theta h M_{JJ}^{-1} p_n^J + h^2 \sum_{i=1}^{s} b_i(\theta) M_{JJ}^{-1} F^J(Y_i), \\ p_{n+1}^J &= p_n^J + h \sum_{i=1}^{s} \overline{b}_i(\theta) F^J(Y_i), \end{aligned} \tag{44}$$

for $J = 1,\ldots,N$.

We want to use the preservation of the differential 2-form defined by (39), i.e., $dq_{n+1} \wedge dp_{n+1} = dq_n \wedge dp_n$, to prove the following theorem.

Theorem 7.2 *An s-stage continuous Nyström method is symplectic if*

$$\begin{aligned} \overline{b}_i(\theta) - \theta b_i(\theta) + b_i(\theta) c_i &= 0, \quad 1 \le i \le s, \\ b_i(\theta) a_{ij} - b_j(\theta) a_{ji} + \overline{b}_i(\theta) b_j(\theta) - \overline{b}_j(\theta) b_i(\theta) &= 0, \quad 1 \le i < j \le s \end{aligned} \tag{45}$$

These conditions must hold for every $\theta \in [0,1]$.

Proof: Let $k_i^J = F^J(Y_i)$. After some computation quite similar to that in Okunbor and Skeel [29], we arrive at

$$\begin{aligned} & dq_{n+1} \wedge dp_{n+1} - dq_n \wedge dp_n \\ &\quad = \sum_J (dq_{n+1}^J \wedge dp_{n+1}^J - dq_n^J \wedge dp_n^J) \\ &\quad = h^2 \sum_i [\overline{b}_i(\theta) - \theta b_i(\theta) + b_i(\theta) c_i] \sum_J M_{JJ}^{-1} dk_i^J \wedge dp_n^J \\ &\qquad + h^3 \sum \sum_{i<j} [b_i(\theta) a_{ij} - b_j(\theta) a_{ji} + \overline{b}_i(\theta) b_j(\theta) - \overline{b}_j(\theta) b_i(\theta)] \\ &\qquad\quad \sum_J M_{JJ}^{-1} dk_i^J \wedge dk_j^J \end{aligned}$$

and the theorem follows. See Marthinsen [27] for details. □

7.2 On Symplectic Dense Output

By using Theorem 7.2, we can construct a symplectic interpolant for the method

$$\begin{array}{c|cc} 0 & & \\ 1 & a_{21} & \\ \hline & \bar{b}_1(\theta) & \bar{b}_2(\theta) \\ \hline & b_1(\theta) & b_2(\theta) \end{array} \tag{46}$$

Theorem 7.3 *The continuous Nyström method (46) gives symplectic dense output if*

$$\begin{aligned} \bar{b}_1(\theta) &= a_{21}\theta \\ \bar{b}_2(\theta) &= \theta^2 - (a_{21}+1)\theta + a_{21} \\ b_1(\theta) &= a_{21} \\ b_2(\theta) &= \theta - a_{21} \end{aligned}$$

This method is only of order 1, and we can not attain greater order with this tableau.

Proof: The conditions for the method to be symplectic are in this case:

$$\begin{aligned} \bar{b}_1(\theta) - \theta b_1(\theta) &= 0 \\ \bar{b}_2(\theta) + (1-\theta)b_2(\theta) &= 0 \\ -b_2(\theta)a_{21} + \bar{b}_1(\theta)b_2(\theta) - \bar{b}_2(\theta)b_1(\theta) &= 0 \end{aligned}$$

These equations can, for instance, be solved with regards to $b_1(\theta)$ and $\bar{b}_1(\theta)$. In order to obtain expressions for the remaining weights, we impose the order one restriction. The order two conditions can not be satisfied with these weights, when requiring A independent of θ. □

The next theorem proves that we, in fact, can never make methods of this kind with higher order.

Theorem 7.4 *An s-stage, continuous, symplectic Nyström method can not be of order greater than one.*

Proof: It suffices to look at the requirements

$$\bar{b}_i(\theta) - \theta b_i(\theta) + b_i(\theta)c_i = 0, \qquad 1 \le i \le s,$$

from Theorem 7.2. They indicate that the weights $b_i(\theta)$, $i = 1, \ldots, s$, must be of one degree less than $\bar{b}_i(\theta)$, $i = 1, \ldots, s$. The continuous order conditions require both families of weights to be of the same degree, and hence, we can not satisfy other order conditions than the first one.

□

This is the same conclusion as in the case of Runge-Kutta methods or partitioned methods. We therefore consider what to do without symplectic dense output. As Amundsen [1] has noted, often the global or long time behavior of preserving the symplectic structure is considered being most important. Therefore, we might use symplectic integrators with non-symplectic interpolation and still obtain quite accurate values compared to nonsymplectic integration.

What makes the problem here, is the definition of the order of a method, see Definition 2.4. We impose a very strong condition since we require the same order for both the approximation to the solution and to the derivative of the solution. If we could relax this definition, we would be able to construct symplectic interpolants of higher orders. But, since the approximation to the derivative of the solution enters the approximation to the solution, a lower order approximation to the derivative will destroy the overall order of the method. What could be done is to define a continuous method to be of order p if $\max_{0\leq\theta\leq 1}|y(x_n+\theta h)-u(x_n+\theta h)| = \mathcal{O}(h^{p+2})$ and $\max_{0\leq\theta\leq 1}|y'(x_n+\theta h)-v(x_n+\theta h)| = \mathcal{O}(h^{p+1})$. We would then obtain the desired difference in power of θ on the two approximations. And, hence, Theorem 7.2 would not imply the order one barrier. But we will not follow this idea any further. The conservation of the symplectic structure over a long period of time is the important task when integrating Hamiltonian problems. What happens within a single step with regards to e.g. output, is not of importance, since we compute the discrete steps with a symplectic, discrete method.

Acknowledgments. We would like to thank Professor Syvert P. Nørsett and Assistant Professors Brynjulf Owren and Anne Kværnø at Department of Mathematical Sciences at the Norwegian Institute of Technology for their always supporting help and encouragement. Our advisor, Ivar Lie, at the Norwegian Defense Research Establishment has also been a great source of inspiration and help during the work with this article.

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