SHORT NOTE

An improvement of two nonstandard finite difference schemes for two population mathematical models

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ABSTRACT
The aim of this paper is to design appropriate nonstandard finite difference (NSFD) schemes for two population mathematical models based on coupled nonlinear ordinary differential equations. Our work clarifies existing constructions of NSFD schemes for these two population models, which are not in full compliance with Mickens' methodology. We select the denominator functions for the discrete first-order derivatives depending on the existence of conservation laws, by following empirical rules suggested by Mickens. We fix nonlocal discretizations that preserve positivity of the schemes, irrespective of the value of the step size. Thus, our NSFD schemes are dynamically consistent with the two population models. We conduct a numerical study to assess the performance of the NSFD method.

KEYWORDS
nonstandard finite difference scheme; population mathematical model; denominator function; positivity preservation; conservation law

1. Introduction

Many biological models are based on systems of coupled ordinary differential equations [1–3]. These systems do not usually possess closed-form solutions, hence approximations must be sought. Numerical-based methods are usually employed for producing approximate solutions. The time domain is discretized and the estimates are obtained at the mesh points. Theoretically, there is convergence as the step size value tends to zero. But it is desirable that, apart from convergence, biological properties of the system are preserved. These properties are usually related to positivity of subpopulations, their asymptotic limit (e.g. extinction or other equilibrium states), and conservation laws (e.g. some restriction for the total population size). Preserving these features is not only a matter of biological consistency, but also a way to improve the convergence performance.

In this paper, we construct appropriate nonstandard finite difference (NSFD) schemes for two population mathematical models [4], within Mickens' general methodology [5–11]. The authors of [4] use versions of the NSFD discretization that are not fully consistent with Mickens' rules. Namely, appropriate choice of denominator functions for the discrete first-order derivatives depending on the existence of certain expressions and conservation laws, and suitable nonlocal discretizations for positivity

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preservation. In particular, positivity of their discretizations only holds when the step size is lower than a certain critical value. Besides, their numerical scheme for the second model does not obey the general conservation law. The two NSFD schemes that we propose in this paper do not show these limitations. It is noted the similarity on purpose and methodology of the present work with [12], although that contribution deals with a mathematical model for respiratory virus transmission and does not conduct a numerical study.

2. Population mathematical models

The following systems of coupled, nonlinear ordinary differential equations have been used in [4] to model the dynamics of phytoplankton–nutrient interaction under nutrient recycling and the whooping cough in the human population (pertussis), respectively:

$$\begin{cases} N'(t) = aP(t) + bZ(t) - cN(t)P(t), \\ P'(t) = cN(t)P(t) - dP(t)Z(t) - aP(t), \\ Z'(t) = dP(t)Z(t) - bZ(t), \end{cases} \tag{1}$$

$$\begin{cases} S'(t) = \mu - \mu S(t) - \beta S(t)I(t), \\ I'(t) = \beta S(t)I(t) - (\mu + \nu)I(t), \\ R'(t) = \nu I(t) - \mu R(t). \end{cases} \tag{2}$$

Here the time t is nonnegative, $t \geq 0$. All coefficients, denoted by lower-case and Greek letters, are assumed to be positive. The three time-dependent functions $(N(t), P(t), Z(t))$ and $(S(t), I(t), R(t))$ denote subpopulations (compartments). The first triple represents concentrations of nitrogen, phytoplankton and zooplankton. The second triple represents the proportion of susceptible, infected and recovered individuals.

3. Design of NSFD schemes

For the analysis of new integrators, basic scalar models are first considered. It is hoped that the conclusions possess some relevance in more complex situations. In fact, methods that do not succeed for basic scalar models should not be applied to real problems.

Consider the simple scalar equations $Y'(t) = \lambda Y(t)$, $Y'(t) = \lambda Y(t)^2$ and $Y'(t) = \lambda_1 Y(t) - \lambda_2 Y(t)^2$. In Biology, Epidemiology and Ecology, these time evolutions correspond to the Malthusian exponential growth model, the Malthusian growth model taking into account squared abundance, and Verhulst's logistic growth model. These equations, because of having closed-form solutions, possess exact schemes. Discretize $t_n = nh$, $n \geq 0$, $h = \Delta t > 0$, $Y_n = Y(t_n)$:

$$\frac{Y_{n+1} - Y_n}{\frac{\mathrm{e}^{\lambda h} - 1}{\lambda}} = \lambda Y_n, \quad \frac{Y_{n+1} - Y_n}{h} = \lambda Y_{n+1} Y_n, \quad \frac{Y_{n+1} - Y_n}{\frac{\mathrm{e}^{\lambda_1 h} - 1}{\lambda_1}} = \lambda_1 Y_n - \lambda_2 Y_{n+1} Y_n. \tag{3}$$

These difference equations may be viewed as modifications of the explicit-Euler rule,

by employing nonlocal discretizations and by modifying the classical denominator h by a function $\phi(h) = h + \mathcal{O}(h^2)$. Nonlocal discretizations usually ensure A-stability. They can also be used for positivity of the schemes, whenever the governing differential equation model satisfies a positivity condition. In terms of the corresponding denominator function $\phi(h)$, the three exact schemes read explicitly as follows:

$$Y_{n+1} = (1 + \lambda\phi(h))Y_n, \quad Y_{n+1} = \frac{Y_n}{1 - \lambda\phi(h)Y_n}, \quad Y_{n+1} = \frac{Y_n(1 + \lambda_1\phi(h))}{1 + \lambda_2\phi(h)Y_n}. \tag{4}$$

As can be seen, $\phi(h)$ is given by $(\mathrm{e}^{\alpha h} - 1)/\alpha$ when the expression $1 + \alpha\phi(h)$ occurs (α depends on parameters). Otherwise $\phi(h) = h$.

For systems of coupled differential equations with a conservation law, the nonlocal discretizations and the denominator function selections for each equation should also make the scheme obey that law.

NSFD schemes are constructed on the basis of these ideas. It is expected that the nonlocal discretizations and the denominator function selections improve dynamic consistency (preservation of conservation laws, positivity and asymptotic behavior) and accelerate the decay of the integration error.

4. Design of the NSFD schemes for the two population mathematical models

If the initial conditions at time zero are nonnegative, then the time-dependent functions are nonnegative on the whole domain. This is a "positivity condition". On the other hand, by adding the three equations for the two systems, we obtain

$$M'(t) = 0 \Longrightarrow M(t) = \text{constant} \tag{5}$$

and

$$M'(t) = \mu(1 - M(t)) \Longrightarrow M(t) = 1 + (M(0) - 1)\mathrm{e}^{-\mu t}, \tag{6}$$

respectively, where $M(t)$ is the total population (the sum of the three time-dependent functions). These are conservation laws. An important comment for the second case (2), (6), must be made here. When the initial proportions of susceptible, infected and recovered individuals add up to 1, that is, $M(0) = 1$, the equality $M(t) = 1$ holds for all t, as stated in [4]. However, considering the general conservation law (6) has significant advantages. As will be seen later, (6) gives rise to a certain choice of denominator functions for the discrete first-order derivatives, which greatly improves the convergence of the numerical scheme in applications.

To construct the two NSFD schemes, we discretize

$$t \longleftarrow t_n = nh, \ n \geq 0, \quad h = \Delta t > 0, \tag{7}$$

$$(N(t), P(t), Z(t)) \longleftarrow (N_n, P_n, Z_n), \tag{8}$$

$$(S(t), I(t), R(t)) \longleftarrow (S_n, I_n, R_n), \tag{9}$$

$$M(t) \longleftarrow M_n. \tag{10}$$

Let $\phi_1(h)$, $\phi_2(h)$ and $\phi_3(h)$ be three denominator functions for the three discrete first-order derivatives, which are specified later. A priori, these are nonnegative monotonically increasing functions satisfying the condition $h + \mathcal{O}(h^2)$. On the other hand, we use the following nonlocal representations:

$$N(t)P(t) \longleftarrow N_{n+1}P_n, \tag{11}$$

$$P(t)Z(t) \longleftarrow P_{n+1}Z_n, \tag{12}$$

$$aP(t) \longleftarrow aP_{n+1}, \tag{13}$$

$$bZ(t) \longleftarrow bZ_{n+1}, \tag{14}$$

$$S(t)I(t) \longleftarrow S_{n+1}I_n, \tag{15}$$

$$\mu S(t) \longleftarrow \mu S^{n+1}, \tag{16}$$

$$\mu I(t) \longleftarrow \mu I_{n+1}, \quad \nu I(t) \longleftarrow \nu I_{n+1}, \tag{17}$$

$$\mu R(t) \longleftarrow \mu R_{n+1}. \tag{18}$$

These discretizations are the unique ones that guarantee positivity, regardless of the value h of the step size. They were not set in [4], which placed unnecessary upper bounds on h for positivity. Our NSFD schemes read as follows:

$$\begin{cases} \frac{N_{n+1}-N_n}{\phi_1(h)} = aP_{n+1} + bZ_{n+1} - cN_{n+1}P_n, \\ \frac{P_{n+1}-P_n}{\phi_2(h)} = cN_{n+1}P_n - dP_{n+1}Z_n - aP_{n+1}, \\ \frac{Z_{n+1}-Z_n}{\phi_3(h)} = dP_{n+1}Z_n - bZ_{n+1}, \end{cases} \tag{19}$$

$$\begin{cases} \frac{S_{n+1}-S_n}{\phi_1(h)} = \mu - \mu S_{n+1} - \beta S_{n+1}I_n, \\ \frac{I_{n+1}-I_n}{\phi_2(h)} = \beta S_{n+1}I_n - (\mu+\nu)I_{n+1}, \\ \frac{R_{n+1}-R_n}{\phi_3(h)} = \nu I_{n+1} - \mu R_{n+1}. \end{cases} \tag{20}$$

These schemes are not suitable for computation. After elementary but long calculations, which may be performed on a symbolic software by isolating the $(n+1)$-th

terms, the first NSFD scheme may be expressed as follows:

$$\begin{cases} N_{n+1} = \frac{A_n}{B_n}, \\ P_{n+1} = \frac{P_n + c\phi_2(h) N_{n+1} P_n}{1+\phi_2(h)[dZ_n + a]}, \\ Z_{n+1} = \frac{Z_n + d\phi_3(h) P_{n+1} Z_n}{1+\phi_3(h) b}, \end{cases} \tag{21}$$

where

$$\begin{aligned} A_n = {} & a\phi_1(h)[P_n + bP_n\phi_3(h) + b\phi_2(h)Z_n] + N_n[1 + b\phi_3(h)][1 + a\phi_2(h) + d\phi_2(h)Z_n] \\ & + b\phi_1(h)Z_n[1 + d\phi_3(h)P_n + d\phi_2(h)Z_n], \end{aligned} \tag{22}$$

$$B_n = [1 + b\phi_3(h)][1 + a\phi_2(h) + d\phi_2(h)Z_n] + c\phi_1(h)P_n[1 + b\phi_3(h) + d\phi_2(h)Z_n]. \tag{23}$$

The second NSFD scheme is

$$\begin{cases} S_{n+1} = \frac{S_n + \phi_1(h)\mu}{1+\phi_1(h)[\mu + \beta I_n]}, \\ I_{n+1} = \frac{I_n + \beta\phi_2(h) S_{n+1} I_n}{1+\phi_2(h)[\mu+\nu]}, \\ R_{n+1} = \frac{R_n + \nu\phi_3(h) I_{n+1}}{1+\phi_3(h)\mu}. \end{cases} \tag{24}$$

Inspection of the difference equations (21) and (24) demonstrates that the positivity condition holds for every step size. On the other hand, notice that the difference equations need to be solved in a particular order. For system (21), first N_{n+1} is determined from N_n, P_n and Z_n, second P_{n+1} is found from N_{n+1}, P_n and Z_n, and third Z_{n+1} is obtained from P_{n+1} and Z_n. For system (24), first S_{n+1} is determined from S_n and I_n, second I_{n+1} is found from S_{n+1} and I_n, and third R_{n+1} is obtained from I_{n+1} and R_n. Once the correct order is followed, the recurrences are solved explicitly and at really cheap cost. There is no need to numerically solve nonlinear algebraic systems, as usually occurs with implicit standard finite difference schemes (backward-Euler, trapezoid, etc.).

Regarding the denominator functions, we deal with each model separately. We base on [10] (consult Section 3 as well). For the first model (1), since $M'(t) = 0$, necessarily $\phi_1 = \phi_2 = \phi_3 = \phi$. There is no common term of the form $1 + \alpha\phi(h)$ for the three discrete equations (21), where $\alpha \neq 0$ depends on one or more parameters. Hence the denominator function should be taken as

$$\phi(h) = h. \tag{25}$$

For the second model (2), we use the general conservation law for $M(t)$, (6). By selecting $\phi_1 = \phi_2 = \phi_3 = \phi$, where

$$\phi(h) = \frac{\mathrm{e}^{\mu h} - 1}{\mu}, \tag{26}$$

an exact numerical scheme for $M(t)$ is obtained:

$$\frac{M_{n+1} - M_n}{\phi(h)} = \mu(1 - M_{n+1}). \tag{27}$$

Hence the conservation law is obeyed by the NSFD scheme, irrespective of the step size and the initial condition $M(0)$. Observe also that the expression $1+\mu\phi(h)$ is common for the three discrete equations (24).

5. Discussion: Theoretical and numerical features

An important point is that Mickens' methodology leads to unique NSFD schemes. But the rules need to be appropriately followed. The nonlocal representations of the right-hand side terms are uniquely determined by the positivity condition. The denominator functions $\phi(h)$ of the first-order derivatives are determined by conservation laws and the occurrence of expressions of the form $1+\alpha\phi(h)$, where $\alpha \neq 0$ is composed of one or more parameters. With these rules in mind, we have achieved the purpose of this paper of building NSFD schemes for population models correctly.

We show some enlightening plots. We consider the difference equations (24), fix $\mu = 0.04$, $\nu = 2$, $\beta = 1$, $S(0) = 0.5$, $I(0) = 0.007$ and $R(0) = 0.493$, and compare the traditional denominator function $\phi(h) = h$ with the dynamically consistent choice (26). Let $\epsilon_{*(t)}(h)$ be the absolute error in the approximation of $*(t)$ for step size value h, where $* \in \{S, I, R\}$. Figure 1 reports some of these errors on the time interval $[0, 500]$, for different values of h. Observe that the selection (26) outperforms the classical denominator function for all values of h. On the other hand, these graphs illustrate that the nonlocal discretizations of the schemes give rise to A-stable methods, since the error tends to zero when $t \to \infty$ for every fixed h. This feature, which is characteristic of implicit standard finite difference schemes, is satisfied by our NSFD schemes, which are written explicitly, do not necessitate numerically solving nonlinear algebraic systems, and are recursively run at really cheap cost. NSFD methods seem to take the best of traditional finite difference schemes: from explicit methods, the easy resolution by recursion, and from implicit methods, A-stability. But NSFD schemes do not have their limitations: explicit methods are not A-stable (see Figure 2 on the forward-Euler and explicit Runge-Kutta schemes), and implicit methods require solving nonlinear algebraic systems at each step of the recursion, which entails higher complexity and computational time, especially for large systems. In this regard, Figure 3 is devised to compare the NSFD scheme with implicit standard methods (which are A-stable), specifically backward-Euler (first order) and trapezoid (second order), in terms of error versus CPU time (Mathematica®, version 12.0, year 2019; the nonlinear algebraic systems are solved with the built-in command *FindRoot*). The NSFD approach is clearly superior to backward-Euler, and similar to trapezoid despite the lesser order. Further, NSFD schemes may preserve other qualitative properties of the governing model. In the present case, conservation laws (by denominator selection) and positivity hold for every step size. Positivity is illustrated in Figure 4. For the infectious compartment, the NSFD scheme is compared against a software built-in routine for solving differential equations (Mathematica®, version 12.0, year 2019, *NDSolve*). It is observed that, near extinction of the infectious group, the software routine has an oscillating behavior and takes positive and negative values. By contrast, the NSFD scheme preserves positivity and monotony. The step size $h = 2$ is picked for exemplification, but the same conclusion is reached for any other step size value.

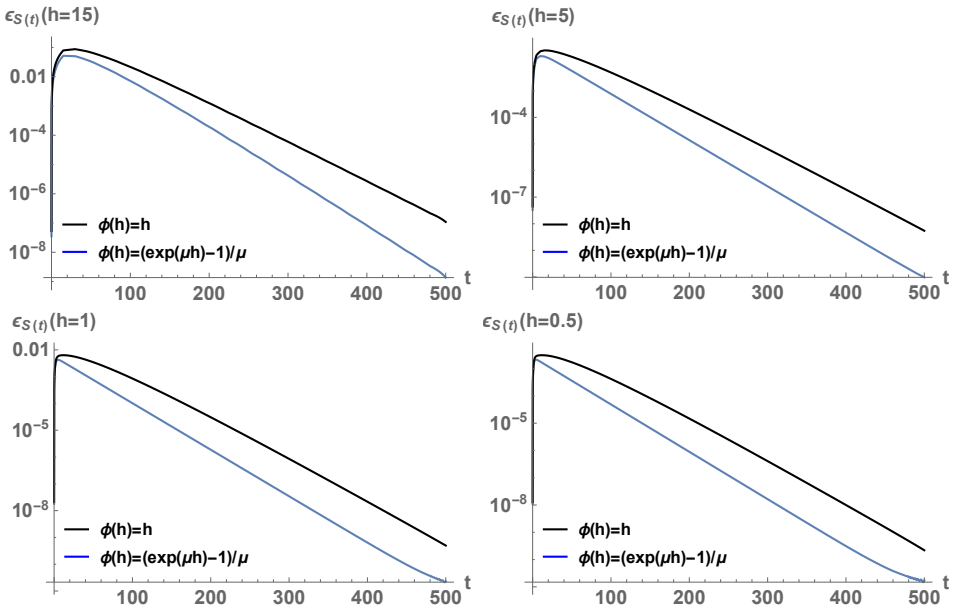

Figure 1. Comparison of performance between the traditional denominator function $\phi(h) = h$ and the dynamically consistent choice (26) for the NSFD scheme (24), with inputs $\mu = 0.04$, $\nu = 2$, $\beta = 1$, $S(0) = 0.5$, $I(0) = 0.007$ and $R(0) = 0.493$. The horizontal axis represents the time variable t on $[0, 500]$. The vertical axis represents $\epsilon_{S(t)}(h)$, which is defined as the absolute error in the approximation of $S(t)$ for step size value h. The selection (26) outperforms the classical denominator function for all values of h.

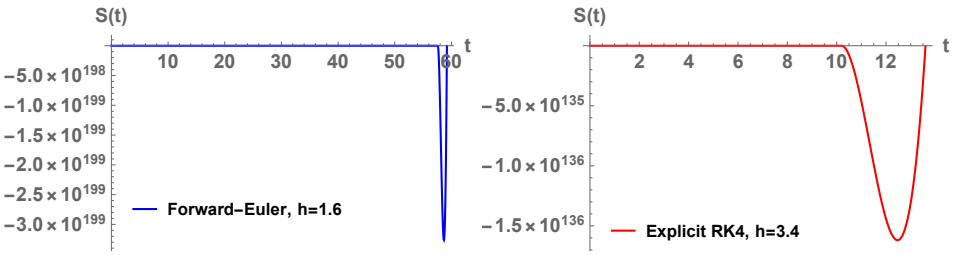

Figure 2. Traditional forward-Euler (left panel) and fourth-order explicit Runge-Kutta (right panel) for model (2), with inputs $\mu = 0.04$, $\nu = 2$, $\beta = 1$, $S(0) = 0.5$, $I(0) = 0.007$ and $R(0) = 0.493$. The horizontal axis represents the time variable t. The vertical axis represents the approximation of $S(t)$, for certain step size values h aimed at highlighting A-instability.

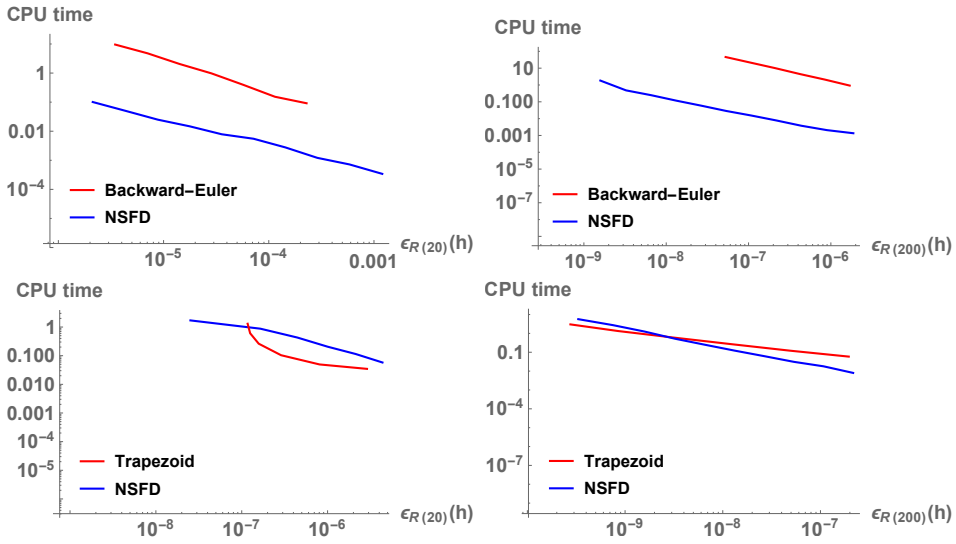

Figure 3. Comparison of performance between the NSFD scheme (24) and the traditional backward-Euler (top panels) and trapezoidal (bottom panels) methods, with inputs $\mu = 0.04$, $\nu = 2$, $\beta = 1$, $S(0) = 0.5$, $I(0) = 0.007$ and $R(0) = 0.493$. The horizontal axis represents $\epsilon_{R(t)}(h)$, which is defined as the absolute error in the approximation of $R(t)$ for step size value h. The vertical axis represents the CPU time in seconds (Mathematica®, version 12.0, year 2019; the nonlinear algebraic systems are solved with the built-in command *FindRoot*). The NSFD approach is clearly superior to backward-Euler, and similar to trapezoid despite the lesser order.

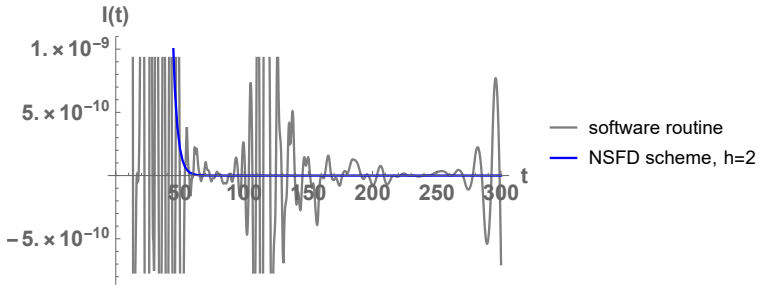

Figure 4. Evolution of the infectious compartment for a software built-in routine (Mathematica®, version 12.0, year 2019, *NDSolve*) and the NSFD scheme (24), with inputs $\mu = 0.04$, $\nu = 2$, $\beta = 1$, $S(0) = 0.5$, $I(0) = 0.007$ and $R(0) = 0.493$. The horizontal axis represents the time variable t on $[0, 300]$. The vertical axis represents $I(t)$. The software routine has an oscillating behavior and takes positive and negative values. By contrast, the NSFD scheme preserves positivity and monotony.

6. Conclusion

NSFD schemes modify classical finite difference schemes on the basis of dynamic consistency. While such consistency depends on the model at hand, preservation of conservation laws, positivity and asymptotic behavior are usual properties to be mimicked for every step size value. This is the case for the two population models considered in the present paper. The first biological system deals with the dynamics of phytoplankton-nutrient interaction under nutrient recycling, and the second one models whooping cough in humans. While NSFD schemes may not be difficult to formulate, a successful implementation must be in agreement with the general NSFD methodology. Compared to traditional schemes, besides dynamic consistency, an important feature of NSFD schemes is that, in general, they can be written explicitly. Hence there are no nonlinear algebraic systems at each step of the recursion, which would incur higher complexity and computational time, especially for large dimension.

In the future, investigation on NSFD schemes should focus on stiff equations (for which explicit standard methods fail) or large systems (for which implicit standard methods are time-consuming or even prohibitive). Those situations should highlight the potential of NSFD integrators even further.

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Conflict of Interest Statement

The authors declare that there is no conflict of interests regarding the publication of this article.

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