

Rosenbrock type methods for solving non-linear second-order in time problems

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Abstract

In this work we present a new class of methods which have been developed in order to numerically solve non-linear second-order in time problems. These methods are of Rosenbrock type, and can be seen as a generalization of these methods when they are applied to second-order in time problems which have been previously transformed into first-order in time problems.

As they follow the ideas of Runge-Kutta-Nyström methods when solving second-order in time problems, we will call them Rosenbrock-Nyström methods.

These new methods present less computational cost than implicit Runge-Kutta-Nyström ones, as the non-linear systems which arises when Runge-Kutta-Nyström methods are used are replaced with sequences of linear ones.

In this article we show the development of Rosenbrock-Nyström methods, as well as the conditions that must be satisfied to get the desired classical order (up to order four) and the main ideas in order to have stability. Besides, we will show some numerical experiments that prove the good behaviour of these new methods.

1 Preliminaries

In this work we are interested in the numerical resolution in time of non-linear second order in time problems of the form

$$\begin{cases} y''(t) &= f(t, y), & 0 \leq t \leq T < \infty, \\ y(0) &= y_0, \\ y'(0) &= v_0. \end{cases} \quad (1)$$

These problems can arise, for example, after the spatial discretization of second-order in time partial differential equations.

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When we solve a problem of this type we have several options in order to choose the numerical temporal integrator. One possibility is to choose a method specially derived to solve second-order in time problems or, in the other hand, we can previously convert the problem to a first order in time problem and then we can use a method specially designed to solve this type of problems.

If we choose the first possibility, we can use, for example, Runge-Kutta-Nyström methods (RKN methods) [?]. When we use this type of methods, we have to choose whether to use explicit or implicit methods. When we use explicit methods we can have stability problems, specially if the problem we are solving is a stiff one. On the other hand, if we choose an implicit method, we can select a method with an infinite stability interval, but by having a high computational cost [?]. This computational cost can be very high when the problem is non-linear or/and multidimensional in space. In order to avoid the high computational cost that implicit RKN methods present when multidimensional problems in space are solved, Fractional Step Runge-Kutta-Nyström methods (FSRKN methods) were developed and studied in [?]. The idea of these methods is to split the spatial operator in a suitable way so that at every intermediate stage the problem to be solved is simpler in a certain way than the original one. However, when the problem we are solving is non-linear, the computational cost can also be very high.

If we prefer to convert the problem to a first order one, then we also have several options. Runge-Kutta methods (RK methods) or Fractional Step Runge-Kutta methods (FSRK methods) are a good option if the problem we have is a linear one but they present a high computational cost when the problem we are solving is a non-linear one. In this case, a good option is to use Rosenbrock methods or Exponential-Rosenbrock type methods [?, ?]... The problem we have when we convert the original problem to a first order one is that the dimension of the problem is doubled, so the computational cost increases.

In order to avoid all the previous drawbacks when solving a problem like (??), in this paper we present a new class of methods, which we call Rosenbrock-Nyström methods. These methods avoid the non-linear systems which arises when RKN methods are used by replacing them by sequences of linear ones. Rosenbrock-Nyström methods arise in a natural way as a generalization of Rosenbrock ones when these are applied to second-order in time equations that have been previously transformed into first-order in time problems. The methods presented here differ very much from the ones that appear in [?], that are of Rosenbrock type and were created to solve second-order nonlinear systems of ordinary differential equations. We remark here three of the most important differences between the methods in [?] and our methods. The first one is that to use the methods presented in [?], we have to define $u = (y, v, t)^T$, with $v = y'(t)$ and then we have to convert the problem to a first order one in the following way:

$$u' = g(y) = \begin{pmatrix} v \\ f(t, y) \\ 1 \end{pmatrix}$$

$$u(0) = \begin{pmatrix} y_0 \\ v_0 \\ t_0 \end{pmatrix}, \quad (2)$$

while with our methods we do not need to convert the problem to a first order one. The second remark is that in [?] we have to solve two linear systems at each intermediate step, instead of the one linear system we have to solve at each intermediate step when using the methods presented here. The last one is that in the mentioned paper, function $g(y)$ and its Jacobian have to be evaluated at every intermediate stage. When using our method, we evaluate function $f(t, y)$ at every intermediate stage, but we use fixed values of $f_t(t, y)$ and $f_y(t, y)$ at every time step, so the number of function evaluations is smaller with our method than with the one presented in [?].

This paper has been structured as follows: in the next section we give a brief description of Rosenbrock-Nyström methods, together with their development. In Section ?? we describe the stability requirements that these methods should satisfy when integrating linear problems. In Section ?? we deal with the consistency of such methods, and we get the conditions that the coefficients of the method should satisfy in order to have up to order four. The construction of such methods is presented in [?]. Finally, in Section ?? we present some numerical experiments in order to test such methods.

2 Development of Rosenbrock-Nyström methods

Non-linear second-order in time problems can be written in an abstract form as follows:

“Find $u : [0, T] \rightarrow \mathcal{H}$ solution of

$$\begin{cases} u''(t) = f(t, u(t)), & 0 \leq t \leq T < \infty, \\ u(0) = u_0, \\ u'(0) = v_0, \end{cases} \quad (3)$$

where, typically, \mathcal{H} is a Hilbert space of functions defined in a certain bounded domain $\Omega \subseteq \mathbb{R}^M$, integer $M \geq 1$ with smooth boundary Γ . This formulation involves lots of different problems: partial differential equations, ordinary differential equations...

Example 2.1 *Let us show here two problems that can be solved by using Rosenbrock-Nyström methods.*

- *The first example is the following partial differential equation [?].*

$$\begin{aligned} u_{tt}(t, x) &= Au(t, x) - \sin(u(t, x)), & x \in [-50, 50], & 0 < t < T, \\ u(0, x) &= 4 \operatorname{atan}\left(\frac{\sqrt{1-w^2}}{w} \frac{\cos(wt)}{\cosh(x\sqrt{1-w^2})}\right), & u_t(0, x) &= 0, \\ u(t, -50) &= u(t, 50), & u_x(t, -50) &= u_x(t, 50), \end{aligned}$$

Operator A is such that $Au = u_{xx}$. This problem can be discretized in space by taking, for example, a pseudo-spectral discretization $u_M(t, x) = \sum_{k=-M}^{M-1} a_k(t) e^{2\pi i k \frac{(x+50)}{100}}$, with M a natural number.

- The second problem appears in [?]. This problem will be solved with our methods in the numerical experiments of Section ??.

$$\begin{aligned} u_j''(t) &= F(u_{j+1} - u_j) - F(u_j - u_{j-1}) + g_j(t), & j = 1, \dots, N, \\ u_j(0) &= \sin\left(\frac{2\pi j}{N+1}\right), & j = 1, \dots, N, \\ u_j'(t) &= 0 & j = 1, \dots, N, \end{aligned} \quad (4)$$

with

$$\begin{aligned} F(u) &= \lambda u + \alpha u^p, \\ u_0(t) &= u_{N+1}(t) = 0, \end{aligned}$$

$g_j(t)$ is such that the exact solution is given by $u_j(t) = \sin\left(\frac{2\pi j}{N+1}\right) \cos(t)$

When we solve a problem like (??) with a Rosenbrock-Nyström method, the numerical approximation to the exact solution and its derivative, $(y(t_n), v(t_n))$ is given by (y_n, v_n) , where $t_n = t_0 + n\tau$, with τ the time-step size. The values y_n and v_n are calculated as

$$\begin{aligned} v_{n+1} &= v_n + k \sum_{i=1}^s b_i f(t_n + \alpha_i k, y_n) + \sum_{j=1}^{i-1} \alpha_{ij} K_{n,j} \\ &\quad + \tau^2 f_t(t_n, y_n) \beta^T \cdot e + \tau f_y(t_n, y_n) \sum_{i=1}^s \beta_i K_{n,i}, \\ y_{n+1} &= y_n + \sum_{i=1}^s b_i K_{n,i}, \end{aligned} \quad (5)$$

where $K_{n,i}$, $i = 1, \dots, s$ are the intermediate stages and $e = (1, \dots, 1)^T$. These intermediate stages are given by the following equations

$$\begin{aligned} K_{n,i} &= \tau v_n + \tau^2 \sum_{j=1}^i \delta_{ij} f(t_n + \alpha_j k, y_n) + \sum_{l=1}^{j-1} \alpha_{jl} K_{n,l} \\ &\quad + \tau^2 \sum_{j=1}^i \gamma_{ij} (\tau f_t(t_n, y_n) + f_y(t_n, y_n) K_{n,j}) \end{aligned} \quad (6)$$

Notice that at every intermediate stage, the problem to be solved is a linear one, so the computational cost is reduced compared with the equations that implicit RKN methods provide when solving this type of problems. When we select the

values $\gamma_{ii} = \gamma$, $i = 1, \dots, s$, then, at every at every intermediate stage $K_{n,i}$ we have to solve a linear problem like

$$(I - k^2 \gamma f_y(t_n, y_n)) K_{n,i} = b_i$$

so the computational cost reduces as the system matrix remains constant for all the intermediate stages.

In what follows, in order to guarantee the solvability of the intermediate stages, we will assume that, for every $t > 0$, $\frac{\partial f}{\partial y}(t, y(t))$ is such that $(I - \mu \frac{\partial f}{\partial y}(t, y(t)))^{-1}$ exists and is bounded for every μ with $\mu \geq 0$.

When we have that for every $t > 0$, $\frac{\partial f}{\partial y}(t, y(t))$ is self-adjoint and negative semi-definite, the solvability and boundedness of the intermediate stages is guaranteed because of the following:

- In the case of $f(t, u(t))$ being a space differential operator, $\frac{\partial f}{\partial y}(t, y(t))$ is the infinitesimal generator of a C_0 -semigroup of type $\tilde{\omega} \leq 0$, so $(\mu I - \frac{\partial f}{\partial y}(t, y(t)))^{-1}$ exists and is bounded for every μ with $\mu \geq \tilde{\omega}$ [?].
- In the case of $f(t, u(t)) : \mathbb{R}^{n+1} \rightarrow \mathbb{R}^n$ being a regular function, then, for every $t > 0$ we have that $\frac{\partial f}{\partial y}(t, y(t))$ is a symmetric negative semi-definite matrix, so $(I - \mu \frac{\partial f}{\partial y}(t, y(t)))^{-1}$ exists for every $\mu \geq 0$

When the problem we are solving is autonomous, that is, of the form

$$\begin{cases} y''(t) &= f(y), \\ y(0) &= y_0, \\ y'(0) &= v_0, \end{cases} \quad (7)$$

the equations which determines the method are

$$\begin{aligned} K_{n,i} &= \tau v_n + \tau^2 \sum_{j=1}^i \delta_{ij} f(y_n + \sum_{l=1}^{j-1} \alpha_{jl} K_{n,l}) + \tau^2 f_y(t_n, y_n) \sum_{j=1}^i \gamma_{ij} K_{n,j} \\ v_{n+1} &= v_n + k \sum_{i=1}^s b_i f(y_n + \sum_{j=1}^{i-1} \alpha_{ij} K_{n,j}) + \tau f_y(t_n, y_n) \sum_{i=1}^s \beta_i K_{n,i}, \\ y_{n+1} &= y_n + \sum_{i=1}^s b_i K_{n,i}. \end{aligned} \quad (8)$$

Similarly as it happens with other classical methods like RK methods, RKN methods, Rosenbrock methods..., the coefficients of these methods can be written in a tableau as follows:

$$\begin{array}{c|c|c|c} \alpha & \mathcal{A}_\alpha & \mathcal{A}_\delta & \mathcal{A}_\gamma \\ \hline & \beta^T & & \\ \hline & b^T & & \end{array} = \begin{array}{c|cccc|cccc|cccc} 0 & 0 & & & & \delta_{11} & & & & \gamma_{11} & & & & & & & \\ \alpha_2 & \alpha_{21} & \ddots & & & \delta_{21} & \delta_{22} & & & \gamma_{21} & \gamma_{22} & & & & & & \\ \vdots & \vdots & \ddots & \ddots & & \vdots & \ddots & \ddots & & \vdots & \ddots & \ddots & & & & & \\ \alpha_s & \alpha_{s1} & \dots & \alpha_{ss-1} & 0 & \delta_{s1} & \delta_{s2} & \dots & \delta_{ss} & \gamma_{s1} & \dots & \gamma_{ss-1} & \gamma_{ss} & & & & \end{array} \quad (9)$$

$$\begin{array}{c|ccc|c} & \beta_1 & \dots & \beta_s \\ \hline & b_1 & \dots & b_s \end{array}$$

where we will assume that $\alpha_i = \sum_{j=1}^{i-1} \alpha_{ij}$.

The way of defining these new methods is the natural one since they can be obtained from Rosenbrock methods applied to problem (??) when it is transformed to a first-order in time problem. Let us remember that the coefficients of Rosenbrock methods are given by an array of the form

$$\frac{\tilde{\alpha} \mid \tilde{\mathcal{A}}_\alpha \parallel \tilde{\gamma} \mid \tilde{\mathcal{A}}_\gamma}{\parallel \tilde{b}^T \parallel} = \frac{\begin{array}{c|ccc|c} \tilde{\alpha}_1 & 0 & & & \parallel \tilde{\gamma}_1 & \tilde{\gamma}_{11} \\ \tilde{\alpha}_2 & \tilde{\alpha}_{21} & \ddots & & \parallel \tilde{\gamma}_2 & \tilde{\gamma}_{21} & \ddots \\ \vdots & \vdots & \ddots & \ddots & \parallel \vdots & \vdots & \ddots & \ddots \\ \tilde{\alpha}_s & \tilde{\alpha}_{s1} & \dots & \tilde{\alpha}_{ss-1} & 0 & \parallel \tilde{\gamma}_s & \tilde{\gamma}_{s1} & \dots & \tilde{\gamma}_{ss-1} & \tilde{\gamma}_{ss} \end{array}}{\parallel \tilde{b}_1 \quad \dots \quad \tilde{b}_s \parallel},$$

and the equations that these methods give when solving a problem like

$$\begin{cases} y'(t) = f(t, y), \\ y(0) = y_0, \end{cases}$$

are

$$Q_{n,i} = \tau f(t_n + \tilde{\alpha}_i \tau, y_n + \sum_{j=1}^{i-1} \tilde{\alpha}_{ij} Q_{n,j}) + \tau^2 \tilde{\gamma}_i f_t(t_n, y_n) + \tau f_y(t_n, y_n) \sum_{j=1}^i \tilde{\gamma}_{ij} Q_{n,j}$$

$$y_{n+1} = y_n + \sum_{j=1}^s \tilde{b}_j Q_{n,j},$$

where $t_n = t_0 + n\tau$, with τ the time-step size and y_n is the numerical approximation to $y(t_n)$. $Q_{n,i}$ are the intermediate stages.

Then, we write problem (??) as a first order one,

$$\begin{cases} \begin{pmatrix} y'(t) \\ v'(t) \end{pmatrix} = \begin{pmatrix} v(t) \\ f(t, y) \end{pmatrix}, \\ \begin{pmatrix} y(0) \\ v(0) \end{pmatrix} = \begin{pmatrix} y_0 \\ v_0 \end{pmatrix}. \end{cases} \quad (10)$$

When we apply a Rosenbrock method to this problem, the intermediate stages are given by

$$\begin{pmatrix} Q_{n,i}^y \\ Q_{n,i}^v \end{pmatrix} = \tau \begin{pmatrix} v_n + \sum_{j=1}^{i-1} \tilde{\alpha}_{ij} Q_{n,j}^v \\ f(t_n + \tau \tilde{\alpha}_i, y_n + \sum_{j=1}^{i-1} \tilde{\alpha}_{ij} Q_{n,j}^y) \end{pmatrix} + \tau^2 \tilde{\gamma}_i \begin{pmatrix} 0 \\ f_t(t_n, y_n) \end{pmatrix} + \tau \begin{pmatrix} 0 & 1 \\ f_y(t_n, y_n) & 0 \end{pmatrix} \begin{pmatrix} \sum_{j=1}^i \tilde{\gamma}_{ij} Q_{n,i}^y \\ \sum_{j=1}^i \tilde{\gamma}_{ij} Q_{n,i}^v \end{pmatrix}$$

and the numerical approximation $(y_{n+1}, v_{n+1})^T$ to the exact solution $(y(t_{n+1}), v(t_{n+1}))^T$ is given by

$$\begin{pmatrix} y_{n+1} \\ v_{n+1} \end{pmatrix} = \begin{pmatrix} y_n \\ v_n \end{pmatrix} + \begin{pmatrix} \sum_{j=1}^s \tilde{b}_j Q_{n,j}^y \\ \sum_{j=1}^s \tilde{b}_j Q_{n,i}^v \end{pmatrix}.$$

We operate in the equations that give the intermediate stages, replacing $Q_{n,j}^v$ by its expression in the equations for $Q_{n,j}^y$. From this, we obtain

$$\begin{aligned}
 Q_{n,i}^y &= kv_n + k^2 \sum_{j=1}^i (\tilde{\alpha}_{ij} + \tilde{\gamma}_{ij}) f(t_n + \tilde{\alpha}_j k, y_n + \sum_{j=1}^{i-1} \tilde{\alpha}_{ij} Q_{n,j}^y) + k^3 \sum_{j=1}^i (\tilde{\alpha}_{ij} + \tilde{\gamma}_{ij}) \tilde{\gamma}_j f_t(t_n, y_n) \\
 &\quad + k^2 \sum_{j=1}^i (\tilde{\alpha}_{ij} + \tilde{\gamma}_{ij}) \sum_{l=1}^j \tilde{\gamma}_l Q_{n,l}^y \\
 v_{n+1} &= v_n + k \sum_{j=1}^s \tilde{b}_j f(t_n + \tilde{\alpha}_j k, y_n + \sum_{l=1}^{j-1} \tilde{\alpha}_{jl} Q_{n,l}^y) \\
 &\quad + k^2 \sum_{j=1}^s \tilde{b}_j \tilde{\gamma}_j f_t(t_n, y_n) + k f_y(t_n, y_n) \sum_{j=1}^s \tilde{b}_j \sum_{l=1}^j \tilde{\gamma}_l \\
 y_{n+1} &= y_n + \sum_{j=1}^s \tilde{b}_j Q_{n,j}^y
 \end{aligned}$$

Now, let us assume that the Rosenbrock method satisfies

$$\begin{aligned}
 \tilde{\alpha}_i &= \sum_{j=1}^{i-1} \tilde{\alpha}_{ij}, \\
 \tilde{\gamma}_i &= \sum_{j=1}^i \tilde{\gamma}_{ij}, \\
 \sum_{j=1}^s \tilde{b}_j &= 1,
 \end{aligned} \tag{11}$$

The first two conditions are usual restrictions satisfied for many Rosenbrock methods and the third one is the condition to have classical order 1. Then, what we obtain is precisely equations (??) if we define

$$\begin{aligned}
 \alpha &= \tilde{\alpha}, \\
 \mathcal{A}_\alpha &= \tilde{\mathcal{A}}_\alpha \\
 \mathcal{A}_\gamma &= (\tilde{\mathcal{A}}_\alpha + \tilde{\mathcal{A}}_\gamma) \tilde{\mathcal{A}}_\gamma, \\
 \mathcal{A}_\delta &= \tilde{\mathcal{A}}_\alpha + \tilde{\mathcal{A}}_\gamma, \\
 b^T &= \tilde{b}^T, \\
 \beta^T &= \tilde{b}^T \tilde{\mathcal{A}}_\gamma,
 \end{aligned} \tag{12}$$

and if we call $K_{n,i} = Q_{n,i}^y$, $i = 1, \dots, s$. Furthermore, we can obtain Rosenbrock-Nyström methods not coming from Rosenbrock ones, which gives much more freedom to obtain the coefficients of the desired methods.

3 Stability when solving linear ordinary differential equations

In this part we deal with the stability of Rosenbrock-Nyström methods when they are applied to a problem like

$$\begin{aligned} U''(t) &= -B^2U(t), \\ U(0) &= U_0, \\ U'(0) &= V_0, \end{aligned} \tag{13}$$

where B is a given symmetric positive defined matrix of order $m \geq 1$ and $U(t)$, $f(t)$, U_0 and $V_0 \in \mathbb{R}^m$.

Here, we study the stability in the energy norm, which is the natural norm for the study of the well-posedness of problem (??). This norm is given by

$$\|(U(t), U'(t))^T\|_B^2 = \|BU(t)\|_2^2 + \|U'(t)\|_2^2,$$

with $\|\cdot\|$ the Euclidean norm in \mathbb{R}^m .

When solving problem (??) with a Rosenbrock-Nyström method, we obtain

$$\begin{bmatrix} U_{n+1} \\ V_{n+1} \end{bmatrix} = \begin{bmatrix} r_{11}(\tau B) & B^{-1}r_{12}(\tau B) \\ Br_{21}(\tau B) & r_{22}(\tau B) \end{bmatrix} \begin{bmatrix} U_0 \\ V_0 \end{bmatrix}, \tag{14}$$

where terms $r_{ij}(kB)$, $1 \leq i, j \leq 2$ are given by

$$\begin{aligned} r_{11}(\tau B) &= I - (b^T \otimes \tau^2 B^2)(\mathcal{I} \otimes I + (\mathcal{A}_\delta \mathcal{A}_\alpha + \mathcal{A}_\gamma) \otimes \tau^2 B^2)^{-1}(\mathcal{A}_\delta e \otimes I), \\ r_{12}(\tau B) &= (b^T \otimes \tau B)(\mathcal{I} \otimes I + (\mathcal{A}_\delta \mathcal{A}_\alpha + \mathcal{A}_\gamma) \otimes \tau^2 B^2)^{-1}(e \otimes I) \\ r_{21}(\tau B) &= -\tau B[(b^T e \otimes I) - ((b^T \mathcal{A}_\alpha + \beta^T) \otimes \tau^2 B^2)(\mathcal{I} \otimes I + (\mathcal{A}_\delta \mathcal{A}_\alpha + \mathcal{A}_\gamma) \otimes \tau^2 B^2)^{-1}(\mathcal{A}_\delta e \otimes I)], \\ r_{22}(\tau B) &= I - ((b^T \mathcal{A}_\alpha + \beta^T) \otimes \tau^2 B^2)(\mathcal{I} \otimes I + (\mathcal{A}_\delta \mathcal{A}_\alpha + \mathcal{A}_\gamma) \otimes \tau^2 B^2)^{-1}(e \otimes I). \end{aligned}$$

These elements form matrix $R(\tau B)$,

$$R(\tau B) = \begin{bmatrix} r_{11}(\tau B) & r_{12}(\tau B) \\ r_{21}(\tau B) & r_{22}(\tau B) \end{bmatrix}.$$

By bounding (??) in the energy norm, we obtain that the proof of stability is related to the boundedness of the powers of matrix $R(\tau B)$. As matrix B is assumed to be symmetric and positive definite, then B is normal and we can use the following spectral result

$$\|R(\tau B)^n\|_2 \leq \sup_{\theta \in \sigma(\tau B)} \|R(\theta)^n\|_2, \tag{15}$$

with $\sigma(\tau B)$ the spectrum of τB . Then, the boundedness of the powers of matrix $R(\tau B)$ is reduced to the study of the boundedness of matrix $R(\theta)$. (Note: if we assume that B is not normal, we can use a similar result to (??), but considering the numerical range instead of the spectrum [?].)

Following the results in [?], the following definitions and theorem can be stated. The proof of Theorem ?? is similar to the one given in [?].

Definition 3.1 The interval $\mathcal{C} = [0, \beta_{stab})$ is the interval of stability of the Rosenbrock-Nyström method if $\beta_{stab} \in \mathbb{R}^+$ is the highest value such that

$$\mathcal{C} \subset \{\theta \in \mathbb{R}^+ \cup \{0\} / \rho(R(\theta)) \leq 1 \text{ and } R(\theta) \text{ is simple when } \rho(R(\theta)) = 1\}.$$

The Rosenbrock-Nyström method is said to be *R-stable* if $\mathcal{C} = \mathbb{R}^+ \cup \{0\}$.

Definition 3.2 The interval $\mathcal{C}^* = [0, \beta_{per})$ is the interval of periodicity of the Rosenbrock-Nyström if $\beta_{per} \in \mathbb{R}^+$ is the highest value such that

$$\mathcal{C}^* \subset \{\theta \in \mathbb{R}^+ \cup \{0\} / R(\theta) \text{ is simple and for all } \lambda \in \sigma(R(\theta)), |\lambda| = 1\}.$$

We will say that the Rosenbrock-Nyström method is *P-stable* if $\mathcal{C}^* = \mathbb{R}^+ \cup \{0\}$.

Theorem 3.3 Under assumptions

(i) The method is *R-stable*.

(ii) $\sigma(\mathcal{A}_\delta \mathcal{A}_\alpha + \mathcal{A}_\gamma) \cap (-\infty, 0] = \emptyset$.

(iii) There exists a value $\bar{\theta} \in \mathbb{R}$ such that $R(\bar{\theta})$ does not have double eigenvalues.

(iv) $(b^T \mathcal{A}_\alpha + \beta^T)(\mathcal{A}_\delta \mathcal{A}_\alpha + \mathcal{A}_\gamma)^{-1}(\mathcal{A}_\delta e) = 1$

Then,

$$\|R(kB)^n\|_2 \leq C, \quad n \in \mathbb{N}.$$

where C is independent of the size of $\sigma(kB)$.

This result can not be obtained if assumption (iv) is not satisfied.

Corollary 3.4 When the Rosenbrock-Nyström method comes from a Rosenbrock one with classical order greater or equal than one, condition

$$(b^T \mathcal{A}_\alpha + \beta^T)(\mathcal{A}_\delta \mathcal{A}_\alpha + \mathcal{A}_\gamma)^{-1}(\mathcal{A}_\delta e) = 1$$

is always satisfied.

Proof.

Let us assume that the Rosenbrock-Nyström method comes from a Rosenbrock one with Butcher array

$$\begin{array}{c|c} \tilde{\alpha} & \tilde{\mathcal{A}}_\alpha \\ \hline \tilde{b}^T & \tilde{\mathcal{A}}_\gamma \end{array}$$

and that the coefficients of the Rosenbrock-Nyström method satisfy relations (??). Then,

$$\begin{aligned} (b^T \mathcal{A}_\alpha + \beta^T)(\mathcal{A}_\delta \mathcal{A}_\alpha + \mathcal{A}_\gamma)^{-1}(\mathcal{A}_\delta e) &= (\tilde{b}^T \tilde{\mathcal{A}}_\alpha + \tilde{b}^T \tilde{\mathcal{A}}_\gamma)((\tilde{\mathcal{A}}_\alpha + \tilde{\mathcal{A}}_\gamma)\tilde{\mathcal{A}}_\alpha + (\tilde{\mathcal{A}}_\alpha + \tilde{\mathcal{A}}_\gamma)\tilde{\mathcal{A}}_\gamma)^{-1}(\tilde{\mathcal{A}}_\alpha + \tilde{\mathcal{A}}_\gamma)e \\ &= \tilde{b}^T(\tilde{\mathcal{A}}_\alpha + \tilde{\mathcal{A}}_\gamma)((\tilde{\mathcal{A}}_\alpha + \tilde{\mathcal{A}}_\gamma)(\tilde{\mathcal{A}}_\alpha + \tilde{\mathcal{A}}_\gamma))^{-1}(\tilde{\mathcal{A}}_\alpha + \tilde{\mathcal{A}}_\gamma)e \\ &= \tilde{b}^T(\tilde{\mathcal{A}}_\alpha + \tilde{\mathcal{A}}_\gamma)((\tilde{\mathcal{A}}_\alpha + \tilde{\mathcal{A}}_\gamma)^2)^{-1}(\tilde{\mathcal{A}}_\alpha + \tilde{\mathcal{A}}_\gamma)e \\ &= \tilde{b}^T e = 1 \end{aligned}$$

□

4 Order conditions for Rosenbrock-Nyström methods

Let us see the conditions that Rosenbrock-Nyström methods should satisfy to obtain the highest possible order when integrating a problem like (??). In a similar way as with Runge-Kutta-Nyström methods, a Rosenbrock-Nyström method is said to have classical order p if

$$\begin{aligned}\rho_{n+1} &= y(t_{n+1}) - \hat{y}_{n+1} = O(\tau^{p+1}), \\ \xi_{n+1} &= y'(t_{n+1}) - \hat{v}_{n+1} = O(\tau^{p+1}),\end{aligned}$$

where $(\hat{y}_{n+1}, \hat{v}_{n+1})^T$ is the numerical solution obtained from the exact solution $(y(t_n), y'(t_n))^T = (\tilde{y}_{n+1}, \tilde{v}_{n+1})^T$ with time step size τ .

In order to study the order conditions, it is useful to write the equations as in the autonomous case, given by (??), in the following way,

$$\begin{aligned}g_{n,i}^J &= y_n^J + \sum_{j=1}^{i-1} \alpha_{ij} K_{n,j}^J, \\ K_{n,i}^J &= \tau v_n^J + \tau^2 \sum_{j=1}^i \delta_{ij} f^J(g_j) + \tau^2 \sum_K f_K^J(y_n) \sum_{j=1}^i \gamma_{ij} K_{n,j}^K, \\ v_{n+1}^J &= v_n^J + \tau \sum_{i=1}^s b_i f^J(g_i) + \tau \sum_K f_K^J(y_n) \sum_{i=1}^s \beta_i K_{n,i}^K, \\ y_{n+1}^J &= y_n^J + \sum_{i=1}^s b_i K_{n,i}^J,\end{aligned}$$

where the superscripts indices in capital letters indicates the component of the vector we are using (in this part the notation is similar to the one used in [?]). In the following, $\partial f^J / \partial y^K$ will be denoted by f_K^J , $\partial^2 f^J / \partial y^K \partial y^L$ by f_{KL}^J and so on.

To get the order conditions we are going to compare the Taylor series of \hat{y}_{n+1} and \hat{v}_{n+1} obtained from the exact solution $(\tilde{y}_n, \tilde{v}_n)^T$ with the Taylor series of the exact solution.

In this part the following formulae are used:

$$\begin{aligned}(\tau\varphi(\tau))^{(q)}|_{\tau=0} &= q\varphi^{(q-1)}(\tau)|_{\tau=0}, \quad q \geq 1, \\ (\tau^2\varphi(\tau))^{(q)}|_{\tau=0} &= q(q-1)\varphi^{(q-2)}(\tau)|_{\tau=0}, \quad q \geq 2.\end{aligned}$$

These formulae are obtained by using that

$$\begin{aligned}(\tau\varphi(\tau))^{(q)} &= q\varphi^{(q-1)}(\tau) + \tau\varphi^{(q)}(\tau), \quad q \geq 1, \\ (\tau^2\varphi(\tau))^{(q)} &= q(q-1)\varphi^{(q-2)}(\tau) + 2q\tau\varphi^{(q-1)}(\tau) + \tau^2\varphi^{(q)}(\tau), \quad q \geq 2.\end{aligned}$$

These formulae can be proved in a recursive manner.

We differentiate by using the notation $\varphi(\tau) = \sum_{j=1}^i (\delta_{ij} f^J(g_j) + \gamma_{ij} \sum_K f_K^J(\tilde{y}_n) K_{n,j}^K)$ together with the previous formulae. Then, we obtain

$$\begin{aligned}
 (K_{n,i}^J)^{(0)}|_{\tau=0} &= 0, \\
 (K_{n,i}^J)^{(1)}|_{\tau=0} &= \tilde{v}_n^J|_{\tau=0} + \left(2\tau \sum_{j=1}^i (\delta_{ij} f^J(g_j) + \gamma_{ij} \sum_K f_K^J(\tilde{y}_n) K_{n,j}^K) \right) |_{\tau=0} \\
 &\quad + \left(\tau^2 \sum_{j=1}^i (\delta_{ij} f^J(g_j) + \gamma_{ij} \sum_K f_K^J(\tilde{y}_n) K_{n,j}^K)^{(1)} \right) |_{\tau=0} \\
 &= \tilde{v}_n^J, \\
 (K_{n,i}^J)^{(2)}|_{\tau=0} &= 2 \sum_{j=1}^i (\delta_{ij} f^J(g_j) + \gamma_{ij} \sum_K f_K^J(\tilde{y}_n) K_{n,j}^K) |_{\tau=0} \\
 &= 2 \sum_{j=1}^i \delta_{ij} f^J(\tilde{y}_n) \\
 (K_{n,i}^J)^{(3)}|_{\tau=0} &= 6 \sum_{j=1}^i (\delta_{ij} f^J(g_j)^{(1)} + \gamma_{ij} \sum_K f_K^J(\tilde{y}_n) (K_{n,j}^K)^{(1)}) |_{\tau=0} \\
 &= 6 \sum_{j=1}^i (\delta_{ij} \alpha_j \sum_K f_K^J(\tilde{y}_n) \tilde{v}_n^K + \gamma_{ij} \sum_K f_K^J(\tilde{y}_n) \tilde{v}_n^K) \\
 &= 6 \sum_{j=1}^i (\delta_{ij} \alpha_j + \gamma_{ij}) \sum_K f_K^J(\tilde{y}_n) \tilde{v}_n^K, \\
 (K_{n,i}^J)^{(4)}|_{\tau=0} &= 12 \sum_{j=1}^i (\delta_{ij} (f^J(g_j))^{(2)} + \gamma_{ij} \sum_K f_K^J(\tilde{y}_n) (K_{n,j}^K)^{(2)}) |_{\tau=0} \\
 &= 12 \sum_{j=1}^i \delta_{ij} \alpha_j^2 \sum_{K,L} f_{KL}^J(\tilde{y}_n) \tilde{v}_n^K \tilde{v}_n^L + 24 \sum_{j=1}^i \sum_{l=1}^{i-1} \sum_{m=1}^l \delta_{ij} \alpha_j \delta_{lm} \sum_K f_K^J(\tilde{y}_n) f^K(\tilde{y}_n) \\
 &\quad + 24 \sum_{j=1}^i \sum_{l=1}^j \gamma_{ij} \delta_{jl} \sum_K f_K^J(\tilde{y}_n) f^K(\tilde{y}_n),
 \end{aligned}$$

where we have used that

$$\begin{aligned}
 f^J(g_i)|_{\tau=0} &= f^J(\tilde{y}_n), \\
 (f^J(g_i))^{(1)}|_{\tau=0} &= \sum_K \alpha_i f_K^J(\tilde{y}_n) \tilde{v}_n^K, \\
 (f^J(g_i))^{(2)}|_{\tau=0} &= \sum_{K,L} \alpha_i^2 f_{K,L}^J(\tilde{y}_n) \tilde{v}_n^K \tilde{v}_n^L + 2 \sum_K f_K^J(\tilde{y}_n) f^K(\tilde{y}_n) \sum_{j=1}^{i-1} \sum_{l=1}^j \alpha_{ij} \delta_{jl},
 \end{aligned}$$

together with

$$\begin{aligned}
 (g_i^K)^{(0)}|_{\tau=0} &= \tilde{y}_n^K, \\
 (g_i^K)^{(1)}|_{\tau=0} &= \sum_{j=1}^{i-1} \alpha_{ij} (K_{n,j}^J)^{(1)}|_{\tau=0} \\
 &= \sum_{j=1}^{i-1} \alpha_{ij} \tilde{v}_n^J \\
 &= \alpha_i \tilde{v}_n^J, \\
 (g_i^K)^{(2)}|_{\tau=0} &= \sum_{j=1}^{i-1} \alpha_{ij} (K_{n,j}^J)^{(2)}|_{\tau=0} \\
 &= 2 \sum_{j=1}^{i-1} \sum_{l=1}^j \alpha_{ij} \delta_{jl} f^J(\tilde{y}_n), \\
 (g_i^K)^{(3)}|_{\tau=0} &= \sum_{j=1}^{i-1} \alpha_{ij} (K_{n,j}^J)^{(3)}|_{\tau=0} \\
 &= 6 \sum_{j=1}^{i-1} \sum_{l=1}^j \alpha_{ij} (\delta_{jl} \alpha_l + \gamma_{jl}) \sum_K f_K^J(\tilde{y}_n) \tilde{v}_n^K.
 \end{aligned}$$

Then, by using the expressions obtained for $(K_{n,i}^J)^{(l)}$, $l = 1, \dots, 4$, we have

$$\begin{aligned}
 (\hat{v}_{n+1}^J)^{(1)}|_{\tau=0} &= \sum_{i=1}^s b_i f^J(g_i)|_{\tau=0} + \sum_K f_K^J(\tilde{y}_n) \sum_{i=1}^s \beta_i (K_{n,i}^K)^{(0)}|_{\tau=0} \\
 &= f^J(\tilde{y}_n) \sum_{i=1}^s b_i, \\
 (\hat{v}_{n+1}^J)^{(2)}|_{\tau=0} &= 2 \sum_{i=1}^s b_i (f^J(g_i))^{(1)}|_{\tau=0} + 2 \sum_K f_K^J(\tilde{y}_n) \sum_{i=1}^s \beta_i (K_{n,i}^K)^{(1)}|_{\tau=0} \\
 &= 2 \sum_{i=1}^s b_i \sum_K f_K^J(\tilde{y}_n) \alpha_i \tilde{v}_n^K + 2 \sum_K f_K^J(\tilde{y}_n) \sum_{i=1}^s \beta_i \tilde{v}_n^K \\
 &= 2 \sum_{i=1}^s (b_i \alpha_i + \beta_i) \sum_K f_K^J(\tilde{y}_n) \tilde{v}_n^K, \\
 (\hat{v}_{n+1}^J)^{(3)}|_{\tau=0} &= 3 \sum_{i=1}^s b_i (f^J(g_i))^{(2)}|_{\tau=0} + 3 \sum_K f_K^J(\tilde{y}_n) \sum_{i=1}^s \beta_i (K_{n,i}^K)^{(2)}|_{\tau=0} \\
 &= 3 \sum_{i=1}^s b_i \sum_{K,L} f_{K,L}^J(\tilde{y}_n) \alpha_i^2 \tilde{v}_n^K \tilde{v}_n^L + 6 \sum_{i=1}^s b_i \sum_K f_K^J(\tilde{y}_n) f^K(\tilde{y}_n) \sum_{j=1}^{i-1} \sum_{l=1}^j \alpha_{ij} \delta_{jl}
 \end{aligned}$$

$$\begin{aligned}
 & +6 \sum_K f_K^J(\tilde{y}_n) \sum_{i=1}^s \sum_{j=1}^i \beta_i \delta_{ij} f^K(\tilde{y}_n) \tag{16} \\
 = & 3 \sum_{i=1}^s b_i \alpha_i^2 \sum_{K,L} f_{K,L}^J(\tilde{y}_n) \tilde{v}_n^K \tilde{v}_n^L + 6 \sum_{i=1}^s \sum_K f_K^J(\tilde{y}_n) f^K(\tilde{y}_n) \left(\sum_{j=1}^{i-1} \sum_{l=1}^j b_i \alpha_{ij} \delta_{jl} + \sum_{j=1}^i \beta_i \delta_{ij} \right), \\
 (\hat{v}_{n+1}^J)^{(4)}|_{\tau=0} = & 4 \sum_{i^1}^s b_i (f^J(g_i))^{(3)}|_{\tau=0} + 4 \sum_K f_K^J(\tilde{y}_n) \sum_{i=1}^s \beta_i (K_{n,i}^K)^{(3)}|_{\tau=0} \\
 = & 4 \sum_{i^1}^s b_i \alpha_i^3 \sum_{K,L,M} f_{K,L,M}^J(\tilde{y}_n) \tilde{v}_n^K \tilde{v}_n^L \tilde{v}_n^M \\
 & +16 \sum_{i=1}^s b_i \alpha_i \sum_{j=1}^{i-1} \sum_{l=1}^j \alpha_{ij} \delta_{jl} \sum_{K,L} f_{K,L}^J(\tilde{y}_n) f^K(\tilde{y}_n) \tilde{v}_n^L \\
 & +8 \sum_{i=1}^s b_i \alpha_i \sum_{j=1}^{i-1} \sum_{l=1}^j \alpha_{ij} \delta_{jl} \sum_{K,L} f_{K,L}^J(\tilde{y}_n) f^L(\tilde{y}_n) \tilde{v}_n^K \\
 & +24 \sum_{i=1}^s b_i \sum_{j=1}^{i-1} \sum_{l=1}^j \alpha_{ij} (\delta_{jl} \alpha_l + \gamma_{jl}) \sum_{K,L} f_K^J(\tilde{y}_n) f_L^K(\tilde{y}_n) \tilde{v}_n^L \\
 & +24 \sum_K f_K^J(\tilde{y}_n) \sum_{i=1}^s \beta_i \sum_{j=1}^i (\delta_{ij} \alpha_j + \gamma_{ij}) \sum_L f_L^K(\tilde{y}_n) \tilde{v}_n^L \\
 = & 4 \sum_{i^1}^s b_i \alpha_i^3 \sum_{K,L,M} f_{K,L,M}^J(\tilde{y}_n) \tilde{v}_n^K \tilde{v}_n^L \tilde{v}_n^M \\
 & +16 \sum_{i=1}^s b_i \alpha_i \sum_{j=1}^{i-1} \sum_{l=1}^j \alpha_{ij} \delta_{jl} \sum_{K,L} f_{K,L}^J(\tilde{y}_n) f^K(\tilde{y}_n) \tilde{v}_n^L \\
 & +8 \sum_{i=1}^s b_i \alpha_i \sum_{j=1}^{i-1} \sum_{l=1}^j \alpha_{ij} \delta_{jl} \sum_{K,L} f_{K,L}^J(\tilde{y}_n) f^L(\tilde{y}_n) \tilde{v}_n^K \\
 & +24 \sum_{i=1}^s b_i \sum_{j=1}^{i-1} \sum_{l=1}^j \alpha_{ij} (\delta_{jl} \alpha_l + \gamma_{jl}) \sum_{K,L} f_K^J(\tilde{y}_n) f_L^K(\tilde{y}_n) \tilde{v}_n^L \\
 & +24 \sum_{i=1}^s \sum_{j=1}^i \beta_i (\delta_{ij} \alpha_j + \gamma_{ij}) \sum_{K,L} f_K^J(\tilde{y}_n) f_L^K(\tilde{y}_n) \tilde{v}_n^L \\
 = & \sum_{K,L,M} f_{K,L,M}^J(\tilde{y}_n) \tilde{v}_n^K \tilde{v}_n^L \tilde{v}_n^M \sum_{i^1}^s 4b_i \alpha_i^3 \\
 & + \sum_{K,L} f_{K,L}^J(\tilde{y}_n) f^K(\tilde{y}_n) \tilde{v}_n^L \sum_{i=1}^s \sum_{j=1}^{i-1} \sum_{l=1}^j 24b_i \alpha_i \alpha_{ij} \delta_{jl}
 \end{aligned}$$

$$+24 \sum_{K,L} f_K^J(\tilde{y}_n) f_L^K(\tilde{y}_n) \tilde{v}_n^L \sum_{i=1}^s \left(\sum_{j=1}^{i-1} \sum_{l=1}^j b_i \alpha_{ij} (\delta_{jl} \alpha_l + \gamma_{jl}) + \sum_{j=1}^i \beta_i (\delta_{ij} \alpha_j + \gamma_{ij}) \right)$$

where we have used that

$$\begin{aligned} (f^J(g_i))^{(3)} &= \sum_{K,L,M} f_{K,L,M}^J(g_i) (g_i^K)^{(1)} (g_i^L)^{(1)} (g_i^M)^{(1)} + 2 \sum_{K,L} f_{K,L}^J(g_i) (g_i^K)^{(2)} (g_i^L)^{(1)} \\ &+ \sum_{K,L} f_{K,L}^J(g_i) (g_i^K)^{(1)} (g_i^L)^{(2)} + \sum_K f_K^J(g_i) (g_i^K)^{(3)} \end{aligned}$$

and therefore

$$\begin{aligned} (f^J(g_i))^{(3)}|_{\tau=0} &= \sum_{K,L,M} f_{K,L,M}^J(\tilde{y}_n) \tilde{v}_n^K \tilde{v}_n^L \tilde{v}_n^M \alpha_i^3 + 4 \sum_{K,L} f_{K,L}^J(\tilde{y}_n) \sum_{j=1}^{i-1} \sum_{l=1}^j \alpha_i \alpha_{ij} \delta_{jl} f^K(\tilde{y}_n) \tilde{v}_n^L \\ &+ 2 \sum_{K,L} f_{K,L}^J(\tilde{y}_n) \sum_{j=1}^{i-1} \sum_{l=1}^j \alpha_i \alpha_{ij} \delta_{jl} f^L(\tilde{y}_n) \tilde{v}_n^K \\ &+ 6 \sum_{K,L} f_K^J(\tilde{y}_n) \sum_{j=1}^{i-1} \sum_{l=1}^j \alpha_{ij} (\delta_{jl} \alpha_l + \gamma_{jl}) f_L^K(\tilde{y}_n) \tilde{v}_n^L. \end{aligned}$$

For $(\hat{y}_{n+1}^J)^{(l)}$, $l = 1, \dots, 4$, we get

$$\begin{aligned} (\hat{y}_{n+1}^J)^{(0)}|_{\tau=0} &= \tilde{y}_n^J, \\ (\hat{y}_{n+1}^J)^{(1)}|_{\tau=0} &= \sum_{i=1}^s b_i (K_{n,i}^J)^{(1)}|_{\tau=0} \\ &= \tilde{v}_n^J \sum_{i=1}^s b_i, \\ (\hat{y}_{n+1}^J)^{(2)}|_{\tau=0} &= \sum_{i=1}^s b_i (K_{n,i}^J)^{(2)}|_{\tau=0} \\ &= 2 \sum_{i=1}^s b_i \sum_{j=1}^i \delta_{ij} f^J(\tilde{y}_n) \\ &= 2 f^J(\tilde{y}_n) \sum_{i=1}^s \sum_{j=1}^i b_i \delta_{ij}, \\ (\hat{y}_{n+1}^J)^{(3)}|_{\tau=0} &= \sum_{i=1}^s b_i (K_{n,i}^J)^{(3)}|_{\tau=0} \\ &= 6 \sum_{i=1}^s b_i \sum_{j=1}^i (\delta_{ij} \alpha_j + \gamma_{ij}) \sum_K f_K^J(\tilde{y}_n) \tilde{v}_n^K \\ &= 6 \sum_K f_K^J(\tilde{y}_n) \tilde{v}_n^K \sum_{i=1}^s \sum_{j=1}^i b_i (\delta_{ij} \alpha_j + \gamma_{ij}), \end{aligned} \tag{17}$$

$$\begin{aligned}
 (\hat{y}_{n+1}^J)^{(4)}|_{\tau=0} &= \sum_{i=1}^s b_i (K_{n,i}^J)^{(4)}|_{\tau=0} \\
 &= 12 \sum_{i=1}^s b_i \sum_{j=1}^i \delta_{ij} \alpha_j^2 \sum_{K,L} f_{K,L}^J(\tilde{y}_n) \tilde{v}_n^K \tilde{v}_n^L \\
 &\quad + 24 \sum_{i=1}^s b_i \sum_{j=1}^i \sum_{l=1}^{j-1} \sum_{m=1}^l \delta_{ij} \alpha_{jl} \delta_{lm} \sum_K f_K^J(\tilde{y}_n) f^K(\tilde{y}_n) \\
 &\quad + 24 \sum_{i=1}^s b_i \sum_{j=1}^i \sum_{l=1}^j \gamma_{ij} \delta_{jl} \sum_K f_K^J(\tilde{y}_n) f^K(\tilde{y}_n) \\
 &= 12 \sum_{K,L} f_{K,L}^J(\tilde{y}_n) \tilde{v}_n^K \tilde{v}_n^L \sum_{i=1}^s \sum_{j=1}^i b_i \delta_{ij} \alpha_j^2 \\
 &\quad + 24 \sum_K f_K^J(\tilde{y}_n) f^K(\tilde{y}_n) \sum_{i=1}^s \sum_{j=1}^i \sum_{l=1}^j b_i (\gamma_{ij} \delta_{jl} + \delta_{ij} \alpha_{jl} \sum_{m=1}^l \delta_{lm}).
 \end{aligned}$$

Now, we calculate the derivatives of the exact solution, by taking into account that $y''(t_n) = f(\tilde{y}_n)$,

$$\begin{aligned}
 (\tilde{y}_n^J)^{(1)} &= \tilde{v}_n^J, \\
 (\tilde{y}_n^J)^{(2)} &= (\tilde{v}_n^J)^{(1)} = f^J(\tilde{y}_n), \\
 (\tilde{y}_n^J)^{(3)} &= (\tilde{v}_n^J)^{(2)} = (f^J(\tilde{y}_n))^{(1)} = \sum_K f_K^J(\tilde{y}_n) \tilde{v}_n^K, \tag{18} \\
 (\tilde{y}_n^J)^{(4)} &= (\tilde{v}_n^J)^{(3)} = (f^J(\tilde{y}_n))^{(2)} \\
 &= \sum_{K,L} f_{KL}^J(\tilde{y}_n) \tilde{v}_n^K (\tilde{y}_n^L)^{(1)} + \sum_K f_K^J(\tilde{y}_n) (\tilde{v}_n^K)^{(1)} \\
 &= \sum_{K,L} f_{KL}^J(\tilde{y}_n) \tilde{v}_n^K \tilde{v}_n^L + \sum_K f_K^J(\tilde{y}_n) f^K(\tilde{y}_n), \\
 (\tilde{y}_n^J)^{(5)} &= (\tilde{v}_n^J)^{(4)} = (f^J(\tilde{y}_n))^{(3)} \\
 &= \sum_{K,L,M} f_{K,L,M}^J(\tilde{y}_n) \tilde{v}_n^K \tilde{v}_n^L (\tilde{y}_n^M)^{(1)} + \sum_{K,L} f_{K,L}^J(\tilde{y}_n) (\tilde{v}_n^K)^{(1)} \tilde{v}_n^L \\
 &\quad + \sum_{K,L} f_{K,L}^J(\tilde{y}_n) \tilde{v}_n^K (\tilde{v}_n^L)^{(1)} + \sum_{K,L} f_{K,L}^J(\tilde{y}_n) (\tilde{y}_n^L)^{(1)} f^K(\tilde{y}_n) \\
 &\quad + \sum_{K,L} f_K^J(\tilde{y}_n) f_L^K(\tilde{y}_n) (\tilde{y}_n^L)^{(1)} \\
 &= \sum_{K,L,M} f_{K,L,M}^J(\tilde{y}_n) \tilde{v}_n^K \tilde{v}_n^L \tilde{v}_n^M + \sum_{K,L} f_{K,L}^J(\tilde{y}_n) f^K(\tilde{y}_n) \tilde{v}_n^L \\
 &\quad + \sum_{K,L} f_{K,L}^J(\tilde{y}_n) \tilde{v}_n^K f^L(\tilde{y}_n) + \sum_{K,L} f_{K,L}^J(\tilde{y}_n) f^K(\tilde{y}_n) \tilde{v}_n^L
 \end{aligned}$$

$$\begin{aligned}
 & + \sum_{K,L} f_K^J(\tilde{y}_n) f_L^K(\tilde{y}_n) \tilde{v}_n^L \\
 = & \sum_{K,L,M} f_{K,L,M}^J(\tilde{y}_n) \tilde{v}_n^K \tilde{v}_n^L \tilde{v}_n^M + 3 \sum_{K,L} f_{K,L}^J(\tilde{y}_n) f^K(\tilde{y}_n) \tilde{v}_n^L \\
 & + \sum_{K,L} f_K^J(\tilde{y}_n) f_L^K(\tilde{y}_n) \tilde{v}_n^L
 \end{aligned}$$

Then, by comparing the results in (??) and (??) with the results in (??), the order conditions up to order four are:

Order 1: We compare $(\hat{v}_n^J)^{(1)}$ with $(\tilde{v}_n^J)^{(1)}$ and $(\hat{y}_n^J)^{(1)}$ with $(\tilde{y}_n^J)^{(1)}$

$$\sum_{i=1}^s b_i = 1.$$

Order 2: We compare $(\hat{v}_n^J)^{(2)}$ with $(\tilde{v}_n^J)^{(2)}$ and $(\hat{y}_n^J)^{(2)}$ with $(\tilde{y}_n^J)^{(2)}$

$$\begin{aligned}
 \sum_{i=1}^s (b_i \alpha_i + \beta_i) &= \frac{1}{2}, \\
 \sum_{i=1}^s \sum_{j=1}^i b_i \delta_{ij} &= \frac{1}{2}.
 \end{aligned}$$

Order 3: We compare $(\hat{v}_n^J)^{(3)}$ with $(\tilde{v}_n^J)^{(3)}$ and $(\hat{y}_n^J)^{(3)}$ with $(\tilde{y}_n^J)^{(3)}$

$$\begin{aligned}
 \sum_{i=1}^s b_i \alpha_i^2 &= \frac{1}{3}, \\
 \sum_{i=1}^s \sum_{j=1}^{i-1} \sum_{l=1}^j b_i \alpha_{ij} \delta_{jl} + \sum_{i=1}^s \sum_{j=1}^i \beta_i \delta_{ij} &= \frac{1}{6}, \\
 \sum_{i=1}^s \sum_{j=1}^i b_i (\delta_{ij} \alpha_j + \gamma_{ij}) &= \frac{1}{6}.
 \end{aligned}$$

Order 4: We compare $(\hat{v}_n^J)^{(4)}$ with $(\tilde{v}_n^J)^{(4)}$ and $(\hat{y}_n^J)^{(4)}$ with $(\tilde{y}_n^J)^{(4)}$

$$\begin{aligned}
 \sum_{i=1}^s b_i \alpha_i^3 &= \frac{1}{4}, \\
 \sum_{i=1}^s \sum_{j=1}^{i-1} \sum_{l=1}^j b_i \alpha_i \alpha_{ij} \delta_{jl} &= \frac{1}{8}, \\
 \sum_{i=1}^s \sum_{j=1}^{i-1} \sum_{l=1}^j b_i \alpha_{ij} (\delta_{jl} \alpha_l + \gamma_{jl}) + \sum_{i=1}^s \sum_{j=1}^i \beta_i (\delta_{ij} \alpha_j + \gamma_{ij}) &= \frac{1}{24}, \\
 \sum_{i=1}^s \sum_{j=1}^i b_i \delta_{ij} \alpha_j^2 &= \frac{1}{12},
 \end{aligned}$$

$$\sum_{i=1}^s \sum_{j=1}^i \sum_{l=1}^{j-1} \sum_{m=1}^l b_i \delta_{ij} \alpha_{jl} \delta_{lm} + \sum_{i=1}^s \sum_{j=1}^i \sum_{l=1}^j b_i \gamma_{ij} \delta_{jl} = \frac{1}{24}.$$

By using notation $\alpha^j = (\alpha_1^j, \dots, \alpha_s^j)^T$ and $(b\alpha)^T = (b_1\alpha_1, \dots, b_s\alpha_s)$, these order conditions can be written as follows:

Order 1:

$$b^T e = 1.$$

Order 2:

$$b^T \alpha + \beta^T e = \frac{1}{2}, \quad b^T \mathcal{A}_\delta e = \frac{1}{2}.$$

Order 3:

$$b^T \alpha^2 = \frac{1}{3}, \quad (b^T \mathcal{A}_\alpha + \beta^T) \mathcal{A}_\delta e = \frac{1}{6}, \quad b^T (\mathcal{A}_\delta \alpha + \mathcal{A}_\gamma e) = \frac{1}{6}.$$

Order 4:

$$\begin{aligned} b^T \alpha^3 &= \frac{1}{4}, & (b\alpha)^T \mathcal{A}_\alpha \mathcal{A}_\delta e &= \frac{1}{8}, & (b^T \mathcal{A}_\alpha + \beta^T) (\mathcal{A}_\delta \alpha + \mathcal{A}_\gamma e) &= \frac{1}{24}, \\ b^T \mathcal{A}_\delta \alpha^2 &= \frac{1}{12}, & b^T (\mathcal{A}_\delta \mathcal{A}_\alpha + \mathcal{A}_\gamma) \mathcal{A}_\delta e &= \frac{1}{24}. \end{aligned}$$

5 Numerical experiments

This section is devoted to the numerical experiments we have made in order to prove the advantages of these methods when solving a non-linear equation.

The Rosenbrock-Nyström methods we have chosen is the one that is developed in [?]. This method is a method with 2 stages and classical order 3. The coefficients of this method are given by the following array:

$$\begin{array}{c|cc||c|c|c} 0 & 0 & 0 & \frac{2}{3} & \frac{2}{3} & 0 \\ \frac{\sqrt{2}}{\sqrt{3}} & \frac{\sqrt{2}}{\sqrt{3}} & -\frac{1}{3} & \frac{2}{3} & \frac{-9-2\sqrt{6}}{9} & \frac{2}{3} \\ \hline & -\frac{\sqrt{6}}{6} & \frac{1}{2} & & & \\ \hline & \frac{1}{2} & \frac{1}{2} & & & \end{array} \quad (19)$$

We have compared this method with the one given in [?] for the method with 2 stages and classical order four. Although this method has higher order than our method, we have selected it because of the same number of stages in order to compare the computational cost. The equations that our two-stage methods give when solving a problem like (??), with $f(t, y(t)) : \mathbb{R}^{n+1} \rightarrow \mathbb{R}$ being such that for every $t > 0$ and $\gamma > 0$, matrix $I - \gamma f_y(t, y(t))$ is invertible. Then, the equations with time step size τ are given by

$$\begin{aligned} (I - \tau^2 \gamma_{11} f_y(t_n, y_n)) K_{n,1} &= \tau v_n + \tau^2 \delta_{11} f(t_n, y_n) + \tau^3 \gamma_{11} f_t(t_n, y_n), \\ (I - \tau^2 \gamma_{22} f_y(t_n, y_n)) K_{n,2} &= \tau v_n + \tau^2 \delta_{21} f(t_n, y_n) + \tau^2 \delta_{22} f(t_n + \alpha_{2\tau}, y_n + \alpha_{21} K_{n,1}) \\ &\quad + \tau^2 \gamma_{21} (\tau f_t(t_n, y_n) + f_y(t_n, y_n) K_{n,1}) + \tau^3 \gamma_{22} f_t(t_n, y_n), \end{aligned}$$

and then,

$$\begin{aligned} v_{n+1} &= v_n + \tau b_1 f(t_n, y_n) + \tau b_2 f(t_n + \alpha_2 \tau, y_n + \alpha_{21} K_1) + \tau^2 f_t(t_n, y_n) \beta^T e \\ &\quad + \tau f_y(t_n, y_n) (\beta_1 K_{n,1} + \beta_2 K_{n,2}) \\ y_{n+1} &= y_n + b_1 K_{n,1} + b_2 K_{n,2}. \end{aligned}$$

In this way, at every step we only have to solve two linear systems

When solving a problem like (??), we have to define $u = [y, v, t]^T$, with $v = y'$ and then, we consider the autonomous system given by (??). For a two-stage method, we define, for $\gamma^2 \geq 0$ a real parameter

$$E \equiv I - \gamma^2 h^2 g_u^2(u_0), \quad , i = 1, 2,$$

Then, we obtain vectors k_1 and k_2 by using the following formulae

$$\begin{aligned} Ek_1 &= g(u_n) + \phi_1 h g_u(u_n) g(u_n) + \theta_1 h g_u(u_n) g(u_n), \\ Ek_2 &= g(u_n + h a_{21} k_1) + \phi_2 h g_u(u_n) g(u_n + h e_{21} k_1) + \theta_2 h g_u(u_n + h b_{21} k_1) g(u_n + h d_{21} k_1) + c_{21} k_1 \end{aligned}$$

And then, u_{n+1} is given by

$$u_{n+1} = u_n + h m_1 k_1 + m_2 k_2$$

An alternative given in this article is to implement the algorithm as:

- Let $L = I - \gamma^2 h^2 f_y$.
- Determine $\{p_i, q_i\}$, for $i = 1, 2$ via

$$\begin{aligned} Lp_1 &= v_n + \eta_1 h f(t_n, y_n) + \gamma^2 h^2 f_t(t_n, y_n), \\ Lq_1 &= f(t_n, y_n) + \eta_1 (f_y(t_n, y_n) v_n + f_t(t_n, y_n)) \\ Lp_2 &= \gamma^2 h^2 (1 + c_{21}) f_t(t_n, y_n) + v_n + a_{21} h q_1 + \phi_2 h f(t_n + e_{21} h, y_n + e_{21} h p_1) \\ &\quad + \theta_2 h f(t_n + d_{21} h, y_n + d_{21} h p_1) + c_{21} p_1, \\ Lq_2 &= \phi_2 h f_y(t_n, y_n) (y_n + e_{21} h q_1) + f(t_n + a_{21} h, y_n + a_{21} h p_1) + \phi_2 h f_t(t_n, y_n) \\ &\quad + \theta_2 h f_y(t_n + b_{21} h, y_n + b_{21} h p_1) (v_n + h d_{21} q_1) + \theta_2 h f_t(t_n + b_{21} h, y_n + b_{21} h p_1) + c_{21} q_1, \end{aligned}$$

and then

$$\begin{aligned} y_{n+1} &= y_n + h(m_1 p_1 + m_2 p_2), \\ v_{n+1} &= v_n + h(m_1 q_1 + m_2 q_2). \end{aligned}$$

We have selected the method that the authors consider in their numerical experiments. The coefficients of this method are:

$$\begin{aligned} d_{21} &= 0, & e_{21} &= a_{21}, & a_{21} &= -0.7777536224724765, \\ b_{21} &= 1.117655988539988, & c_{21} &= -1.109377052294547, & \eta_1 = \theta_1 &= 0.5444631141603234, \\ \phi_2 &= 0.6622450174040982, & \theta_2 &= 0.4462326530351922 & \gamma^2 &= \frac{3 + \sqrt{7}}{12}, \\ m_1 &= 1.022753184288266, & m_2 &= 0.2080352101413627. \end{aligned}$$

The first problem we have solved is the equation presented in example ???. This problem is a modification of the nonlinear wave-propagation suggested in [?]. Here, we have selected the same parameters that were chosen in [?],

$$N = 20, \quad \lambda = 10000, \quad \alpha = 2, \quad p = 3.$$

The second problem was also studied in [?] and is the equation of motion of a soliton in an exponential lattice. This problem was firstly proposed in [?] and it is a highly nonlinear system.

$$\begin{aligned} u_j''(t) &= 2e^{-u_j} - e^{-u_{j-1}} - e^{-u_{j+1}}, \quad j = 1, \dots, N \\ u_j(0) &= -\ln(1 + \beta^2 \operatorname{sech}^2(\alpha j)), \\ u_j'(0) &= \frac{2\beta^3 \operatorname{sech}^2(\alpha j) \tanh(\alpha j)}{1 + \beta^2 \operatorname{sech}^2(\alpha j)}. \end{aligned}$$

with $\alpha = 2$, $\beta = \sinh(\alpha)$ and $N = 20$. The solution of this problem is $u_j(t) = -\ln(1 + \beta^2 \operatorname{sech}^2(\alpha j + \beta t))$.

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