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Using Approximations of Unity in the Construction of Positivity-Preserving NSFD Schemes

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Abstract

We present examples of nonstandard finite difference (NSFD) schemes that preserve positivity while simultaneously exploiting various ways unity (i.e. the number "1") can be represented algebraically in these expressions. NSFD schemes (also known as "Mickens discretizations") use nonstandard numerical techniques to approximate derivatives and other features in ordinary and partial differential equations. These NSFD schemes can often be used to produce numerical solutions to differential equations that have particular desired properties like increased accuracy, preserving positivity, and maintaining boundedness.

AMS Subject Classifications: 65L05, 65L12.
Keywords: Numerical analysis, finite differences, nonstandard finite differences, differential equations, positivity-preserving, Mickens discretization.

1 Introduction

In this paper we construct a number of nonstandard finite difference (NSFD) schemes with certain desired properties and demonstrate their use in the numerical solution of ordinary differential equations (ODEs). NSFD schemes are specialized finite difference methods that can be used to approximate numerical solutions of differential equations. There are various kinds of NSFD schemes, which are often constructed using rules articulated by Mickens [13,14,16]. Our motivation for the work in this paper is to expand the repertoire of possible NSFD schemes available for solving ODEs by incorporating approximations of unity that utilize expressions like $\frac{x_k}{x_{k+1}}$ or $\frac{x_{k+1}}{x_k}$. Our goal is to identify

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NSFD schemes for our selected ODE whose numerical solutions have a specific desired property, i.e., we want to identify NSFD schemes that result in numerical solutions that are positivity preserving, i.e. they remain nonnegative over the entirety of their domain. This is especially important for differential equations that represent physical quantities such as density or time and contain square roots of the independent variable.

There are many examples of ODE models of nature such as the Lotka–Volterra model (describes predator-prey dynamics) [22] or the SIR epidemic model (investigates the propagation of infectious disease) [7]. Only a limited number of models use ODEs that can be solved analytically in terms of a finite combination of elementary functions and so solutions are often found using numerical approximation techniques. In the past forty years NSFD schemes [1,2,10–12,15] have gained popularity for use in the development of numerical solutions to such models. This is due to their ability to give rise to numerical solutions that preserve the same qualitative features as the corresponding differential equation modeling the phenomena of interest; These desired features include dynamic consistency [18], preserving positivity of the solution [17,23], maintaining the stability behaviour of fixed points [8] and having the same fixed points [20] to name a few.

There are other examples of NSFD schemes that take advantage of approximations of unity previously published in the research literature. In [3], this idea is used in the numerical solution of partial differential equations that involve cross-diffusion. In [6] approximations of unity are used in the construction of NSFD schemes to numerically solve productive-destructive systems of ODEs. In [4], they examine ODE models in population dynamics using NSFD schemes that take advantage of the "1" approximation and that preserve qualitative features of the dynamical system.

Specifically, in this paper we present multiple NSFD schemes that utilize approximations of unity and preserve positivity of the solution for a selected ODE example where this is required due to the nature of the equation, which contains square roots of the dependent variable. We find that although there are numerous *possible* NSFD schemes that can be derived from the unity approximation, only a few satisfy our requirements to produce positivity-preserving solutions.

The rest of this article is organized as follows. In Section 2 we present all possible NSFD schemes that use expressions equivalent to unity and use them to obtain numerical solutions to a simple first-order initial-value problem (IVP). The eight possible NSFD schemes that utilize approximations of unity are classified into six distinct schemes, which we analyze to identify the schemes that have the positivity-preserving property we desire. In Subsection 2.3 we present the numerical performance for each scheme. We conclude with a summary of results and discussion of possible future work in Section 3. Our results show that for our selected ODE, our newly created NSFD schemes do not have improved accuracy over a well-known NSFD scheme, the implicit Euler method.

2 NSFD Schemes Using Approximations of Unity

Among various techniques for approximating ordinary differential equations numerically, nonstandard finite difference schemes have been proved to be one of the most efficient and versatile approaches in recent years [19, 21]. In this section, we derive and apply NSFD schemes that use approximations of unity to obtain numerical solutions of a particular simple initial-value problem (2.1) and (2.2), that we call Example A.

2.1 A Simple ODE Example

Below we consider a number of possible NSFD schemes that exploit various ways the number "1" can be approximated algebraically as we discretize Example A, which is the initial value problem below:

$$\frac{dx}{dt} = -\lambda\sqrt{x}, \tag{2.1}$$

for $t \geq 0$ with $\lambda > 0$ and with initial condition

$$x(0) = x_0 > 0. \tag{2.2}$$

From Equations (2.1) and (2.2) we know that the solution must be nonnegative, bounded and monotonically decreasing for all $t \geq 0$. These results follow from the following observations:

- Clearly $x(t) = 0$ is a solution to Equation (2.1) and is the fixed point.
- Since $x(0) > 0$ and $\dfrac{dx}{dt} < 0$, the solution $x(t)$ can only decrease.

The exact solution is

$$x(t) = \begin{cases} \left(\sqrt{x_0} - \dfrac{\lambda}{2}t\right)^2, & 0 < t \leq t_c = \dfrac{2\sqrt{x_0}}{\lambda} \\ 0 & , \quad t > t_c. \end{cases} \tag{2.3}$$

Note that the exact solution in Equation (2.3) is nonnegative, bounded and monotonically decreasing for all $t \geq 0$. This is illustrated by the graph in Figure (2.1) below for the case $\lambda = 1$ and $x_0 = 1$. Observe that Example A in (2.1) has one fixed point, at $x = 0$. We will try to find NSFD schemes that match these properties of Example A.

Roeger and Mickens [23] first studied IVPs of the form $\dfrac{dx}{dt} = -\lambda x^{\alpha}, \quad x(t_0) = x_0 > 0$ for $\lambda > 0$ and $\alpha > 0$, and such equations often appear in the modelling of a broad range of physical and engineering phenomena [13, 16]. In [23] Roeger and Mickens proved the existence of an exact finite difference scheme when $\alpha > 0$. Our Example A

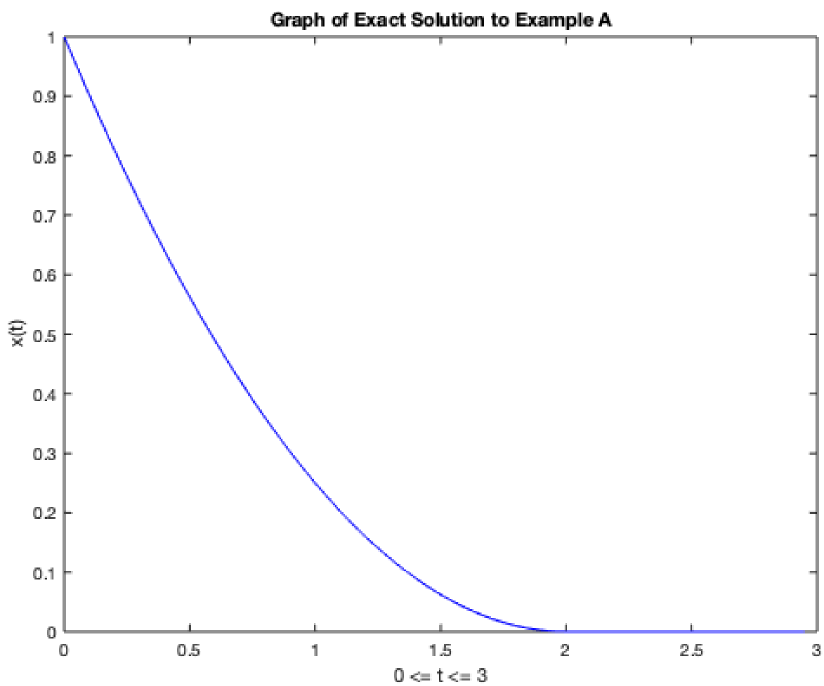

Figure 2.1: Graph of exact solution to Example A

is the special case when $\alpha = 1/2$ and the corresponding exact finite difference scheme is

$$x_{k+1} = \left(\sqrt{x_k} - \frac{\lambda h}{2} \right)^2. \tag{2.4}$$

Note the exact finite difference scheme can also be written

$$\frac{x_{k+1} - x_k}{h} = -\lambda \sqrt{x_k} + \frac{\lambda^2 h}{4}. \tag{2.5}$$

The exact scheme in Equation (2.4) is clearly positivity-preserving.

2.2 All Possible NSFD Schemes For Example A Utilizing The "1" Approximation

In this subsection we shall tabulate and categorize possible NSFD schemes utilizing the "1" approximation that we can apply to solve Example A. We can view Equation (2.1) as:

$$\frac{dx}{dt} = -\lambda \sqrt{x} \left(\frac{x}{x} \right), \tag{2.6}$$

where "1" i.e. "$\left(\frac{x}{x} \right)$" is treated as the expression in the parenthesis given in Equation (2.6) and is the source of the unity approximation idea.

Possible discretizations of "1" in the right-hand side of Equation (2.6) can be explored using various choices for A, B and C in Equation (2.7), which is a discretized version of Equation (2.1):

$$\frac{x_{k+1} - x_k}{h} \approx -\lambda\sqrt{x_A}\left(\frac{x_B}{x_C}\right). \tag{2.7}$$

Assuming a 2-point stencil, A, B and C can all be either k or $k+1$. This results in a total of eight possibilities (i.e. we have three parameters each of which can take on two possible values $=2^3$) leading to the six distinct numerical schemes presented in Table 2.1.

Table 2.1: All Possible Finite Difference Schemes for Example A

A	B	C	$\sqrt{x}$	Label	Scheme
k	k	k	$\sqrt{x_k}$	Scheme 0	Explicit Forward Euler
$k+1$	k	k	$\sqrt{x_{k+1}}$	Scheme 1	Implicit Euler
k	$k+1$	k	$\frac{x_{k+1}}{\sqrt{x_k}}$	Scheme 2	NSFD
k	k	$k+1$	$\frac{(x_k)^{\frac{3}{2}}}{x_{k+1}}$	Scheme 3	NSFD
$k+1$	$k+1$	$k+1$	$\sqrt{x_{k+1}}$	Scheme 1	Implicit Euler
k	$k+1$	$k+1$	$\sqrt{x_k}$	Scheme 0	Explicit Forward Euler
$k+1$	k	$k+1$	$\frac{x_k}{\sqrt{x_{k+1}}}$	Scheme 4	NSFD
$k+1$	$k+1$	k	$\frac{(x_{k+1})^{\frac{3}{2}}}{x_k}$	Scheme 5	NSFD

We will analyze each of the six distinct schemes in the subsequent sub-subsections.

2.2.1 Scheme 0

For Scheme 0, we can choose $A = k, B = k$ and $C = k$ or $A = k, B = k + 1$ and $C = k + 1$ in Equation (2.7) which results in a scheme that is the explicit forward Euler method [9]:

$$\frac{x_{k+1} - x_k}{h} \approx -\lambda\sqrt{x_k}\left(\frac{x_k}{x_k}\right) = -\lambda\sqrt{x_k}. \tag{2.8}$$

Upon rearranging Equation (2.8), this results in the following scheme:

$$x_{k+1} = \sqrt{x_k}(\sqrt{x_k} - \lambda h). \tag{2.9}$$

To preserve positivity $\sqrt{x_k}$ must be greater than or equal to λh for all k. However Scheme 0 is not a positivity-preserving scheme because for some $k > 0$, x_k will be less than $(\lambda h)^2$.

2.2.2 Scheme 1

Choosing $A = k + 1, B = k$ and $C = k$ or $A = k + 1, B = k + 1$ and $C = k + 1$ in Equation (2.7) results in Scheme 1 which is equivalent to the implicit backward Euler scheme [9].

$$\frac{x_{k+1} - x_k}{h} \approx -\lambda\sqrt{x_{k+1}}\left(\frac{x_k}{x_k}\right) = -\lambda\sqrt{x_{k+1}} \tag{2.10}$$

or,

$$x_{k+1} + \lambda h\sqrt{x_{k+1}} - x_k = 0. \tag{2.11}$$

Let $u_k = \sqrt{x_k}$, then Equation (2.11) becomes

$$u_{k+1}^2 + (\lambda h)u_{k+1} - u_k^2 = 0. \tag{2.12}$$

Solving the quadratic Equation (2.12) in u_{k+1} for the positive root gives,

$$u_{k+1} = \frac{1}{2}\left[-\lambda h + \sqrt{\lambda^2 h^2 + 4u_k^2}\right] \tag{2.13}$$

and therefore,

$$x_{k+1} = u_{k+1}^2 = \frac{1}{4}\left[-\lambda h + \sqrt{\lambda^2 h^2 + 4x_k}\right]^2. \tag{2.14}$$

From Equation (2.14), it is clear that x_{k+1} is always positive since the term in the radical is always greater than λh when $x_0 > 0$ and thus **Scheme 1 is a positivity-preserving scheme**. Note Scheme 1 has a fixed point at $x = 0$.

2.2.3 Scheme 2

For Scheme 2, we chose $A = k, B = k + 1$ and $C = k$ in Equation (2.7) which results in

$$\frac{x_{k+1} - x_k}{h} \approx -\lambda\sqrt{x_k}\left(\frac{x_{k+1}}{x_k}\right) = -\lambda\frac{x_{k+1}}{\sqrt{x_k}}. \tag{2.15}$$

Solving Equation (2.15) for x_{k+1} and simplifying gives

$$x_{k+1} = \left(\frac{\sqrt{x_k}}{h\lambda + \sqrt{x_k}}\right)x_k. \tag{2.16}$$

Since $\lambda > 0$, $h > 0$ and $x_0 > 0$ it is clear $x_k > 0$ for all k so **Scheme 2 is a positivity preserving NSFD scheme**. Further, since in Equation (2.16) the numerator is clearly always less than the denominator, $x_{k+1} < x_k$ for all k so the numerical solution also decreases smoothly to zero as k increases. Note, Scheme 2 has a fixed point at $x = 0$.

2.2.4 Scheme 3

Scheme 3 is formed by selecting $A = k, B = k$ and $C = k + 1$ in Equation (2.7) to produce

$$\frac{x_{k+1} - x_k}{h} \approx -\lambda\sqrt{x_k}\left(\frac{x_k}{x_{k+1}}\right) = -\lambda\frac{x_k^{3/2}}{x_{k+1}}. \tag{2.17}$$

Re-arranging Equation (2.17) forms a quadratic in x_{k+1} given by

$$x_{k+1}^2 - x_k x_{k+1} + \lambda h x_k^{3/2} = 0. \tag{2.18}$$

Solving Equation (2.18) for x_{k+1} we obtain

$$x_{k+1} = \frac{1}{2}\left\{x_k \pm \sqrt{x_k^2 - 4\lambda h x_k^{3/2}}\right\} \tag{2.19}$$

where we choose the positive root. We know that x_k decreases monotonically because it is clear that the expression $\dfrac{x_{k+1}}{x_k} = \dfrac{1}{2}\left\{1 + \sqrt{1 - \dfrac{4\lambda h}{\sqrt{x_k}}}\right\} < 1$ for all k. When $\sqrt{x_k} - 4\lambda h < 0$ or $x_k < 16\lambda^2 h^2$ the expression in Equation (2.19) will produce complex values when the term in the radical becomes negative as x_k decreases to zero. So Scheme 3 is not positivity-preserving.

2.2.5 Scheme 4

Selecting $A = k + 1, B = k$ and $C = k + 1$ in Equation (2.7) results in another distinct scheme that we label Scheme 4. Thus, Scheme 4 is:

$$\frac{x_{k+1} - x_k}{h} \approx -\lambda\sqrt{x_{k+1}}\left(\frac{x_k}{x_{k+1}}\right) = -\lambda\frac{x_k}{\sqrt{x_{k+1}}} \tag{2.20}$$

Letting $x_k = u_k^2$ in Equation (2.20), results in

$$\frac{u_{k+1}^2 - u_k^2}{h} = -\lambda \frac{u_k^2}{u_{k+1}}. \tag{2.21}$$

An explicit expression for Scheme 4 is obtained by using the standard formula [5] for the solution to the cubic polynomial $at^3 + bt^2 + ct + d = 0$ where $a = 1, b = 0, c = -u_k^2, d = \lambda h u_k^2$ and the variable is $t = u_{k+1}$:

$$u_{k+1}^3 - u_k^2 u_{k+1} + \lambda h u_k^2 = 0. \tag{2.22}$$

Since we can't easily write down an explicit expression for x_{k+1} in terms of x_k we verified through numerical experiments that Scheme 4 is not positivity-preserving.

2.2.6 Scheme 5

The last unique scheme, Scheme 5 is formed by selecting $A = k+1, B = k+1$ and $C = k$ in Equation (2.7) which results in

$$\frac{x_{k+1} - x_k}{h} \approx -\lambda \sqrt{x_{k+1}} \left(\frac{x_{k+1}}{x_k} \right) = -\lambda \frac{x_{k+1}^{3/2}}{x_k}. \tag{2.23}$$

Letting $x_k = u_k^2$ and re-arranging we obtain the following cubic

$$\lambda h u_{k+1}^3 + u_k^2 u_{k+1}^2 - u_k^4 = 0 \tag{2.24}$$

which we will solve again using the formula for the solution to the generic cubic with coefficients $a = \lambda h, b = u_k^2, c = 0$, and $d = -u_k^4$. **Scheme 5 is a positivity-preserving NSFD scheme**, which is verified through numerical experimentation with the results given in Subsection 2.3. By examining Equation (2.23) we find that the fixed point for Scheme 5 is $x = 0$.

2.3 Numerical Results

In this section we analyse the qualitative nature and computational performance of each of the six distinct finite difference Schemes 0 through 5 by using each to approximate numerical solutions to Example A with parameter $\lambda = 1$ and an initial value of $x_0 = 1$, which corresponds to $t_c = 2$. In other words, the analysis in this section pertains to the IVP:

$$\frac{dx}{dt} = -\sqrt{x}, \quad x(0) = 1. \tag{2.25}$$

The corresponding true solution is shown in Figure 2.1 and given by:

$$x(t) = \begin{cases} \left(1 - \frac{1}{2}t\right)^2, & 0 < t \leq 2 \\ 0, & t > 2. \end{cases} \tag{2.26}$$

In Table 2.2 below we summarize the six distinct numerical schemes and their status regarding whether their corresponding numerical solutions preserve positivity. Schemes 0 and 1, explicit forward Euler and implicit Euler, respectively, are obtained when B and C in Equation (2.7) are equal, and therefore don't contain an approximation of unity. We don't consider explicit forward Euler to be a NSFD scheme, while technically implicit Euler is a NSFD scheme, since it contains a nonlocal approximation. We note that only Schemes 1, 2 and 5 are NSFD schemes that preserve positivity. All the finite difference schemes considered have the same fixed points as the ODE being approximated. We

Table 2.2: Properties of Numerical Schemes 0 through 5

Scheme	0	1	2	3	4	5
Uses "1" Approximation	No	No	Yes	Yes	Yes	Yes
NSFD Scheme	No	Yes	Yes	Yes	Yes	Yes
Positivity Preserving	No	Yes	Yes	No	No	Yes
Same Fixed Points	Yes	Yes	Yes	Yes	Yes	Yes

conducted numerical experiments using Schemes 0 through 5 but have only presented the numerical results of the schemes that are positivity-preserving in this section. Tables 2.3, 2.4, and 2.5 provide some numerical results implementing the positivity-preserving schemes: Scheme 1, Scheme 2 and Scheme 5 on Example A. Each table presents the L^∞, L^1 and L^2 error norms corresponding to

$$h = 0.05, 0.025, 0.01, 0.005, 0.0025, 0.001.$$

Table 2.3: Scheme 1

Scheme 1	$\|x_{num} - x_{true}\|_{L^\infty}$	$\|x_{num} - x_{true}\|_{L^1}$	$\|x_{num} - x_{true}\|_{L^2}$
$h = 0.0500$	$9.04269906e-03$	$2.49861506e-01$	$4.25803031e-02$
$h = 0.0250$	$4.55941654e-03$	$2.49960864e-01$	$3.02683480e-02$
$h = 0.0100$	$1.83314683e-03$	$2.49992784e-01$	$1.92043351e-02$
$h = 0.0050$	$9.18139387e-04$	$2.49998015e-01$	$1.35939026e-02$
$h = 0.0025$	$4.59458904e-04$	$2.49999459e-01$	$9.61742521e-03$
$h = 0.0010$	$1.83877241e-04$	$2.49999904e-01$	$6.08452185e-03$

3 Conclusion and Future Work

In this article, we examined Mickens discretizations on a specific ODE, while simultaneously exploiting various ways the number "1" can be represented discretely. From the eight possible NSFD schemes that utilize approximations of unity, we obtained six

Table 2.4: Scheme 2

Scheme 2	$\|x_{num} - x_{true}\|_{L^\infty}$	$\|x_{num} - x_{true}\|_{L^1}$	$\|x_{num} - x_{true}\|_{L^2}$
$h = 0.0500$	$2.56724918e-02$	$7.28337343e-01$	$1.22077275e-01$
$h = 0.0250$	$1.32835924e-02$	$7.38528287e-01$	$8.86385799e-02$
$h = 0.0100$	$5.43293498e-03$	$7.45206577e-01$	$5.70338177e-02$
$h = 0.0050$	$2.73745813e-03$	$7.47559691e-01$	$4.05726793e-02$
$h = 0.0025$	$1.37409764e-03$	$7.48766944e-01$	$2.87775662e-02$
$h = 0.0010$	$5.50943336e-04$	$7.49503140e-01$	$1.82345380e-02$

Table 2.5: Scheme 5

Scheme 5	$\|x_{num} - x_{true}\|_{L^\infty}$	$\|x_{num} - x_{true}\|_{L^1}$	$\|x_{num} - x_{true}\|_{L^2}$
$h = 0.0500$	$4.09252162e-02$	$1.18979449e+00$	$1.96435908e-01$
$h = 0.0250$	$2.15975670e-02$	$1.21718416e+00$	$1.44856744e-01$
$h = 0.0100$	$8.95835266e-03$	$1.23596625e+00$	$9.42461363e-02$
$h = 0.0050$	$4.53731893e-03$	$1.24278334e+00$	$6.73222523e-02$
$h = 0.0025$	$2.28375965e-03$	$1.24633140e+00$	$4.78544609e-02$
$h = 0.0010$	$9.17200759e-04$	$1.24851437e+00$	$3.03631095e-02$

different schemes. From these six schemes, the goal was to identify NSFD schemes that produce numerical solutions that preserve positivity.

Our research shows that Scheme 1, Scheme 2 and Scheme 5 are numerical schemes that preserve positivity. In the case of Scheme 1 and Scheme 2 we have provided analysis demonstrating this result. For Scheme 5 we used numerical justification to show it generates positivity-preserving numerical solutions. Our numerical experiments also establish that Scheme 1 outperforms both Scheme 2 and Scheme 5 in terms of the accuracy of the numerical solution when compared to the exact solution. Scheme 2 outperforms Scheme 5. Thus, we write the schemes in order of decreasing accuracy:

$$\text{Scheme } 1 > \text{Scheme } 2 > \text{Scheme } 5.$$

To summarize: Scheme 1, which is the implicit Euler method, generates a numerical solution to Example A that not only preserves positivity, but is also the most accurate. Figure (3.1) compares the error between the exact solution in Equation (2.26) and the numerical solutions generated by Scheme 1, Scheme 2 and Scheme 5. The plots of $\log$(error) versus $\log(h)$ show that all three schemes have the same order of accuracy since the lines in the figure are all parallel. One can also see that all three schemes are second-order schemes, since the slopes of the lines in the figure are roughly equal to 2. The line representing the error in Scheme 1 is the most negative, thus it corresponds to the most accurate scheme.

Future investigations may include examination of other differential equations whose numerical approximation would be likely to include expressions that involve approxi-

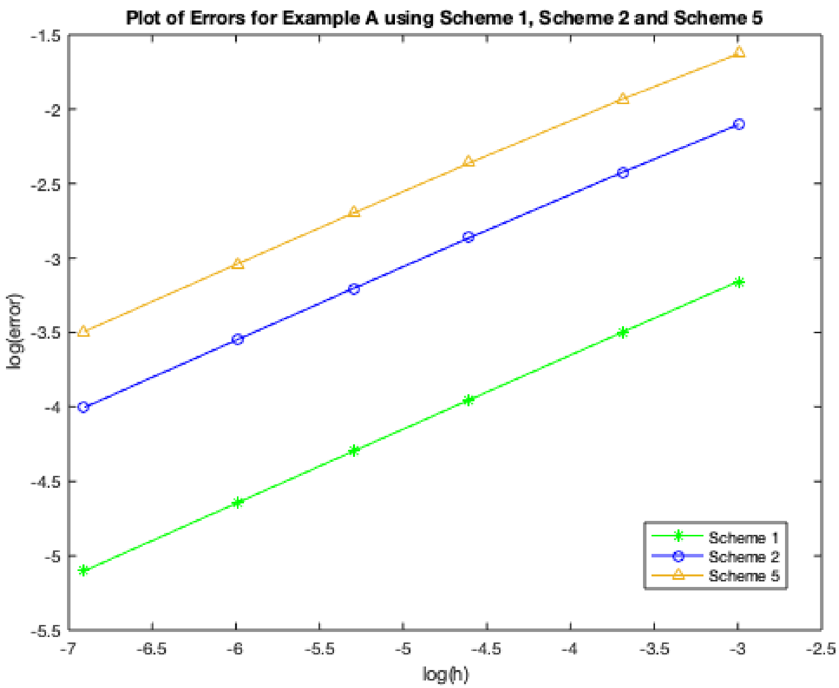

Figure 3.1: Comparing Numerical Errors Of Schemes 1, 2 and 5

mations of unity. For example,

$$\frac{dx}{dt} = -\lambda x^P, \qquad \text{where } P \text{ is rational.} \tag{3.1}$$

was considered by Roeger and Mickens [23], for the case where $\lambda > 0$ and $P > 0$. We believe this work could be extended in multiple ways: applications of approximations of unity and using other nonstandard approximations of the derivative. For example, Equation (3.1) can be re-written as

$$\frac{\Delta x}{\Delta t} \approx -\lambda (x_a)^L \frac{(x_b)^M}{(x_c)^N} \tag{3.2}$$

where a, b, c are either k or $k+1$ and $L + M - N = P$. The left-hand derivative can be approximated in multiple different ways using nonstandard methods. There are an infinite number of possibilities for L, M and N and eight choices for a,b and c that can be explored.

Another suggestion for future work is to increase the size of the stencil used to approximate the differential equation, thus one could examine unity approximations with $\frac{x_{k+1}}{x_{k-1}}$. This would provide a larger number of possible NSFD approximations to evaluate that we have considered here.

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