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High order nonstandard finite-difference methods

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ABSTRACT

Nonstandard finite difference (NSFD) methods have been considered to overcome some issues of standard methods, particularly when the numerical solution must preserve important properties of the exact solution. These issues increase for high order methods.

In this paper we first derive a general procedure to obtain unconditionally positive second order NSFD methods. Furthermore, by suitably adding some parameters α_i within these schemes, we show that it is still possible to get positivity, and also to preserve other qualitative properties of the exact solution. In fact, for each particular problem we can get optimal values of α_i that guarantee positivity, elementary stability and the minimization of the local truncation error, being possible to achieve also third order nonstandard schemes, which are not present in the literature.

As an example of use, we employ the developed theory to derive positive and elementary stable NSFD methods of order one, two and three for a predator-prey model, showing their advantages over other nonstandard methods from the literature.

1. Introduction

Numerical methods based on nonstandard finite differences (NSFD) have been considered for the solution of ordinary differential equations (ODEs) and partial differential equations (PDEs), particularly when the physical model requires that the numerical scheme preserves some relevant properties, like positivity or elementary stability. This is the case, for example, in chemical reactions, evolution of epidemics or biological models [1–10].

In this work, we focus on the most general autonomous nonlinear differential system

$$x' = f(x), \qquad x(t_0) = x_0, \tag{1}$$

where $f : \mathbb{R}^{N+1} \to \mathbb{R}^N$ is a sufficiently smooth function, and the exact solution $x(t)$ is positive, this is

$$x_0 \geqslant 0 \quad \Rightarrow \quad x(t) \geqslant 0 \quad \text{for all } t \in \left[t_0, T\right], \tag{2}$$

where the inequalities are meant to be componentwise.

Forward Euler method preserves positivity under some step-size restrictions, while backward Euler is unconditionally positive. In general, unconditionally positive Runge-Kutta methods (RKM) must have order less than or equal to one [11]. We are interested in higher-order numerical methods that preserve this property. Furthermore, we are also concerned about the preservation of the local asymptotic stability. Many researchers have worked on developing NSFD methods that preserve these properties [3–5,7,12–15]

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in different models. However, in the mentioned works the authors propose NSFD methods that preserve positivity and asymptotic stability with order two at most and, to our knowledge, there are no methods of order three with such characteristics. In this paper, we propose a new general procedure that can improve existing first and second order NSFD methods, preserving positivity and asymptotic stability. Furthermore, thanks to the new procedure, we show that it is also possible to obtain third order NSFD methods.

Let us describe below a biological model and an epidemiological system, both of which are often discussed in the literature.

Rosenzweig-MacArthur predator-prey model is studied in detail in [4,5,16]. There the authors consider a logistic intrinsic growth of the prey population of the form

$$\begin{aligned} \frac{dx^1}{dt} &= f^1(x^1,x^2) := bx^1(1-x^1) - ag(x^1)x^1x^2, \quad x^1(0) = x^1_0 \geq 0, \\ \frac{dx^2}{dt} &= f^2(x^1,x^2) := g(x^1)x^1x^2 - dx^2, \quad x^2(0) = x^2_0 \geq 0\,. \end{aligned} \tag{3}$$

We summarize below the main features of system (3). For more details, see [4,5,16]. If all the parameters are positive and the function g satisfies

$$g(x^1) \geq 0, \quad g'(x^1) \leq 0, \quad \left(x^1 g(x^1)\right)' \geq 0, \quad x^1 g(x^1) \text{ is bounded as } x^1 \to \infty,$$

then, the solution is positive. The origin $E_0 = (0,0)$ is always an equilibrium point (unstable). The boundary point $E_1 = (1,0)$ is also an equilibrium point (asymptotically stable if $g(1) < d$, and unstable if $g(1) > d$). Finally, if $g(1) > d$, there exists an interior equilibrium point $\bar{E} = (\bar{x}^1, \bar{x}^2)$ given by

$$\bar{x}^1\, g(\bar{x}^1) = d, \qquad \bar{x}^2 = \frac{b\bar{x}^1(1-\bar{x}^1)}{ad}\,.$$

This interior point is asymptotically stable if $b + a\bar{x}^2 g'(\bar{x}^1) > 0$ and is unstable if $b + a\bar{x}^2 g'(\bar{x}^1) < 0$.

We also mention a simple version of the compartmental Kermack-McKendrick SIR model [7,13,17,18]. This epidemiological system is described by equations

$$\begin{aligned} \frac{dx^1}{dt} &= f^1(x^1,x^2,x^3) := \mu(1-x^1) - \beta\, x^2 x^1, \\ \frac{dx^2}{dt} &= f^2(x^1,x^2,x^3) := -\mu\, x^2 - \gamma\, x^2 + \beta\, x^2 x^1, \\ \frac{dx^3}{dt} &= f^3(x^1,x^2,x^3) := -\mu\, x^3 + \gamma\, x^2, \end{aligned} \tag{4}$$

where $x^1(t)$, $x^2(t)$ and $x^3(t)$ represent positive quantities of people over time and μ, β and γ are positive parameters of the model.

Observe that in systems like (3) or (4) the right hand side $f = f_+ + f_-$ can be split into two terms, where f_+ is the positive part and f_- the negative one. In this work we construct general NSFD schemes applied to this kind of problems and obtain second order NSFD methods that can preserve both the positivity of solutions and the local asymptotic stability of equilibria. Besides, we introduce a new class of α-NSFD methods, depending on some parameters α_i, that allows to achieve a third order scheme. The parameters α_i are added in such a way that: when $\alpha_i = 0$ we recover the standard forward Euler scheme, which is not necessarily positive; when $\alpha_i = 1$ we get the classical NSFD method that ensures unconditional positivity of the numerical solution. Finally, we also show the construction of a third order positive NSFD scheme from a two-stage Runge-Kutta method, named α-NSFDRK. As an example of use, the developed theory is employed to derive new methods for the Rosenzweig-MacArthur predator-prey model (3).

The paper is organized as follows. In Section 2 we review NSFD methods applied to models like (3)-(4). In Section 3 we propose a generalization of positive NSFD methods for problem (1) where the function f can be split into positive and negative terms, and, for these methods, we obtain conditions to get second order. A new class of α-NSFD schemes is presented in Section 4, where the parameters α_i allow us to control the positivity of the numerical solution. The new schemes not only preserve the positivity, but also are elementary stable and can achieve third order. In Section 5 we extend these ideas to Runge-Kutta methods in order to obtain other high order positive methods. We illustrate our results by numerical examples in Section 6.

2. Nonstandard finite difference methods

NSFD methods allow to approximate the function f in a different way than the classical case [4,5,7,12,13,15]. By defining the discrete grid $\{t_k = t_0 + k\Delta t,\ k = 0,\dots,K;\ t_K = T\}$, being $x_k \approx x(t_k)$, the two fundamental rules on which these schemes are based can be written for the scalar case as follows.

1. In the approximation of $x'(t_k)$, the discretization step-size Δt is replaced by a non-negative scalar function $\phi(\Delta t) = \Delta t + O\left(\Delta t^2\right)$, giving rise to

$$x'(t_k) \approx \frac{x_{k+1} - x_k}{\phi(\Delta t)}\,.$$

2. The function f in (1) is non-locally modified, i.e. some of its terms can be reshaped using different grid points. For example, terms such as x^2 can be approximated with $x_{k+1}x_k$ instead of x_k^2 (see [4,5,13,15] for more details).

These representations can improve the stability properties of the standard methods, allowing the nonstandard numerical scheme to preserve qualitative characteristics of the model like positivity or elementary stability. We recall below these two desirable properties for the numerical scheme.

We say that the numerical method preserves the positivity of the continuous scheme (2) if the numerical solution satisfies

$$x_k \geq 0, \quad k = 1, \dots, K, \quad \text{given} \quad x_0 \geq 0,$$

where the inequality must be understood componentwise.

Similarly, a numerical method is called elementary stable if, for any value of the step-size Δt, its fixed-points are those of the differential system (1), and if the linear stability properties of each fixed point are the same for both the differential system and the discrete method.

Following the above rules 1 and 2, the NSFD methods present in the literature are constructed for specific problems. We report some examples below and, in the next section, we derive a general class of NSFD methods for systems like (3)-(4), where the function f can be split into positive and negative terms.

NSFD methods were considered in [19] to overcome some difficulties of standard numerical methods on the preservation of the dynamic properties of differential equations. First NSFD schemes correctly preserve these properties but most of them are convergent only up to the first order. Burchard et al. considered the Patankar trick [20] and modified Patankar technique to get positive and conservative second order schemes for fully conservative production-destruction systems in [21]. Based also on the Patankar trick, Dimitrov and Kojouharov [4,14] constructed positive and elementary stable nonstandard (PESN) schemes for the predator-prey model (3) of the form

$$\begin{aligned} \frac{x^1_{k+1} - x^1_k}{\phi^1(\Delta t)} &= b x^1_k - b x^1_{k+1} x^1_k - a g\left(x^1_k\right) x^1_{k+1} x^2_k, \\ \frac{x^2_{k+1} - x^2_k}{\phi^2(\Delta t)} &= g\left(x^1_k\right) x^1_k x^2_k - d x^2_{k+1}, \end{aligned} \tag{5}$$

where $\phi^i(\Delta t) = \Delta t + \mathcal{O}(\Delta t^2)$. This scheme preserves positivity and it is elementary stable, though it achieves just order one. Some work has also been done on the SIR model in the field of nonstandard methods. For example, Mickens [15] proposed the following NSFD method for SIR problem (4)

$$\begin{aligned} \frac{x^1_{k+1} - x^1_k}{\phi^1(\Delta t)} &= \mu\left(1 - x^1_{k+1}\right) - \beta\, x^2_k x^1_{k+1}, \\ \frac{x^2_{k+1} - x^2_k}{\phi^2(\Delta t)} &= -\mu\, x^2_{k+1} - \gamma\, x^2_{k+1} + \beta\, x^2_k x^1_{k+1}, \\ \frac{x^3_{k+1} - x^3_k}{\phi^3(\Delta t)} &= -\mu\, x^3_{k+1} + \gamma\, x^2_{k+1}, \end{aligned} \tag{6}$$

with the same functions $\phi^i(\Delta t) = \phi(\Delta t)$ in the denominator. This scheme, analogous to modified Patankar technique [16,20], is positive and preserves the mass $M_k := x^1_k + x^2_k + x^3_k$ of the system.

Blanes et al. got second order methods [1] that unconditionally preserve positivity, but biological problems like (5) have also stability properties that should be preserved. In the recent papers [12,22] the authors obtained new explicit second order modified NSFD methods for solving some biological systems. The new schemes are elementary stable, but nothing is said about other properties of the solution. Also in a recent paper [5], Hoang, et al. obtained a positive second order NSFD method for the Rosenzweig-MacArthur predator-prey model that preserves the asymptotic stability of the equilibrium points.

In this work we obtain a new class of positive, elementary stable and second order α-NSFD methods, depending on some parameters α_i, for general problems. The parameters α_i can be used to minimize the local error, being possible in some problems to achieve positive, elementary stable third order schemes.

3. Second order NSFD for general problems

Eqs. (5) and (6) are particular examples of positive NSFD methods [14,15]. Below we derive a procedure for constructing positive NSFD methods for general problems, by observing that both these schemes can be expressed in a unified framework. For the general nonlinear differential system (1) it is possible to write the corresponding NSFD method like

$$\frac{x^i_{k+1} - x^i_k}{\phi^i(\Delta t, x_k)} = f^i(x_k) + \frac{x^i_{k+1} - x^i_k}{x^i_k} f^i_-(x_k), \quad i = 1, \dots, N, \tag{7}$$

where we have split the function $f = f_+ + f_-$ into a positive f_+ and a negative f_- term. For example, in system (3)

$$f_+(x^1, x^2) = (b x^1, g(x^1) x^1 x^2), \qquad f_-(x^1, x^2) = (-b x^1 x^1 - a g(x^1) x^1 x^2, -d x^2).$$

For large dimension problems it is worth writing the general NSFD scheme (7) in vector notation like this

$$\phi^{-1}(\Delta t, x_k)(x_{k+1} - x_k) = f(x_k) - f_-(x_k) + Df(x_k)\, x_{k+1} = f_+(x_k) + Df(x_k)\, x_{k+1}, \tag{8}$$

where we have denoted $\phi(\Delta t, x_k) = \mathrm{diag}(\phi^i(\Delta t, x_k))$ and $Df(x_k) = \mathrm{diag}(f^i_-(x_k)/x^i_k)$.

Remark 1. Observe that, if $\phi^i(\Delta t, x_k) = \Delta t$ in Eq. (7), then this scheme coincides with Patankar Euler scheme (PE) considered in [21] for fully conservative problems.

We prove below the positivity of the general NSFD scheme (7) derived in this section.

Theorem 1. *The NSFD method (7) preserves the numerical positivity of the model (1) for all the values of the step-size Δt, that is, $x_k \geq 0$ for all $k \geq 1$ whenever $x_0 \geq 0$.*

Proof. The proof is done by induction. Since $x_0 \geq 0$, we assume that $x_k \geq 0$ and show that $x_{k+1} \geq 0$. To get that we write Eq. (7) into explicit form by collecting the x_{k+1} terms

$$x^i_{k+1}\left(1 - \frac{\phi^i f^i_-}{x^i_k}\right) = x^i_k + \phi^i f^i - \phi^i f^i_- = x^i_k + \phi^i (f^i - f^i_-) = x^i_k + \phi^i f^i_+ \quad \Rightarrow \quad x^i_{k+1} = \frac{x^i_k + \phi^i f^i_+}{1 - \phi^i f^i_-/x^i_k},$$

where all the functions f are evaluated at x_k, and $\phi^i \geq 0$ is evaluated at $(\Delta t, x_k)$. As the difference $f - f_- = f_+$ is always positive, we conclude $x^i_{k+1} \geq 0$. $\square$

Remark 2. Note that, from the last equation, we can write x^i_{k+1} as

$$x^i_{k+1} = \frac{x^i_k + \phi^i f^i_+}{1 - \phi^i f^i_-/x^i_k} = \frac{x^i_k + \phi^i f^i - \phi^i f^i_-}{1 - \phi^i f^i_-/x^i_k} = x^i_k + \frac{\phi^i f^i}{1 - \phi^i f^i_-/x^i_k},$$

or in vector notation

$$x_{k+1} = \left(I - \phi\, Df(x_k)\right)^{-1}\left(x_k + \phi\, f_+\right) = x_k + \left(I - \phi\, Df(x_k)\right)^{-1} \phi\, f.$$

This will be useful in the following to get the Taylor series of x_{k+1}.

Next we get conditions on the functions $\phi^i(\Delta t, x)$ in the denominator of (7) so that the scheme achieves second order. To get that we need the expansion of the exact and the numerical solutions. Then, as an example, we will apply this general result to the differential problems (3) and (4).

Theorem 2. *If the functions ϕ^i, $i = 1, \dots, N$, of the NSFD method (7) satisfy the conditions*

$$(\phi^i)''(0, x) = \frac{\partial f^i(x)}{\partial x^i} + \sum_{\substack{j=1 \\ j\neq i}}^{N} \frac{\partial f^i(x)}{\partial x^j}\, \frac{f^j(x)}{f^i(x)} - 2\frac{f^i_-(x)}{x^i_k}, \tag{9}$$

for all $x \in \mathbb{R}^N_+$ and $f^i(x) \neq 0$, $i = 1, \dots, N$, then, the local truncation error of the NSFD method (7) is $\mathcal{O}(\Delta t^3)$.

Proof. Expanding the exact solution of (1) into a Taylor series, we get

$$x^i(\Delta t) = x^i(0) + \Delta t\, f^i(x_0) + \frac{1}{2}\sum_{j=1}^{N} \frac{\partial f^i(x_0)}{\partial x^j} f^j(x_0)\, \Delta t^2 + \mathcal{O}(\Delta t^3). \tag{10}$$

If we consider $\phi^i(\Delta t, x) = \Delta t + \frac{1}{2}(\phi^i)''(0, x)\, \Delta t^2 + \mathcal{O}(\Delta t^3)$, then, from Remark 2 and the expansion of the function $1/(1-x) = 1 + x + x^2 + \cdots$, it is easy to get the Taylor expansion of the numerical solution x^i_1 in (7)

$$x^i_1 = x^i_0 + \Delta t\, f^i(x_0) + \left(\frac{f^i(x_0) f^i_-(x_0)}{x^i_0} + \frac{1}{2} f^i(x_0)(\phi^i)''(0, x_0)\right)\Delta t^2 + \mathcal{O}(\Delta t^3). \tag{11}$$

Comparing both series (10) and (11), we get the conditions (9) on the second derivative. $\square$

Example 1. In the particular case $N = 2$, the conditions (9) coincide with the ones obtained in [5, Eq. (22)] for the predator-prey scheme (5). If $N = 3$, we can apply the result to the discretized SIR model (6), and the conditions (9) on the second derivative $(\phi^i)''$ are

$$(\phi^1)''\left(0, x^1_k, x^2_k, x^3_k\right) = \frac{\mu^2(x^1_k - 1) + \mu\,\beta(x^1_k - 1)x^2_k + \beta\, x^1_k x^2_k(\beta(x^1_k + x^2_k) - \gamma)}{\mu(x^1_k - 1) + \beta x^1_k x^2_k},$$

$$(\phi^2)''\left(0, x^1_k, x^2_k, x^3_k\right) = \frac{\mu^2 + 2\,\mu\,\gamma + \gamma^2 + \mu\,\beta(x^1_k - 1) + \beta^2 x^1_k(x^2_k - x^1_k)}{\mu + \gamma - \beta x^1_k},$$

$$(\phi^3)''\left(0, x^1_k, x^2_k, x^3_k\right) = \frac{\gamma(\gamma - \beta x^1_k)x^2_k + \mu^2 x^3_k}{-\gamma\, x^2_k + \mu\, x^3_k}.$$

4. α-NSFD methods

Theorems 1 and 2 ensure positivity and second order for the numerical solution in (7). However, the continuous problem (1) may have other properties that should be preserved. In [5,12,13,15,22] the authors consider NSFD schemes like (5) or (6) with particular elections of the functions ϕ^i for different purposes. In [12] second order NSFD methods that preserve elementary stability are obtained, while in [5] the addition of some weights in the discretization allows to preserve both, positivity and elementary stability, for the new second order NSFD methods proposed.

The general scheme (7), based on the Patankar-trick [20,21], is unconditionally positive, but in some problems it may lead to time lag effects on the numerical solution (see [21, Figs. 13 and 14] for details). It is possible to relax the positivity requirement by adding some parameters $\alpha^i \geq 0$, $i = 1, \ldots, N$, in the numerical scheme (7) in the following way

$$\frac{x^i_{k+1} - x^i_k}{\phi^i(\Delta t, x_k)} = f^i(x_k) + \alpha^i \, \frac{x^i_{k+1} - x^i_k}{x^i_k} f^i_-(x_k), \quad i = 1, \ldots, N\,. \tag{12}$$

As shown below, the new schemes, namely α-NSFD methods, can still be second order for any value of the parameters and, what is more, for certain values of α^i, these methods are unconditionally positive.

Remark 3. Observe that the case $\alpha^i = 0$, $i = 1, \ldots, N$, corresponds with the basic explicit Euler method (if $\phi^i = \Delta t$), while $\alpha^i = 1$, $i = 1, \ldots, N$, gives us the unconditionally positive scheme (7).

Theorem 3. *The α-NSFD method (12) preserves the numerical positivity of the model (1) if $\alpha^i \geq f^i(x)/f^i_-(x)$, $i = 1, \ldots, N$, $x \geq 0$.*

Proof. The proof is analogous to that in Theorem 1. Now, Eq. (12) in explicit form is

$$x^i_{k+1}\left(1 - \alpha^i \, \frac{\phi^i f^i_-}{x^i_k}\right) = x^i_k + \phi^i f^i - \alpha^i \phi^i f^i_- = x^i_k + \phi^i \left(f^i - \alpha^i f^i_-\right),$$

$$x^i_{k+1} = \frac{x^i_k + \phi^i \left(f^i - \alpha^i f^i_-\right)}{1 - \alpha^i \phi^i f^i_-/x^i_k}, \tag{13}$$

where all the functions f and ϕ are evaluated at x_k and $(\Delta t, x_k)$, respectively. As the denominator is positive, we get the following inequality

$$x^i_{k+1} \geq 0 \quad \Longleftrightarrow \quad x^i_k + \phi^i \left(f^i - \alpha^i f^i_-\right) \geq 0\,.$$

In particular we get positivity if $\alpha^i \geq \frac{f^i}{f^i_-}$, $i = 1, \ldots, N$. □

Remark 4. The Taylor series of the numerical solution in (12) is easy to get if we write (13) like

$$x^i_{k+1} = \frac{x^i_k + \phi^i \left(f^i - \alpha^i f^i_-\right)}{1 - \alpha^i \phi^i f^i_-/x^i_k} = x^i_k + \phi^i f^i \, \frac{1}{1 - \alpha^i \phi^i f^i_-/x^i_k}.$$

Then, from the expansion of the function $1/(1-x) = 1 + x + x^2 + \cdots$, we get

$$x^i_{k+1} = x^i_k + \phi^i f^i \left(1 + \alpha^i \phi^i f^i_-/x^i_k + (\alpha^i \phi^i f^i_-/x^i_k)^2 + \cdots\right).$$

Considering the expansion of ϕ^i up to third order $\phi^i = \Delta t + \frac{1}{2}(\phi^i)'' \Delta t^2 + \frac{1}{6}(\phi^i)''' \Delta t^3 + \mathcal{O}(\Delta t^4)$, we can finally write

$$x^i_{k+1} = x^i_k + f^i \Delta t + \left(\tfrac{1}{2}(\phi^i)'' f^i + \alpha^i f^i f^i_-/x^i_k\right) \Delta t^2 \tag{14}$$

$$+ \left(\tfrac{1}{6}(\phi^i)''' f^i + \alpha^i (\phi^i)'' f^i f^i_-/x^i_k + (\alpha^i f^i_-/x^i_k)^2 f^i\right) \Delta t^3 + \mathcal{O}(\Delta t^4). \tag{15}$$

Theorem 4. *If the functions ϕ^i, $i = 1, \ldots, N$, of the α-NSFD method (12) satisfy the conditions*

$$(\phi^i)''(0, x) = \frac{\partial f^i(x)}{\partial x^i} + \sum_{\substack{j=1\\ j\neq i}}^{N} \frac{\partial f^i(x)}{\partial x^j} \frac{f^j(x)}{f^i(x)} - 2\,\alpha^i \, \frac{f^i_-(x)}{x^i_k}, \tag{16}$$

for all $x \in \mathbb{R}^N_+$ and $f^i(x) \neq 0$, $i = 1, \ldots, N$, then, the local truncation error of the α-NSFD method (12) is $\mathcal{O}(\Delta t^3)$.

Proof. The proof is analogous to that in Theorem 2. Now, according to (14), the Taylor expansion of x^i_1 in (12) is

$$x^i_1 = x^i_0 + \Delta t \, f^i(x_0) + \left(\frac{1}{2} f^i(x_0)(\phi^i)''(0, x_0) + \frac{\alpha^i \, f^i(x_0) f^i_-(x_0)}{x^i_0}\right) \Delta t^2 + \mathcal{O}(\Delta t^3)\,. \tag{17}$$

Finally, by subtracting the expansions (10) and (17), we get the statement (16). □

Remark 5. The election of the functions ϕ^i such that (16) is satisfied, allows to get second order for any value of the parameters α^i. Note that, in particular, we can reach second order by choosing $\phi^i = \Delta t$ and

$$\alpha^i \left(= \alpha^i(x)\right) = \frac{x^i_k}{2 f^i_-(x)} \left(\frac{\partial f^i(x)}{\partial x^i} + \sum_{\substack{j=1\\ j\neq i}}^{N} \frac{\partial f^i(x)}{\partial x^j} \frac{f^j(x)}{f^i(x)}\right),$$

i.e. by varying the values of α^i during the time integration. In the numerical tests, we have used also this method, namely $\alpha^i(x)$-NSFD2.

Once we have guaranteed second order and positivity, we analyze conditions on the parameters so that the α-NSFD method also preserves other properties of the problem. In the theorem below we give sufficient conditions on the parameters so that the scheme (12), applied to the predator-prey model (3), is elementary stable.

Theorem 5. *For the discrete scheme (12), applied to differential system (3), the following holds true.*

1. *The trivial equilibrium point $E_0 = (0,0)$ is always unstable.*
2. *If $g(1) > d$, then the boundary equilibrium point $E_1 = (1,0)$ is unstable.*
3. *If $g(1) < d$ and $\alpha^i \geq \bar{\alpha}^i$, with $\bar{\alpha}^i = 1/2$, $i = 1,2$, then the boundary equilibrium point E_1 is locally asymptotically stable.*
4. *Suppose the interior equilibrium point $\bar{E} = (\bar{x}^1, \bar{x}^2)$ exists ($g(1) > d$) and $b + a\bar{x}^2 g'(\bar{x}^1) > 0$. Then the point $\bar{E}$ is locally asymptotically stable if*

$$\alpha^1 \geq \bar{\alpha}^1 := \frac{\bar{x}^1\left(b + a\,\bar{x}^2 g'(\bar{x}^1)\right)}{2b} \qquad \text{and} \qquad \alpha^2 \geq \bar{\alpha}^2 := \frac{a\,\bar{x}^2\left(g(\bar{x}^1) + \bar{x}^1 g'(\bar{x}^1)\right)}{\bar{x}^1\left(b + a\,\bar{x}^2 g'(\bar{x}^1)\right)}. \tag{18}$$

5. *If $g(1) < d$ and $b + a\bar{x}^2 g'(\bar{x}^1) < 0$, then the point $\bar{E}$ is unstable.*

Proof. The proof is similar to that in [5, Theorem 4]. In this case, the scheme (12) can be written like

$$x^i_{k+1} = x^i_k + \frac{\phi^i f^i}{1 - \alpha^i \phi^i f^i_- / x^i_k}, \qquad i = 1,2. \tag{19}$$

Consequently, the set of equilibria of the α-NSFD method (12) coincides with the set of equilibria of the continuous-time predator-prey model (3). If $x = (x^1, x^2)$ is an equilibrium point of the system (12), applied to problem (3), then from (19) the Jacobian matrix of (12) evaluated at this point is $J^D(x) = (J^D_{ij}(x))$, where

$$J^D_{ij}(x) = \delta_{ij} + \frac{\phi^i(\Delta t, x)\, J^C_{ij}(x)}{1 - \alpha^i\, \phi^i(\Delta t, x)\, f^-_i(\Delta t, x)/x^i}, \tag{20}$$

and $J^C = (J^C_{ij})$ being the Jacobian of the predator-prey system (3). Finally, we obtain

$$J^D(x) = \begin{pmatrix} 1 + \dfrac{\phi^1(\Delta t, x)\,(b - 2bx^1 - ax^2(x^1 g'(x^1) + g(x^1)))}{1 + \alpha^1\, \phi^1(\Delta t, x)(bx^1 + ag(x^1)x^2)} & \dfrac{\phi^1(\Delta t, x)\,(-ag(x^1)x^1)}{1 + \alpha^1\, \phi^1(\Delta t, x)(bx^1 + ag(x^1)x^2)} \\ \dfrac{\phi^2(\Delta t, x)\,(x^2(x^1 g'(x^1) + g(x^1)))}{1 + \alpha^2\, \phi^2(\Delta t, x)\, d} & 1 + \dfrac{\phi^2(\Delta t, x)\,(g(x^1)x^1 - d)}{1 + \alpha^2\, \phi^2(\Delta t, x)\, d} \end{pmatrix}.$$

1. Evaluating the Jacobian matrix at the point $E_0 = (0,0)$ we get

$$J^D(0,0) = \begin{pmatrix} 1 + b\,\phi^1(\Delta t, 0, 0) & 0 \\ 0 & 1 - \dfrac{\phi^2(\Delta t, 0, 0)\, d}{1 + \alpha^2\, \phi^2(\Delta t, 0, 0)\, d} \end{pmatrix}.$$

   Clearly we get $\lambda_1 = 1 + b\,\phi^1 > 0$, and the point E_0 is unstable.
2. Evaluating J^D at the boundary point $E_1 = (1,0)$ we obtain

$$J^D(1,0) = \begin{pmatrix} 1 - \dfrac{b\,\phi^1(\Delta t, 1, 0)}{1 + \alpha^1\, \phi^1(\Delta t, 1, 0)\, b} & \dfrac{-a\, g(1)\phi^1(\Delta t, 1, 0)}{1 + \alpha^1\, \phi^1(\Delta t, 1, 0)\, b} \\ 0 & 1 + \dfrac{\phi^2(\Delta t, 1, 0)\,(g(1) - d)}{1 + \alpha^2\, \phi^2(\Delta t, 1, 0)\, d} \end{pmatrix}.$$

   If $g(1) - d > 0$, then $\lambda_2 > 1$, and the point E_1 is unstable.
3. Under the assumption $g(1) - d < 0$, the inequalities $-1 < \lambda_1 < 1$ and $-1 < \lambda_2 < 1$ are equivalent to

$$\alpha^1 > \frac{1}{2} - \frac{1}{b\,\phi^1} \qquad \text{and} \qquad \alpha^2 > \frac{1}{2} - \frac{2 + \phi^2}{2d\,\phi^2},$$

   respectively. Consequently, If $g(1) < d$ and $\alpha^i \geq 1/2$, $i = 1,2$, then the boundary equilibrium point E_1 is locally asymptotically stable.
4. Remember that the point $\bar{E} = (\bar{x}^1, \bar{x}^2)$ exists just if $g(1) < d$. The Jacobian matrix at $\bar{E}$ is

$$J^D(\bar{E}) = \begin{pmatrix} 1 - \dfrac{\phi^1 \bar{x}^1 (b + a\bar{x}^2\, g'(\bar{x}^1))}{1 + b\,\alpha^1\, \phi^1} & \dfrac{-a\, d\, \phi^1}{1 + b\,\alpha^1\, \phi^1} \\ \dfrac{\phi^2 \bar{x}^2 (g(\bar{x}^1) + \bar{x}^1\, g'(\bar{x}^1))}{1 + d\,\alpha^2\, \phi^2} & 1 \end{pmatrix},$$

   where the functions ϕ^i are evaluated at $(\Delta t, \bar{x}^1, \bar{x}^2)$. The characteristic polynomial of this matrix is

$$\begin{aligned}p(\lambda) &= \lambda^2 - \mathrm{Tr}(J^D(\bar{E}))\,\lambda + \det(J^D(\bar{E}))\\ &= \lambda^2 - \left(2 - \frac{\phi^1\bar{x}^1(b+a\bar{x}^2\,g')}{1+b\,\alpha^1\,\phi^1}\right)\lambda + \left(1 - \frac{\phi^1\bar{x}^1(b+a\bar{x}^2\,g')}{1+b\,\alpha^1\,\phi^1} + \frac{a\,d\,\phi^1}{1+b\,\alpha^1\,\phi^1}\,\frac{\phi^2\bar{x}^2(g+\bar{x}^1\,g')}{1+d\,\alpha^2\,\phi^2}\right),\end{aligned}$$

where both, g and g', are evaluated at $\bar{x}^1$ henceforth. According to Theorem 2 in [5] inequalities $-1<\lambda_1<1$ and $-1<\lambda_2<1$ are equivalent to

$$\det(J^D(\bar{E}))<1,\quad 1\pm\mathrm{Tr}(J^D(\bar{E}))+\det(J^D(\bar{E}))>0\,.$$

From the first inequality we get

$$\begin{aligned}\det(J^D(\bar{E}))<1 &\Leftrightarrow -\frac{\phi^1\bar{x}^1(b+a\bar{x}^2\,g')}{1+b\,\alpha^1\,\phi^1} + \frac{a\,d\,\phi^1}{1+b\,\alpha^1\,\phi^1}\,\frac{\phi^2\bar{x}^2(g+\bar{x}^1\,g')}{1+d\,\alpha^2\,\phi^2} < 0\\ &\Leftrightarrow \frac{a\,d}{1}\,\frac{\phi^2\bar{x}^2(g+\bar{x}^1\,g')}{1+d\,\alpha^2\,\phi^2} < \frac{\bar{x}^1(b+a\bar{x}^2\,g')}{1}\\ &\Leftrightarrow a\,g\,\bar{x}^1\phi^2\bar{x}^2(g+\bar{x}^1\,g') < \bar{x}^1(b+a\bar{x}^2\,g')(1+d\,\alpha^2\,\phi^2)\\ &\Leftrightarrow -(b+a\bar{x}^2\,g') - (b+a\bar{x}^2\,g')(d\,\alpha^2\,\phi^2) + a\,g\,\phi^2\bar{x}^2(g+\bar{x}^1\,g') < 0\,. \end{aligned}\tag{21}$$

Remember that $(\bar{x}^1\ g)' = g+\bar{x}^1g' \geq 0$ and $b+a\bar{x}^2g' \geq 0$ by hypothesis. Consequently, if

$$-(b+a\bar{x}^2g')d\,\alpha^2 + a\,g\,\bar{x}^2(g+\bar{x}^1g') = -(b+a\bar{x}^2g')\bar{x}^1\,\alpha^2 + a\,\bar{x}^2(g+\bar{x}^1g') \leq 0 \tag{22}$$

holds, then inequality (21) is true. Finally, we can write the sufficient condition (22) as

$$\alpha^2 \geq \frac{a\,\bar{x}^2(g+\bar{x}^1\,g')}{\bar{x}^1(b+a\bar{x}^2\,g')}\,.$$

Second inequality $1-\mathrm{Tr}(J^D(\bar{E}))+\det(J^D(\bar{E}))>0$ is immediate: we just have to write

$$1-\mathrm{Tr}(J^D(\bar{E}))+\det(J^D(\bar{E})) = \frac{a\,d\,\phi^1}{1+b\,\alpha^1\,\phi^1}\,\frac{\phi^2\bar{x}^2(g+\bar{x}^1\,g')}{1+d\,\alpha^2\,\phi^2} > 0\,.$$

For the last inequality, $1+\mathrm{Tr}(J^D(\bar{E}))+\det(J^D(\bar{E}))>0$, we have

$$1+\mathrm{Tr}(J^D(\bar{E}))+\det(J^D(\bar{E})) = 4-2\,\frac{\phi^1\bar{x}^1(b+a\bar{x}^2\,g')}{1+b\,\alpha^1\,\phi^1} + \frac{a\,d\,\phi^1}{1+b\,\alpha^1\,\phi^1}\,\frac{\phi^2\bar{x}^2(g+\bar{x}^1\,g')}{1+d\,\alpha^2\,\phi^2} > 0\,.$$

As the last term is positive, we obtain the condition

$$4-2\,\frac{\phi^1\bar{x}^1(b+a\bar{x}^2\,g')}{1+b\,\alpha^1\,\phi^1} \geq 0.$$

And this inequality holds if

$$\alpha^1 \geq \frac{\bar{x}^1(b+a\bar{x}^2\,g')}{2b}.$$

5. If $b+a\bar{x}^2g'<0$, it is immediate that $\det(J^D(\bar{E}))-1>0$, and this implies that the interior equilibrium point $\bar{E}$ is unstable. □

4.1. A third order positive and elementary stable α-NSFD method

Theorems 3 and 4 ensure positivity and second order for the method (12). Also, Theorem 5 ensures elementary stability for the method (12) on problem (3). Observe that we can still use the parameters α^i, $i=1,\dots,N$, to minimize, for example, the local truncation error (LTE). In fact, it is also possible to annihilate the main term of the LTE along the integration process, thus getting an explicit third order nonstandard method, namely $\alpha^i(x)$-NSFD3. We briefly describe below the general procedure for the election of parameters α^i to obtain this third order α-NSFD scheme.

Consider the next $\mathcal{O}(\Delta t^3)$ terms in the Taylor expansion of the exact solution (10)

$$\frac{1}{6}\left(\sum_{j_1,j_2=1}^{N}\frac{\partial^2 f^i(x_0)}{\partial x^{j_1}\,\partial x^{j_2}}\,f^{j_1}(x_0)\,f^{j_2}(x_0) + \sum_{j=1}^{N}\frac{\partial f^i(x_0)}{\partial x^j}\Big(\sum_{\ell=1}^{N}\frac{\partial f^j(x_0)}{\partial x^\ell}\,f^\ell(x_0)\Big)\right)\Delta t^3 + \mathcal{O}(\Delta t^4), \tag{23}$$

and the corresponding terms in numerical solution already obtained in (15)

$$\left(\frac{1}{6}(\phi^i)'''(0,x_0)f^i + \frac{\alpha^i(\phi^i)''(0,x_0)f^i\,f^i_-(x_0)}{x^i_0} + \left(\frac{\alpha^i\,f^i_-(x_0)}{x^i_0}\right)^2 f^i\right)\Delta t^3 + \mathcal{O}(\Delta t^4). \tag{24}$$

Comparing (23) and (24), and annihilating the $\mathcal{O}(\Delta t^3)$ coefficients, the α-NSFD method (12), with ϕ^i satisfying (16), reaches order three.

For the particular case $N = 2$, like the predator-prey model (3), we report below the values of α^1 and α^2 that annihilate the $\mathcal{O}(\Delta t^3)$ terms. The corresponding third order method $\alpha^i(x)$-NSFD3 is obtained by choosing

$$\alpha^i \left(= \alpha^i(x)\right) = \frac{\sum_{j=1}^2 f^i_{x^j} f^j + \sqrt{\alpha^i_{\text{num}}}}{2\, f^i f^i_- / x^i}, \qquad i = 1, 2\,, \tag{25}$$

with

$$\alpha^1_{\text{num}} = -2(f^1)^3 f^1_{x^1x^1} + 3(f^1_{x^2} f^2)^2 - (f^1)^2\left(4 f^2 f^1_{x^1x^2} + 2 f^1_{x^2} f^2_{x^1} - (f^1_{x^1})^2\right) - 2 f^1 f^2 (f^1_{x^2x^2} f^2 + f^1_{x^2} f^2_{x^2} - 2 f^1_{x^1} f^1_{x^2}),$$

$$\alpha^2_{\text{num}} = -2(f^2)^3 f^2_{x^2x^2} + 3(f^2_{x^1} f^1)^2 - (f^2)^2\left(4 f^1 f^2_{x^1x^2} + 2 f^1_{x^2} f^2_{x^1} - (f^2_{x^2})^2\right) - 2 f^2 f^1 (f^2_{x^1x^1} f^1 + f^2_{x^1} f^1_{x^1} - 2 f^2_{x^2} f^2_{x^1}),$$

where, for brevity, we have used the notation

$$f^i = f^i(x), \qquad f^i_{x^j} = \frac{\partial f^i(x)}{\partial x^j}, \qquad f^i_{x^j x^\ell} = \frac{\partial^2 f^i(x)}{\partial x^j \partial x^\ell}\,.$$

In the numerical experiments, we have used the $\alpha^i(x)$-NSFD3 method to solve the predator-prey problem (3). The corresponding numerical results are shown in Figs. 1–4 and Tables 3 and 6. The implementation of the $\alpha^i(x)$-NSFD3 third order method is summarized in Algorithm 1, and briefly described below.

Algorithm 1 Pseudocode for the third order $\alpha^i(x)$-NSFD3 method (to solve problem (3)).

Input: t_0, x_0, T, Δt, δ, $\bar{\alpha}^i$, $\bar{x}^i$, f^i, $f^i_{x^j}$, $f^i_{x^j x^\ell}$ $(i, j, \ell = 1, 2)$
1: **initialize** $t \leftarrow t_0$, $k \leftarrow 0$, $x_k \leftarrow x_0$
2: **while** $t < T$ **do**
3: $\quad f^i \leftarrow f^i(x_k)$, $f^i_- \leftarrow f^i_-(x_k)$, $f^i_{x^j} \leftarrow \dfrac{\partial f^i(x_k)}{\partial x^j}$, $f^i_{x^j x^\ell} \leftarrow \dfrac{\partial^2 f^i(x_k)}{\partial x^j \partial x^\ell}$, $\qquad i, j, \ell = 1, 2$
4: $\quad \alpha^i \leftarrow \alpha^i(x_k)$, $\qquad i = 1, 2$ ▷ see (25)
5: $\quad$ **if** $\left(\exists\, i = 1, 2 : (\alpha^i < \bar{\alpha}^i \vee \alpha^i \in \mathbb{C})\right) \wedge (\forall\, i = 1, 2 : |x^i_k - \bar{x}^i| < \delta\, |\bar{x}^i|)$ **then**
6: $\qquad \alpha^i \leftarrow \max(0, \bar{\alpha}^i)$, $\qquad i = 1, 2$ ▷ elementary stability control, see Theorem 5
7: $\quad$ **end if**
8: $\quad \tau^i \leftarrow (\phi^i)''(0, x_k)$, $\qquad i = 1, 2$ ▷ see (16)
9: $\quad \phi^i \leftarrow \phi^i(\Delta t, x_k)$, $\qquad i = 1, 2$ ▷ see e.g. next (31)
10: $\quad$ **compute** x^i_{k+1} as in (13), $i = 1, 2$
11: $\quad$ **if** $\exists\, i = 1, 2 : (x^i_{k+1} < 0 \vee x^i_{k+1} \in \mathbb{C})$ **then**
12: $\qquad \alpha^i \leftarrow \max(0, f^i / f^i_-)$, $\qquad i = 1, 2$ ▷ positivity control, see Theorem (3)
13: $\qquad \tau^i \leftarrow (\phi^i)''(0, x_k)$, $\qquad i = 1, 2$ ▷ see (16)
14: $\qquad \phi^i \leftarrow \phi^i(\Delta t, x_k)$, $\qquad i = 1, 2$ ▷ see e.g. next (31)
15: $\qquad$ **compute** x^i_{k+1} as in (13), $i = 1, 2$
16: $\quad$ **end if**
17: $\quad t \leftarrow t + \Delta t$, $k \leftarrow k + 1$
18: **end while**

- The inputs are: the initial condition x_0; the bounds of the time interval t_0 and T; the step-size Δt; the equilibrium points $(\bar{x}^1, \bar{x}^2)$; the related values $\bar{\alpha}^1$ and $\bar{\alpha}^2$ from Theorem 5; a parameter $\delta > 0$, used to control the elementary stability; the functions f^i and their first and second order derivatives $f^i_{x^j}$, $f^i_{x^j x^\ell}$.
- Lines 3–4: we select α^i to obtain order three, according to (25).
- Lines 5–7 (elementary stability control): when the solution is close to the equilibrium point (i.e., when their relative distance is smaller than δ), we check the elementary stability conditions in Theorem 5 and, if necessary, change the α^i coefficients accordingly.
- Line 10: we compute the numerical solution using the chosen α^i.
- Lines 11–16 (positivity control): if the numerical solution x_{k+1} is negative or complex, exploiting the positivity conditions in Theorem 3, we change the coefficients α^i accordingly and recompute the solution.

The main goal of the proposed implementation lies in preserving positivity and elementary stability by exploiting the conditions given in Theorems 3 and 5, that provide the values of the α^i coefficients in the $\alpha^i(x)$-NSFD method guaranteeing this. Note that if the numerical solution never becomes negative, and the coefficients $\alpha^i(x)$ in (25) at each step are such as to guarantee elementary stability, we also reach order three. Therefore, always looking primarily at the positivity and stability of the solution, we do not even sacrifice accuracy unless necessary. A similar idea has been used in [21], where the authors derive unconditionally positive methods based on the Patankar trick, but propose to slightly modify them by relaxing the positivity requirement when not needed. Indeed, unconditional positivity can lead to lag effects in the numerical solution, and thus to inaccurate results, see [21, Figs. 13 and 14].

Finally, note that Algorithm 1 is generalizable for any problem, once the user provides the $\bar{\alpha}^i$ values related to the elementary stability control, as done here in Theorem 5 for the model (3).

5. α-NSFDRK methods

The NSFD methods (5) and (6) are based on forward Euler scheme, where Δt has been changed by $\phi^i(\Delta t)$, $i = 1, \dots, N$, and the function f has been non-locally modified. We have generalized this technique by means of formula (7), and finally we have added some parameters in (12) to get the new α-NSFD methods. These ideas can also be applied to higher order Runge-Kutta methods as we describe below. For simplicity, we have considered a simple second order explicit RK method, this is Heun's method or explicit trapezoidal rule. The coefficients of the scheme can be displayed in a Butcher tableau

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array} \tag{26}$$

and the equations of one Δt-step applied to the autonomous problem (1), from $x_k \approx x(t_k)$ to $x_{k+1} \approx x(t_k + \Delta t)$, are

$$\begin{aligned} X_1 &= x_k, \\ X_2 &= x_k + \Delta t\, f(X_1), \\ x_{k+1} &= x_k + \tfrac{1}{2}\,\Delta t\, f(X_1) + \tfrac{1}{2}\,\Delta t\, f(X_2), \end{aligned} \tag{27}$$

where $X_1, X_2 \in \mathbb{R}^N$ are the internal stages and $x_{k+1} \in \mathbb{R}^N$ is the numerical solution at $t = t_k + \Delta t$. This approach is second order, but does not preserve the positivity of the system. In [21] the authors applied the Patankar trick to Heun's method to get positivity for fully conservative problems. In this section we extend the α-NSFD ideas in Section 4 to RK methods. The equations of the new second order scheme, namely α-NSFDRK method, are

$$\frac{X_2^i - x_k^i}{\phi^i(\Delta t, x_k)} = f^i(x_k) + \alpha^i\, \frac{X_2^i - x_k^i}{x_k^i} f_-^i(x_k), \quad i = 1, \dots, N, \tag{28a}$$

$$\frac{x_{k+1}^i - x_k^i}{\phi^i(\Delta t, x_k)} = \tfrac{1}{2} f^i(x_k) + \tfrac{1}{2}\alpha^i\, \frac{x_{k+1}^i - X_2^i}{X_2^i} f_-^i(x_k) + \tfrac{1}{2} f^i(X_2) + \tfrac{1}{2}\alpha^i\, \frac{x_{k+1}^i - X_2^i}{X_2^i} f_-^i(X_2), \quad i = 1, \dots, N\,. \tag{28b}$$

Remark 6. If $\alpha^i = 0$, $i = 1, \dots, N$, and $\phi^i = \Delta t$, then the internal stage X_2 in (28a) is nothing but the numerical approach after a forward Euler step. Consequently, Eq. (28a) for the stage X_2 coincides with Eq. (12) for the numerical solution x_{k+1}.

Remark 7. Observe that the case $\alpha^i = 0$, $i = 1, \dots, N$, and $\phi^i = \Delta t$, corresponds with the basic Heun's method (27), while for $\alpha = 1$, and $\phi^i = \Delta t$, we recover the second order Patankar-Runge-Kutta scheme considered in [21] for fully conservative problems.

Below we extend Theorems 3 and 4 in Section 4, now for the new α-NSFDRK method (28). Positivity is obtained under the same hypothesis made in Theorem 3, while second order can be obtained for the simple case $\phi^i = \Delta t$, not being necessary to calculate second derivatives $(\phi^i)''(0)$ like those in Theorem 4.

Theorem 6. *The α-NSFDRK method (28) preserves the numerical positivity of the model (1) if $\alpha^i \geq f^i(x)/f_-^i(x)$, $i = 1, \dots, N$, $x \geq 0$.*

Proof. Similarly to the proof of the Theorem 3, it is possible to obtain an explicit scheme for the internal stage X_2 in (28a)

$$X_2^i = \frac{x_k^i + \phi^i\big(f^i(x_0) - \alpha^i f_-^i(x_0)\big)}{1 - \alpha^i \phi^i f_-^i / x_k^i}. \tag{29}$$

Then, we can also get an explicit expression for the numerical solution x_{k+1} in (28b)

$$x_{k+1}^i = \frac{x_k^i + \frac{1}{2}\phi^i\big(f^i(x_0) - \alpha^i f_-^i(x_0)\big) + \frac{1}{2}\phi^i\big(f^i(X_2) - \alpha^i f_-^i(X_2)\big)}{1 - \frac{1}{2}\alpha^i \phi^i f_-^i(x_0)/X_2^i - \frac{1}{2}\alpha^i \phi^i f_-^i(X_2)/X_2^i}. \tag{30}$$

In both cases, the denominator is positive for any value of the parameters α^i. From the numerator we get the sufficient condition for positivity, this is $f^i(x) - \alpha^i f_-^i(x) \geq 0$. $\square$

Theorem 7. *If the functions ϕ^i, $i = 1, \dots, N$, of the α-NSFDRK method (28) satisfy $\phi^i(0) = \Delta t$, then the method achieves second order for any value of the parameters α^i, $i = 1, \dots, N$.*

Proof. Taylor expansion of the internal stage X_2^i in (29) gives us

$$X_2^i = x_k^i + \Delta t\, f^i(x_k) + \frac{\alpha^i\, f^i(x_0) f_-^i(x_0)}{x_0^i} \Delta t^2 + \mathcal{O}(\Delta t^3).$$

Then, the expansion for the numerical solution x_{k+1}^i in (30) is

$$x_{k+1}^i = x_k^i + \Delta t\, f^i(x_k) + \frac{1}{2} \sum_{j=1}^{N} \frac{\partial f^i(x_0)}{\partial x^j} f^j(x_0)\, \Delta t^2 + \mathcal{O}(\Delta t^3).$$

The parameters α^i vanished up to Δt^2 and the method is second order. $\square$

Table 1
Errors and rates of convergence for first order methods in case $g(1) < d$; for α-NSFD1 we used $\alpha = 0.928$, and for α^i-NSFD1 we used $\alpha^1 = 0.8$, $\alpha^2 = 0.5$.

	EE1		PESN1 [4]		α-NSFD1		α^i-NSFD1	
Δt	Error	Rate	Error	Rate	Error	Rate	Error	Rate
10^{-1}	1.73e-01	–	3.43e-02	–	2.27e-02	–	1.96e-03	–
10^{-2}	7.86e-03	1.34	2.75e-03	1.10	1.95e-03	1.07	4.23e-04	0.67
10^{-3}	7.90e-04	1.00	2.69e-04	1.01	1.92e-04	1.01	4.59e-05	0.96
10^{-4}	7.90e-05	1.00	2.68e-05	1.00	1.92e-05	1.00	4.62e-06	1.00

For the new α-NSFDRK method (28), Theorems 6 and 7 ensure positivity and second order. As done in Section 4 for α-NSFD methods, also for the α-NSFDRK proposed in this section we have analyzed conditions on the parameters so that the scheme also preserves the behavior of the equilibrium points on problem (3). However, we got that the scheme (28) is not elementary stable, and the same happens with any other second order RK method. Therefore, in the numerical experiments we have chosen the parameters α^i to annihilate, when possible, the main term of the local error, thus achieving third order. We have named $\alpha^i(x)$-HEUN3 to this positive third order α-NSFDRK method.

6. Numerical simulations

All the theoretical findings related to positivity, elementary stability and accuracy of the new α-NSFD and α-NSFDRK methods have been tested in the numerical simulations. We have compared our new schemes with other NSFD methods existing in the literature to show the advantages of the new ones. In order to make the comparison possible, we have considered the same functions ϕ^i used in [4,5], defined by

$$\phi^i(\Delta t, x) = \begin{cases} \dfrac{e^{\tau^i(x)\Delta t} - 1}{\tau^i(x)} & \text{if} \quad \tau^i(x) \neq 0, \\ \Delta t & \text{if} \quad \tau^i(x) = 0, \end{cases} \tag{31}$$

where $\tau^i(x) = (\phi^i)''(0, x)$ is the one in Theorem 4 that guarantees order two for any α^i. All the numerical methods used in the simulations are listed below. In each case, the ending number denotes the order of the method.

EEE: explicit Euler method.
PESN1: the positive and elementary stable NSFD given in [4,14]. This method coincides with (12) for the particular case $\phi^i = \Delta t$ and $\alpha = 1$.
α-NSFD1: the α-NSFD method (12), with $\alpha^i = \alpha$, where α is a-priori fixed, and $\phi^i = \Delta t$.
α^i-NSFD1: the α-NSFD method (12), where the α^i coefficients are a-priori fixed, and $\phi^i = \Delta t$.
PRK2: the positive second order Patankar-Runge-Kutta scheme considered in [21]. This method coincides with (28) for the particular case $\phi^i = \Delta t$ and $\alpha = 1$.
PESN2: the positive and elementary stable NSFD scheme given in [5]. This method coincides with (12) just for the particular case $\omega^i = 0$ (in [5, Eq. (8)]) and $\alpha^i = 1$.
α-NSFD2: the α-NSFD method (12), with $\alpha^i = \alpha$, where α is a-priori fixed, and ϕ^i are given in (31).
α^i-NSFD2: the α-NSFD method (12), where the α^i coefficients are a-priori fixed and ϕ^i are given in (31).
$\alpha^{i(x)}$-NSFD2:] the α-NSFD method (12) from Remark 5, where the α^i coefficients vary along the time integration so as to guarantee second order, and $\phi^i = \Delta t$. Its implementation has been performed following the same ideas as in Algorithm 1 for method $\alpha^i(x)$-NSFD3.
$\alpha^i(x)$-NSFD3: the α-NSFD method derived in Subsection 4.1, where ϕ^i are given in (31).
$\alpha^i(x)$-HEUN3: the α-NSFDRK method derived in Section 5, where $\phi^i = \Delta t$.

For the α-NSFD methods with non-variable coefficients, we prefixed α or α^i by taking into account the elementary stability conditions in Theorem 5. Also, all these methods have been implemented with a control on positivity. That is, if at a given grid point the numerical solution is not positive, then, only at that point, we use $\alpha = \max\left(0, f^i/f^i_-\right)_{i=1}^N$, or $\alpha^i = \max\left(0, f^i/f^i_-\right)$, $i = 1, \dots, N$, according to Theorem 3.

All the methods have been implemented in Matlab, version R2023b. To calculate a reference solution for the performed tests, we have used the Matlab function `ode15s` requiring absolute and relative tolerance equal to `eps`.

In all simulations we have considered the Rosenzweig-MacArthur predator-prey system (3), like in [4,5], with $g(x) = 1/(c + x)$, and we have examined two different situation: the first one, $g(1) < d$, in which there does not exist interior equilibrium point, and the second one, $g(1) > d$, with an interior equilibrium point that is asymptotically stable.

6.1. Predator-prey problem when $g(1) < d$

We consider system (3) with the following set of the parameters:

$$a = 1.0, \quad b = 2.0, \quad c = 0.5, \quad d = 6.0\,.$$

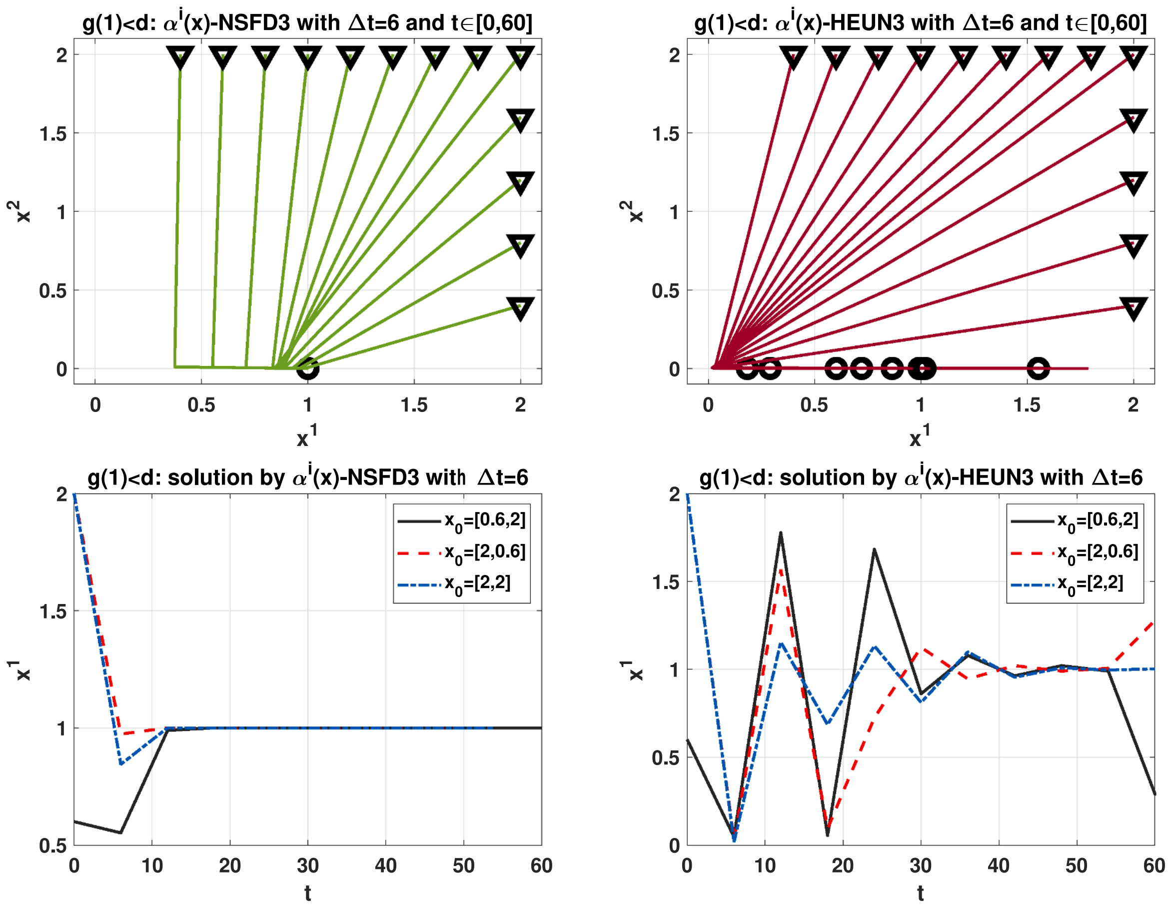

Fig. 1. Phase plots (top) and x^1-solution (bottom) for $\alpha^i(x)$-NSFD3 and $\alpha^i(x)$-HEUN3 methods in case $g(1) < d$. In the phase plots, the symbol '∇' denotes the initial condition, and '$\circ$' denotes the numerical solution at $t = 60$.

Table 2
Errors and rates of convergence for second order methods in case $g(1) < d$; for α-NSFD2 we used $\alpha = 0.661$, and for α^i-NSFD2 we used $\alpha^1 = 0.5$, $\alpha^2 = 0.873$. Also, according to [5, p. 9], we used $\omega^1 = \omega^2 = 0$ (in [5, Eq. (8)]) for PESN2.

	PRK2 [21]		PESN2 [5]		α-NSFD2		α^i-NSFD2		$\alpha^i(x)$-NSFD2	
Δt	Error	Rate	Error	Rate	Error	Rate	Error	Rate	Error	Rate
10^{-1}	1.64e-02	–	2.29e-03	–	9.22e-04	–	9.56e-04	–	1.67e-03	–
10^{-2}	2.20e-04	1.87	2.33e-05	1.99	1.22e-05	1.88	1.83e-07	3.72	1.62e-05	2.01
10^{-3}	2.29e-06	1.98	2.34e-07	2.00	1.25e-07	1.99	9.70e-09	1.27	1.61e-07	2.00
10^{-4}	2.30e-08	2.00	2.34e-09	2.00	1.25e-09	2.00	1.07e-10	1.96	1.62e-09	2.00

Table 3
Errors and rates of convergence for third order methods in case $g(1) < d$.

	$\alpha^i(x)$-NSFD3		$\alpha^i(x)$-HEUN3	
Δt	Error	Rate	Error	Rate
10^{-1}	2.40e-05	–	1.97e-03	–
10^{-2}	1.91e-09	4.10	3.78e-06	2.72
10^{-3}	4.16e-12	2.66	4.10e-09	2.96
10^{-4}	4.58e-12	–	1.32e-12	3.49

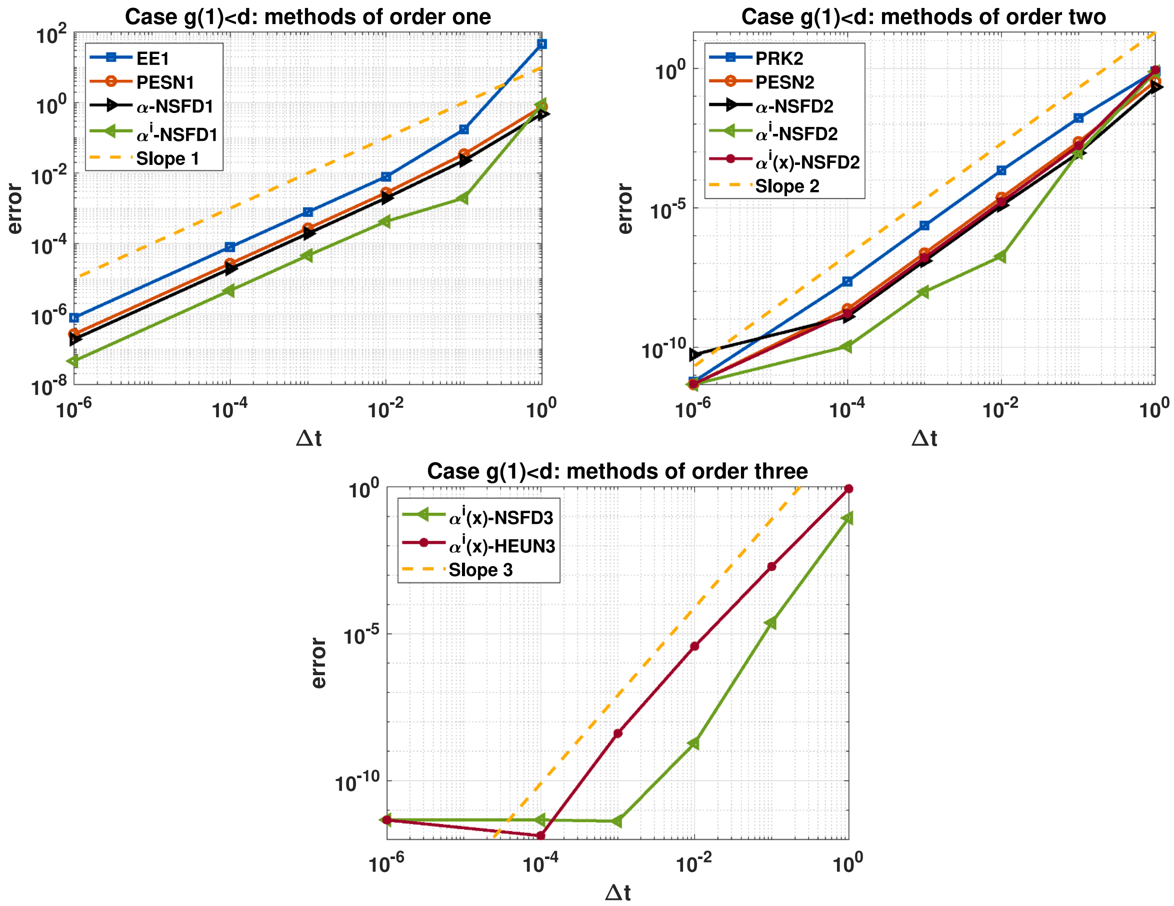

Fig. 2. Convergence results for the first, second and third order methods in case $g(1) < d$.

Table 4
Errors and rates of convergence for first order methods in case $g(1) > d$; for α-NSFD1 we used $\alpha = 0.944$, and for α^i-NSFD1 we used $\alpha^1 = 0.901$, $\alpha^2 = 0.751$.

	EE1		PESN1 [4]		α-NSFD1		α^i-NSFD1	
Δt	Error	Rate	Error	Rate	Error	Rate	Error	Rate
10^{-1}	1.57e+00	–	6.73e-02	–	2.72e-02	–	1.20e-02	–
10^{-2}	8.21e-02	1.84	7.23e-03	0.97	2.40e-03	1.06	7.65e-04	1.20
10^{-3}	8.07e-03	1.28	7.28e-04	1.00	2.36e-04	1.01	7.19e-05	1.03
10^{-4}	8.06e-04	1.01	7.28e-05	1.00	2.36e-05	1.00	7.14e-06	1.00

In this case there does not exist interior equilibrium point and the boundary equilibrium point $E_1 = (1, 0)$ is asymptotically stable. The numerical results are summarized in Figs. 1 and 2, and in Tables 1–3.

In particular, in Fig. 1 we report the behavior of the solution also using phase plots to show the stability properties of the new proposed $\alpha^i(x)$-NSFD3 and $\alpha^i(x)$-HEUN3 methods. To get that we have integrated the problem in the time interval [0,60] with several choices of the initial conditions. As expected, note that, although the α^i coefficients vary along the numerical integration with the aim of increasing the order of convergence, positivity and elementary stability are maintained by the $\alpha^i(x)$-NSFD3 method. Instead, the $\alpha^i(x)$-HEUN3 method is not elementary stable, in accordance with the developed theory. In any case, to show the non-elementary stability of the $\alpha^i(x)$-HEUN3 method we had to use a very large time step, as this method preserved the behavior of the equilibrium points for $\Delta t < 6$. The positivity is instead preserved by $\alpha^i(x)$-HEUN3 method for any choice of Δt, as expected.

Fig. 2, and Tables 1–3, show the absolute errors in 1-norm obtained by all numerical methods at the point $t = 1$ with initial condition $(x_0, y_0) = (5, 2)$, by varying the step-size Δt, similarly to [5, Section 4, Example 1]. The obtained results testify that the first and second order α-NSFD methods derived in this paper achieve lower errors than the other schemes from the scientific literature with which they have been compared. In particular, note that the methods characterized by the lowest errors are those for which it is possible to choose a different coefficient α^i for each component x^i_{k+1} of the solution. Furthermore, observe that the $\alpha^i(x)$-NSFD3 and

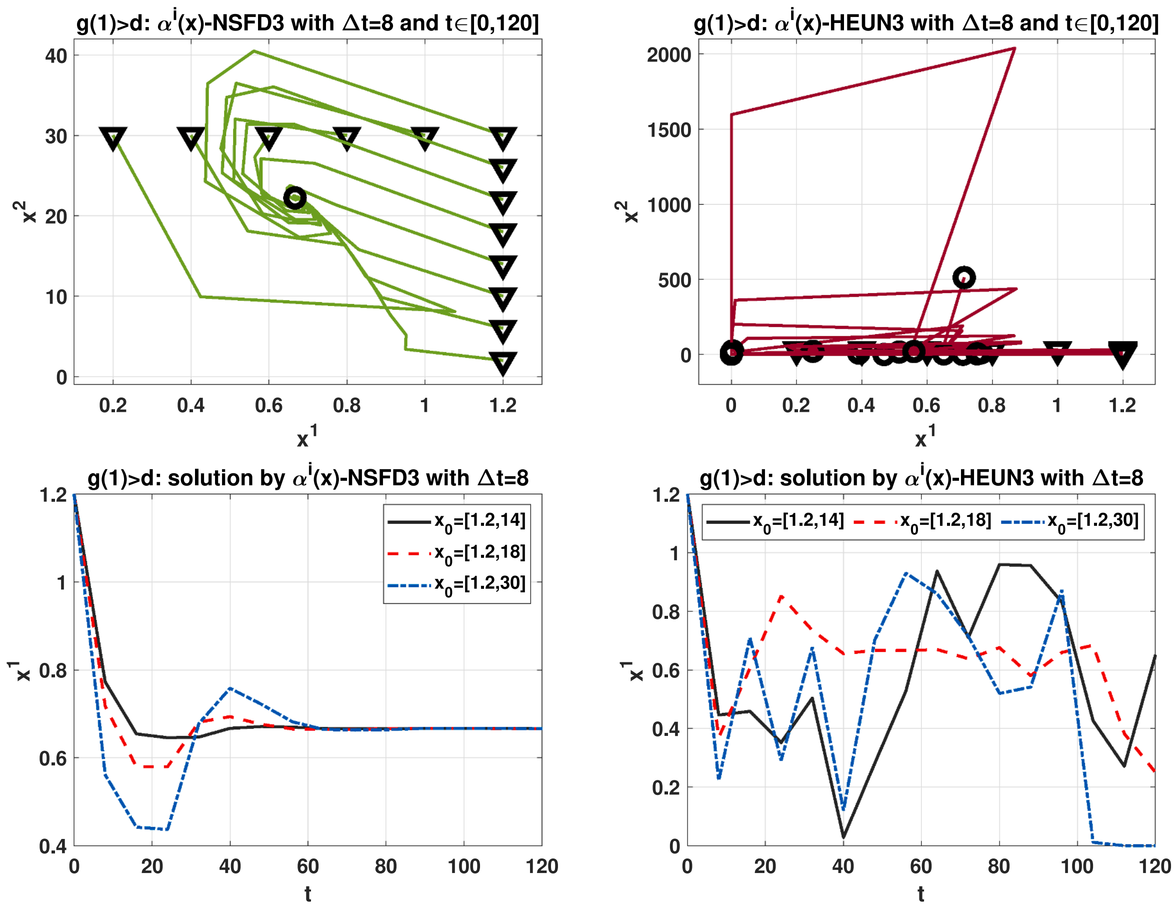

Fig. 3. Phase plots (top) and x^1-solution (bottom) for $\alpha^i(x)$-NSFD3 and $\alpha^i(x)$-HEUN3 methods in case $g(1) > d$. In the phase plots, the symbol '∇' denotes the initial condition, and '$\circ$' denotes the numerical solution at $t = 120$.

Table 5
Errors and rates of convergence for second order methods in case $g(1) > d$; for α-NSFD2 we used $\alpha = 0.834$, and for α^i-NSFD2 we used $\alpha^1 = 0.834$, $\alpha^2 = 0.74$. Also, according to [5, p. 11], we used $\omega^1 = 0.15$ and $\omega^2 = 0.11$ (in [5, Eq. (8)]) for PESN2.

	PRK2 [21]		PESN2 [5]		α-NSFD2		α^i-NSFD2		$\alpha^i(x)$-NSFD2	
Δt	Error	Rate	Error	Rate	Error	Rate	Error	Rate	Error	Rate
10^{-1}	1.33e-01	–	1.55e-03	–	1.58e-03	–	1.57e-03	–	1.13e-03	–
10^{-2}	1.61e-03	1.92	1.44e-05	2.03	5.47e-06	2.46	5.36e-06	2.47	1.11e-05	2.01
10^{-3}	1.64e-05	1.99	1.43e-07	2.00	4.57e-08	2.08	4.57e-08	2.07	1.11e-07	2.00
10^{-4}	1.64e-07	2.00	1.43e-09	2.00	5.55e-10	1.91	4.33e-10	2.02	1.11e-09	2.00

Table 6
Errors and rates of convergence for third order methods in case $g(1) > d$.

	$\alpha^i(x)$-NSFD3		$\alpha^i(x)$-HEUN3	
Δt	Error	Rate	Error	Rate
10^{-1}	6.84e-05	–	1.98e-02	–
10^{-2}	6.64e-08	3.01	3.13e-05	2.80
10^{-3}	6.43e-11	3.01	3.52e-08	2.95
10^{-4}	2.63e-11	–	9.51e-12	3.57

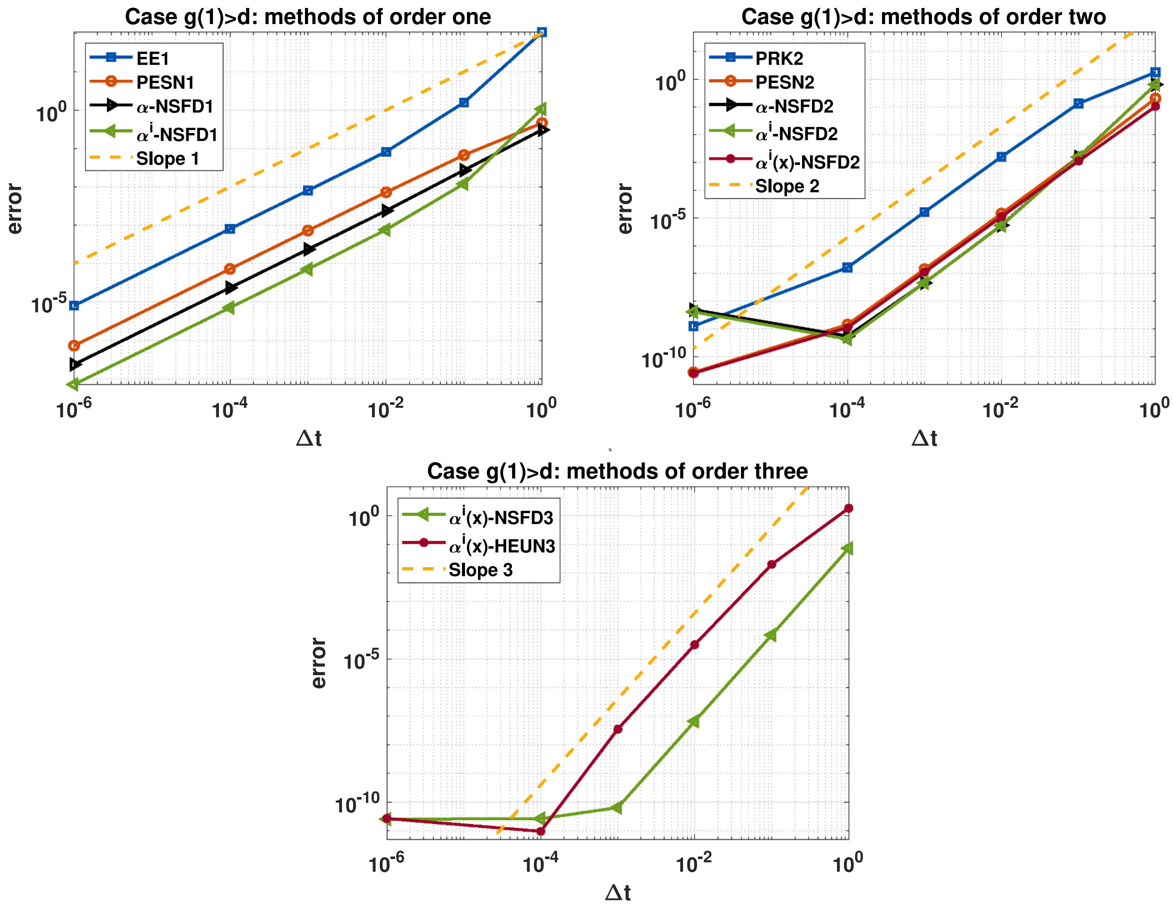

Fig. 4. Convergence results for the first, second and third order methods in case $g(1) > d$.

$\alpha^i(x)$-HEUN3 methods reach order three, as expected from the developed theory. Although they are of the same order, $\alpha^i(x)$-NSFD3 provides much lower errors than $\alpha^i(x)$-HEUN3. We emphasize that, to our knowledge, this is the first paper in which a positive and elementary stable nonstandard method, namely $\alpha^i(x)$-NSFD3, is derived also for order three.

6.2. *Predator-prey problem when* $g(1) > d$

In this second situation, we consider system (3) with the following set of the parameters:

$$a = 0.02, \quad b = 0.5, \quad c = 2.0, \quad d = 0.25\,.$$

In this case, $g(1) > d$, and there is an interior equilibrium point at $\bar{E} = (2/3, 200/9)$ that is asymptotically stable. The numerical results are summarized in Figs. 3 and 4, and in Tables 4–6. They confirm what has already been discussed in the previous case.

Note, from Fig. 3, that the $\alpha^i(x)$-NSFD3 method preserves the stability properties of the internal equilibrium point even for the big time step-size $\Delta t = 8$, according to its elementary stability, unlike the $\alpha^i(x)$-HEUN3 method.

It is remarkable that despite not being elementary stable, $\alpha^i(x)$-HEUN3 still preserves positivity for $\Delta t = 8$, as expected. In any case, we have experimentally seen that for $\Delta t < 8$, also the $\alpha^i(x)$-HEUN3 method is able to preserve the equilibrium points of the model and the related properties.

Furthermore, Fig. 4, and Tables 4–6, show the absolute errors in 1-norm obtained by all the numerical methods at the point $t = 1$ with initial condition $(x_0, y_0) = (16, 9)$, by varying the step-size Δt, similarly to [5, Section 4, Example 3]. As in the previous case $g(1) < d$, also for $g(1) > d$ the methods of order one and two characterized by the lowest errors are the new ones derived in this paper, for which it is possible to choose different α^i coefficients for each component of the numerical solution. Furthermore, as expected, $\alpha^i(x)$-NSFD3 and $\alpha^i(x)$-HEUN3 show order three, but the former seems to be much more convenient than the latter since, as in the previous case, it achieves significantly lower errors.

7. Conclusions

In this work, we have proposed a general technique for the construction of positive nonstandard finite difference methods for initial value problems. We have also considered the introduction of some parameters α^i within these new numerical schemes, possibly variable along the time integration in order to annihilate or minimize the local truncation error at each step, while still ensuring the preservation of the desired properties of the continuous model, such as the positivity of the solution and/or the stability of the equilibrium points. This technique has allowed the derivation of nonstandard positivity preserving and elementary stable numerical methods of order three. To our knowledge, this is the first manuscript in which methods with these features are proposed. Although this is the major contribution of the paper, we emphasize that, thanks to the proposed technique, we were also able to derive positivity preserving and elementary stable methods of order one and two which generalize and improve existing numerical schemes of nonstandard type of the same order. Numerical experiments conducted on a predator-prey model confirmed the theoretical results proved in the manuscript, and showed the advantages of the new methods with respect to others taken from the scientific literature.

Future research works starting from this paper could concern the use of the new technique for different models of interest, or its generalization for the preservation of other properties of the solution.

Data availability

No data was used for the research described in the article.

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References

[1] S. Blanes, A. Iserles, S. Macnamara, Positivity-preserving methods for ordinary differential equations, ESAIM: Math. Model. Numer. Anal. 56 (6) (2022) 1843–1870.
[2] H. Burchard, E. Deleersnijder, A. Meister, Application of modified Patankar schemes to stiff biogeochemical models for the water column, Ocean Dyn. 55 (3-4) (2005) 326–337.
[3] D. Conte, G. Pagano, B. Paternoster, Nonstandard finite differences numerical methods for a vegetation reaction–diffusion model, J. Comput. Appl. Math. 419 (2023) 114790.
[4] D.T. Dimitrov, H.V. Kojouharov, Positive and elementary stable nonstandard numerical methods with applications to predator–prey models, J. Comput. Appl. Math. 189 (1-2) (2006) 98–108.
[5] M.T. Hoang, M. Ehrhardt, A second-order nonstandard finite difference method for a general Rosenzweig–MacArthur predator–prey model, J. Comput. Appl. Math. 444 (2024) 115752.
[6] S. Kopecz, A. Meister, A comparison of numerical methods for conservative and positive advection-diffusion-production-destruction systems, PAMM 19 (1) (2019) e201900209.
[7] R.E. Mickens, Numerical integration of population models satisfying conservation laws: NSFD methods, J. Biol. Dyn. 1 (4) (2007) 427–436.
[8] S. Nüßlein, H. Ranocha, D.I. Ketcheson, Positivity-preserving adaptive Runge-Kutta methods, Commun. Appl. Math. Comput. Sci. 16 (2) (2021) 155–179.
[9] A. Sandu, Positive numerical integration methods for chemical kinetic systems, J. Comput. Phys. 170 (2) (2001) 589–602.
[10] L.F. Shampine, S. Thompson, J.A. Kierzenka, G.D. Byrne, Non-negative solutions of ODEs, Appl. Math. Comput. 170 (1) (2005) 556–569.
[11] C. Bolley, M. Crouzeix, Conservation de la positivité lors de la discrétisation des problèmes d'évolution paraboliques, RAIRO. Analyse numérique 12 (3) (1978) 237–245.
[12] F.K. Alalhareth, M. Gupta, H.V. Kojouharov, S. Roy, Second-order modified nonstandard explicit Euler and explicit Runge–Kutta methods for n-dimensional autonomous differential equations, Computation 12 (9) (2024) 183.
[13] D. Conte, N. Guarino, G. Pagano, B. Paternoster, On the advantages of nonstandard finite difference discretizations for differential problems, Numer. Anal. Appl. 15 (3) (2022) 219–235.
[14] D.T. Dimitrov, H.V. Kojouharov, Stability-preserving finite-difference methods for general multi-dimensional autonomous dynamical systems, Int. J. Numer. Anal. Model. 4 (2) (2007) 282–292.
[15] R.E. Mickens, Nonstandard Finite Difference Schemes: Methodology and Applications, World Scientific, 2020.
[16] F. Brauer, C. Castillo-Chavez, C. Castillo-Chavez, Mathematical Models in Population Biology and Epidemiology, 2, Springer, 2012, 40.
[17] W.O. Kermack, A.G. McKendrick, Contributions to the mathematical theory of epidemics–I. 1927, Bull. Math. Biol. 53 (1-2) (1991) 33–55.
[18] J.D. Murray, Mathematical Biology: I. an Introduction, 17, Springer Science & Business Media, 2007.
[19] R.E. Mickens, Nonstandard Finite Difference Models of Differential Equations, World Scientific, 1993.
[20] S.V. Patankar, Numerical Heat Transfer and Fluid Flow, McGraw-Hill, New York, 1980.
[21] H. Burchard, E. Deleersnijder, A. Meister, A high-order conservative Patankar-type discretisation for stiff systems of production–destruction equations, Appl. Numer. Math. 47 (1) (2003) 1–30.
[22] H.V. Kojouharov, S. Roy, M. Gupta, F. Alalhareth, J.M. Slezak, A second-order modified nonstandard theta method for one-dimensional autonomous differential equations, Appl. Math. Lett. 112 (2021) 106775.