Numerical instabilities in finite-difference models of ordinary differential equations

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NUMERICAL INSTABILITIES IN FINITE-DIFFERENCE MODELS OF ORDINARY DIFFERENTIAL EQUATIONS

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ABSTRACT
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NUMERICAL INSTABILITIES IN INFINITE-DIFFERENCE MODELS OF ORDINARY DIFFERENTIAL EQUATIONS

Advisor: Professor Ronald E. Mickens

Thesis dated June 1989

We investigate various mechanisms for the occurrence of numerical instabilities in the discrete modeling of ordinary differential equations by finite-differences. The Logistic equation is used to illustrate the three types of numerical instabilities. Our results can be easily generalized to arbitrary first-order differential equations.
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CHAPTER ONE

INTRODUCTION

1.1. Statement of the Problem

Many dynamic systems can be modeled in terms of ordinary differential equations. The general lack of exact solutions in finite, closed form means that numerical approximations must be used to determine the possible solution behaviors of the differential equation. The method of finite-differences is one of the most widely used procedures for numerical integration.

The purpose of this thesis is to investigate various mechanisms for the occurrence of numerical instabilities in the discrete modeling of ordinary differential equations by finite-differences.

1.2. Summary of Results

Linear stability analysis was used to determine the existence of numerical instabilities in the Logistic differential equation for three finite-difference schemes: forward Euler, central difference and a fourth-order Runge-Kutta. Our major conclusion is that numerical instabilities can arise whenever one or more of the following conditions occur:

(i) the step-size, \( h = \Delta t \), becomes equal to or larger than a threshold value \( h_0 \), i.e., \( h \geq h_0 \);
(ii) the order of the discrete finite-difference model is larger than the order of the corresponding differential equation;

(iii) the number of fixed points (constant solutions) of the finite-difference scheme is larger than the number of fixed points of the corresponding differential equation.

1.3. Finite-Difference Models

Consider the following ordinary, first-order, differential equation

\[ \frac{dx}{dt} = f(x,t), \quad x(0) = x_0 = \text{given}, \tag{1.1} \]

where the function \( f(x,t) \) has the necessary properties such that Eq. (1.1) has a solution.\(^2,^4\) This equation can be modeled by the finite-difference scheme

\[ \frac{x_{k+1} - x_k}{h} = f(x_k, hk), \quad x_0 = \text{given}, \tag{1.2} \]

where \( h = \Delta t \) is the step-size, \( k \) is an integer, and \( x_k \) is the discrete analogue of \( x(t) \) evaluated at the discrete time \( t = t_k = hk \). Note that in constructing Eq. (1.2) from Eq. (1.1), the following replacements were made

\[ (1.3a) \quad t \to hk, \quad x(t) \to x_k \]
There are other possibilities for constructing discrete models of Eq. (1.1). These will be considered in Chapter Two. However, for the moment, we only wish to indicate that the general modeling process consists of the steps:

(a) replacement of the derivative in Eq. (1.1) by a discrete finite-difference;

(b) the substitutions given by Eqs. (1.3);

(c) replacement of the function \( f(x,t) \) by a new function

\[
(1.4) \quad f(x,t) \rightarrow f(x_k,t_k) + hg(x_k,t_k,h),
\]

where the exact nature of \( g(x_k,t_k,h) \) depends on the particular procedure used.

1.4. **Numerical Instabilities**

A finite-difference model has numerical instabilities when it has solutions that do not correspond to any solution of the differential equation.

A particular form of numerical instability is the existence of chaotic solutions. A chaotic solution, of
a finite-difference equation or scheme, is an unstable solution that is bounded and does not approach (as $k \to \infty$) any constant solution of either the difference or differential equation.

1.5. Linear Stability Analysis

An important tool needed to investigate numerical instabilities is linear stability analysis. This procedure consists of determining the local stability properties of the constant solutions (fixed points) of Eq. (1.1) and its associated finite-difference model. If the constant solutions of the finite-difference model have different stability properties than the corresponding constant solutions of the differential equation, then numerical instabilities exist. We present only a brief outline of the required procedures; the full details are given in Section 1.5 of the thesis by Arthur L. Smith.9

Consider the first-order difference equation

$$x_{k+1} = F(x_k)$$  \hspace{1cm} (1.5)

The fixed-points or constant solutions are determined by the condition

$$\bar{x} = F(\bar{x}).$$  \hspace{1cm} (1.6)
Denote these solutions by

\[(1.7) \ \{\bar{x}_\ell\}, \ \ell = 1,2,\ldots,M,\]

where \(M\) may be unbounded. It is assumed that all the zeros of Eq. (1.6) are simple. Now select a particular constant solution, say \(\bar{x}_i\), and consider neighboring solutions

\[(1.8) \ x_k = \bar{x}_i + \epsilon_k,\]

where

\[(1.9) \ |\epsilon_0| \ll |\bar{x}_i - \bar{x}_{i-1}| \quad \text{and} \quad |\bar{x}_{i+1} - \bar{x}_i|.\]

If \(\epsilon_k\) satisfies the condition

\[(1.10) \ \lim_{k \to \infty} |\epsilon_k| = 0,\]

then \(x_k = \bar{x}_i\) is said to be a stable constant solution. Otherwise, it is an unstable constant solution. The substitution of Eq. (1.8) into Eq. (1.5) gives

\[(1.11) \ \bar{x}_i + \epsilon_{k+1} = F(\bar{x}_i + \epsilon_k) = F(\bar{x}_i) + B\epsilon_k + O(\epsilon_k^2),\]

where the constant \(B\) is
(1.12) \( B \equiv \frac{dF(x)}{dx} \bigg|_{x=\bar{x}_i} \).

Using Eq. (1.6) and retaining only the linear term on the right-side of Eq. (1.11), the following equation is obtained

(1.13) \( \epsilon_{k+1} = B\epsilon_k \).

Its solution is

(1.14) \( \epsilon_k = \epsilon_0(B)^k \).

Comparison of Eq. (1.14) with the condition of Eq. (1.10) gives the linear analysis result for stability

(1.15) \(|B| < 1\).

Consequently, \( x_k = \bar{x}_i \) is linearly stable if the following inequality is satisfied

(1.16) \( \left| \frac{dF(x)}{dx} \bigg|_{x=\bar{x}_i} \right| < 1 \).

1.6. Outline of Thesis

In Chapter Two, three discrete models of the Logistic differential equation are constructed. Each model illus-
trates a different mechanism for the occurrence of numerical instabilities. A discussion of the major results of this thesis is given at the end of the chapter. Finally, Chapter Three states a number of related issues that can form the basis for future investigations into the existence of numerical instabilities for both ordinary and partial differential equations.
2.1. The Logistic Differential Equation

The "simplest" nonlinear first-order differential equation is

\[ \frac{dx}{dt} = x(1-x), \quad x(0) = x_0 \text{ given.} \]

This equation is named the Logistic equation and provides an elementary model of a population interacting with itself.² Both Ushiki ⁸ and Mickens ⁷,¹² have done much work on this differential equation in their investigations of how numerical instabilities occur.

Examination of Eq. (2.1) shows that it has two constant solutions.

\[ x_1 = 0 \quad \text{and} \quad x_2 = 1. \]

The first solution is (linearly) unstable, while the second solution is (linearly) stable. Applying the method of separation of variables allows a determination of the exact general solution to Eq. (2.1); it is

\[ x(t) = \frac{x_0}{x_0 + (1-x_0)e^{-t}}. \]
Note that

\[(2.4) \lim_{t \to \infty} x(t) = 1, \text{ for } x_0 > 0,\]

\[(2.5) \text{ for } x_0 = 0, \quad x(t) = 0.\]

Both of these results are in agreement with the linear stability analysis.

The remainder of this chapter will be concerned with the construction of three finite-difference models of the Logistic equation and the conditions that permit the existence of numerical instabilities for each model. The obtained results are expected to hold true for the general class of first-order, ordinary differential equations since they only differ from Eq. (2.1) only in having more fixed points (constant solutions). The procedure for investigating the stability of a given fixed point remains the same for a differential equation having an arbitrary number of constant solutions.

2.2. **Forward Euler Scheme**

The so-called forward Euler scheme for the Logistic equation is

\[(2.6) \quad \frac{x_{k+1} - x_k}{h} = x_k(1-x_k).\]
This representation corresponds to the use of the conventional choice for the discrete derivative

\[ \frac{dx}{dt} = \lim_{h \to 0} \frac{x(t+h) - x(t)}{h} = \frac{x_{k+1} - x_k}{h}, \]

and a local modeling of the nonlinear term

\[ F(x) = x(1-x) \to x_k(1-x_k). \]

The fixed-points of Eq. (2.6) are the constant solution \( x_k = \bar{x} \). Substitution of this expression into Eq. (2.6) gives the two constant solutions.

\[ \bar{x}_1 = 0 \quad \text{and} \quad \bar{x}_2 = 1. \]

Comparison with Eq. (2.2) shows that the forward Euler scheme has exactly the same number of fixed-points as the Logistic differential equation. A linear stability analysis can now be applied to Eq. (2.6).

Near \( x_k = \bar{x}_1 = 0 \), we have

\[ x_k = \bar{x}_1 + \epsilon_k \]

and from Eqs. (2.8) and (1.12)
since $h > 0$. Thus, we conclude from Eq. (1.16) that the fixed-point at $x_k = \bar{x}_1 = 0$ is unstable for all (positive) step-sizes. This agrees with the corresponding fixed-point for Eq. (2.1).

Now consider the fixed-point at $x_k = \bar{x}_2 = 1$. A direct calculation gives

\begin{equation}
B = 1 - h.
\end{equation}

Stability requires (see Eqs. (1.15) and (1.16)) that $B$ satisfies the condition

\begin{equation}
|B| < 1.
\end{equation}

This means that $h$ must be restricted to the following interval of step-size values

\begin{equation}
0 < h < 2.
\end{equation}

In summary, the forward Euler scheme for Eq. (2.1) has the same (local) stability properties for the constant solutions as the corresponding differential equation if the step-size lies in the range given by Eq. (2.14). Other-
wise, numerical instabilities will occur.

This particular mechanism for the occurrence of numerical instabilities is a threshold instability, i.e., the step-size has to be larger than a certain value $h_0$ in order for the instability to exist.

2.3. Central Difference Scheme

The central difference scheme for Eq. (2.1) is

\begin{equation}
\frac{x_{k+1} - x_{k-1}}{2h} = x_k(1-x_k).
\end{equation}

This corresponds to the following discrete model for the derivative

\begin{equation}
\frac{dx}{dt} = \lim_{h \to 0} \frac{x(t+h) - x(t-h)}{2h} \to \frac{x_{k+1} - x_{k-1}}{2h}.
\end{equation}

An elementary calculation shows that Eq. (2.15) has fixed-points at

\begin{equation}
x_1 = 0 \quad \text{and} \quad x_2 = 1,
\end{equation}

in agreement with the location of the fixed-point for Eq. (2.1).

A linear stability analysis about the constant solution $x_k = 0$, gives
(2.18) \[ \frac{\epsilon_{k+1} - \epsilon_{k-1}}{2h} = \epsilon_k, \]

or

(2.19) \[ \epsilon_{k+2} - (2h)\epsilon_{k+1} - \epsilon_k = 0. \]

This latter is a second-order linear difference equation with constant coefficients. Its solution can be obtained using standard methods.\(^{10}\) The solution is

(2.20) \[ \epsilon_k = A_1(r_+)^k + A_2(r_-)^k \]

where

(2.21) \[ r_{\pm} = h \pm \sqrt{1 + h^2}, \]

and \((A_1, A_2)\) are arbitrary constants. Note that

(2.22) \[ r_+ > 1 \]

for all \(h > 0\). Hence, the fixed-point at \(x_k = \bar{x}_1 = 0\) is unstable for all values of the step-size.

Also, observe that \(r_-\) satisfies the bounds

(2.23) \[ -1 < r_- < 0, \quad h > 0. \]
Therefore, the second part of the solution for $e_k$, given by Eq. (2.20), can be written

$$(2.24) \quad e_k \sim A_2(-1)^k(\vert r \vert)^k.$$ 

This means that any solution of Eq. (2.15) that starts near $x_k = x_1 = 0$ has two components, one that increases exponentially and a second that decreases exponentially with an oscillating factor $(-1)^k$.

Applying the linear stability procedure about the constant solution $x_k = 1$ gives

$$(2.25) \quad x_k = 1 + \eta_k$$

and

$$(2.26) \quad \eta_{k+2} + (2h)\eta_{k+1} - \eta_k = 0,$$

where the latter difference equation has the solution

$$(2.27) \quad \eta_k = C_1(s_+)^k + C_2(s_-)^k,$$

where $C_1$ and $C_2$ are arbitrary constants, and $s_\pm$ is given by the expression.
(2.28) \[ s_\pm = -h \pm \sqrt{1 + h^2}. \]

Inspection of Eq. (2.28) shows that

(2.29) \[ |s_-| > 1, \quad h > 0. \]

Thus, we conclude that the finite-difference scheme of (2.15) has an unstable constant solution \( x_k = x_2 = 1 \) for all (positive) values of the step-size. This instability gives rise to an exponentially increasing solution (locally) that oscillates with the factor \((-1)^k\).

In summary, the central difference scheme for Eq. (2.1) is unstable for any (positive) step-size. The (local) behavior of the solutions to Eq. (2.15) has been observed in computer experiments.\(^7\)\(^8\) In fact, Ushiki\(^8\) has shown that the finite-difference equation given by the central difference scheme for the Logistic equation has chaotic solutions for all \( h > 0 \).

The numerical instabilities for this case arise from the fact that the difference equation model is of higher order than the corresponding differential equation, i.e., Eq. (2.1) is a first-order equation, while Eq. (2.15) is a second-order equation. (For linear equations, this has the consequence that the finite-difference model has an additional solution as compared to the differential equa-
We call this type of numerical instability an order instability.

2.4. Runge-Kutta Scheme

Our last model is a fourth-order Runge-Kutta scheme. When the technique is applied to Eq. (2.1), the following expression is obtained

\[
X_{k+1} = \left[ 1 + \frac{(2+h)h}{2} \right] X_k - \left[ \frac{(2+3h+h^2)h}{2} \right] X_k^2 \\
+ (1+h)h^2 X_k^3 - \left( \frac{h^3}{2} \right) X_k^4.
\]

Examination of Eq. (2.30) shows that it has four fixed-points or constant solutions! This follows directly from the fact that if \( X_k = \bar{x} \) is substituted into Eq. (2.30), the resulting algebraic equation is of the fourth degree. However, two solutions are already known, namely

\[
\bar{x}_1 = 0, \quad \bar{x}_2 = 1.
\]

Factoring them out gives a quadratic equation; solving it gives the two other solutions

\[
\bar{x}_{3,4} = \frac{2 + h \pm \sqrt{h^2 - 4}}{2h}.
\]
For $0 < h < 2$, the fixed-points $x_3$ and $x_4$ are complex conjugates of each other. For $h \geq 2$, all the fixed-points are real.

The following points should be noted:

(i) The Runge-Kutta finite-difference scheme has four fixed-points, while the Logistic differential equation has only two fixed-points.

(ii) For $0 < h < 2$, the two additional complex conjugate fixed-points do not give rise to numerical instabilities since the solution we seek to calculate is real. However, it is expected that for $h \geq 2$ the fixed points $x_3$ and $x_4$ will cause numerical instabilities.

The following calculations show this analysis to be correct.

First, consider the fixed-point at $x_k = \bar{x}_1 = 0$. Writing

$$x_k = \bar{x}_1 + \epsilon_k = \epsilon_k,$$

and substituting Eq. (2.33) into Eq. (2.30) gives the following (linear) expression

$$\epsilon_{k+1} = \left[1 + \frac{(2+h)h}{2}\right] \epsilon_k \equiv R\epsilon_k.$$
Since $R > 1$, for $h > 0$, $x_k = 0$ is unstable for all positive step-sizes. Thus, for this fixed-point the Runge-Kutta scheme has the same stability property as the Logistic differential equation.

Second, for the fixed-point at $x_k = 1 + \eta_k$, the application of the linear stability procedure gives

$$
(2.35) \quad \eta_{k+1} = \left[1 - h + \frac{h^2}{2}\right] \eta_k \equiv T \eta_k.
$$

A simple calculation shows that

$$
(2.36) \quad \begin{cases} 
0 < T < 1, & \text{for } 0 < h < 2, \\
T \geq 1, & \text{for } h \geq 2.
\end{cases}
$$

Consequently, the Runge-Kutta scheme has the same stability properties as Eq. (2.1) for any value of $h$ in the interval

$$
(2.37) \quad 0 < h < 2.
$$

Consider now the fixed point at $x_k = \bar{x}_3$ for $h \geq 2$. A long and tedious algebraic calculation gives the following expression for $\beta_k$

$$
(2.38) \quad \beta_{k+1} = V \beta_k,
$$

where
(2.39) \( x_k = \bar{x}_3 + \beta_k \),

and

(2.40) \( V = 3 - \left( \frac{h^2}{2} \right) + \left( \frac{h^3}{2} \right)[1 - \sqrt{h^2 - 4}] \).

Except for \( h \approx 2.27 \), \( V(h) \) is large compared to one as illustrated by the values

\[
\begin{align*}
V(2.00) &= 5.000, & V(2.20) &= 1.024, \\
V(3.00) &= -18.187, & V(2.25) &= 0.293, \\
V(4.00) &= -83.851, & V(2.26) &= 0.144, \\
V(10.00) &= -4445.980, & V(2.5) &= -11.844.
\end{align*}
\]

Therefore, for almost all values of \( h \geq 2 \), the fixed-point \( x_k = \bar{x}_3 \) is unstable.

Similar consideration also apply for the fourth fixed point \( x_k = \bar{x}_4 \) for \( h \geq 2 \).

In summary, the Runge-Kutta scheme introduced two "new" fixed-points in addition to the two regular fixed-points of the differential equation. The two "new" fixed-points are complex valued for \( 0 < h < 2 \), but, become real for \( h \geq 2 \). Only for \( 0 < h < 2 \), does the Runge-Kutta scheme have the same stability properties as Eq. (2.1): the fixed-point \( \bar{x}_1 = 0 \) is unstable and the fixed-point
$x_2 = 1$ is stable; the other two (new) fixed-points are complex and thus do not influence directly the stability properties of the real-valued solution. For $h \geq 2$, all the fixed-points become unstable. This latter result implies that if Eq. (2.30) has (globally) bounded solutions, then these solutions are chaotic!

We call the mechanism for numerical instabilities that arise in this case a proliferation instability.

2.5. Discussion

The study and analysis of how numerical instabilities arise in the modeling of differential equations by finite-difference schemes is an important activity of great relevance to modern science and technology. This follows from the fact that almost all the models of dynamic systems in current use are represented mathematically by differential equations. In general, these differential equations do not have exact solutions that can be expressed in terms of a finite number of elementary functions. A knowledge of the relationships among the solutions of the finite-difference schemes and the solutions of the differential equation is thus of fundamental importance for the correct understanding of both the properties of dynamic systems and the prediction of their future behaviors.

The research of this thesis, which extended the
previous work of Mickens,\textsuperscript{7,12} shows that numerical instabilities can occur in the simplest of differential equations, namely the Logistic equation. It is clear that the three mechanisms for instability found in the Logistic equation can also exist in the general class of systems of first-order, ordinary differential equations. Other possible types of numerical instabilities may occur and their existence and characterization needs to be investigated.

Based on the findings of this thesis, we can state the following general conclusions concerning the three types of numerical instabilities "discovered" in the Logistic differential equation:

(i) The step-size $h$ is generally restricted by numerical stability considerations rather than by the accuracy of the finite-difference scheme. In general, there is a threshold value of $h = h_0$ such that for $h \geq h_0$ the finite-difference scheme becomes unstable. We have called this type of instability a \textit{threshold instability}.

(ii) When the order of the finite-difference scheme is larger than the order of the differential equation, then "ghost solutions" or numerical instabilities will occur for any positive step-size $h$.\textsuperscript{6,7,8} This is an \textit{order instability}.

(iii) The use of sophisticated finite-difference schemes such as Runge-Kutta methods will generally give
rise to proliferation instabilities. These occur because the finite-difference equations have a larger number of fixed-points than does the corresponding differential equation.
3.1. Ordinary Differential Equations

Consider the differential equation

\[ \frac{dx}{dt} = F(x,t), \quad x(0) = x_0 = \text{given}, \]

where \( F(x,t) \) has the necessary properties such that Eq. (3.1) has a unique solution. The general goal of numerical analysis is to construct a finite-difference scheme

\[ x_{k+1} = G(x_k, k, h), \]

such that

\[ x_k = x(hk), \quad \text{for all } h > 0. \]

This means that on the computational lattice, \( t_k = hk \), the solution to the finite-difference scheme is exactly equal to the solution to the differential equation for any fixed value of the step-size. Note that no restrictions are placed on the magnitude of the step-size. Finite-difference schemes having this property are called exact. Preliminary work has been done on this problem by Mickens.\(^{12}\) However, these investigations need to be
extended. In the ideal case, rules could be discovered that would allow the construction of an exact finite-difference scheme for an arbitrary ordinary differential equation. However, this is a long term goal and is not likely to be accomplished soon.

A second area of interest is how the derivative terms that appear in the differential equation should be modeled in finite-difference schemes. The recent thesis of Smith\textsuperscript{9} presented certain new results on this problem. However, much more needs to be done on this important problem.

A third issue relates to the modeling of nonlinear terms in the differential equation. For example, the nonlinear expression $x^2$ can be represented by any one (or sum) of the forms

$$x_k^2,$$

$$x^2 \rightarrow \left\{ x_{k+1}x_k, x_k^2, x_{k+1}^2 \right\}.$$  \hspace{1cm} (3.4)

Each form will lead to a different finite-difference scheme. The theory of nonlinear, first-order difference equations\textsuperscript{10} implies that the general solutions of each of these equations will not be the same. Consequently, which model should be used?

Finally, it is of both practical and mathematical
interest to investigate the construction of analytic techniques for obtaining approximations to the exact solutions of nonlinear difference equation. These procedures could be directly applied to the examination of how numerical instabilities arise in finite-difference schemes. In particular, these methods may allow the determination of nonlinear stability conditions.

3.2. Partial Differential Equations

The situation regarding finite-difference models of partial differential equations is complicated. First, there is no ready definition or complete understanding of what constitutes the general solution of an arbitrary partial differential equation. Second, any investigation is further complicated by the fact that multi-step-size parameters occur. For example, the heat equation

\[
\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad u(x,0) = f(x) = \text{given},
\]

has a finite-difference representation

\[
\frac{u^n_m + 1 - u^n_m}{\Delta t} = \frac{u^n_{m+1} - 2u^n_m + u^n_{m-1}}{(\Delta x)^2},
\]

where \( n \) is the discrete time variable, \( t_n = (\Delta t)n; m \) is the discrete space variable, \( x_m = (\Delta x)m; \) and, \( \Delta t \) and \( \Delta x \)
are, respectively, the time-step and the space-step. Stability requires a functional relation between $\Delta t$ and $\Delta x$.

\begin{equation}
\Delta t \leq \frac{(\Delta x)^2}{4}.
\end{equation}

In general, we expect partial differential equations to have a larger number of possible types of numerical instabilities than ordinary differential equations. Linear stability analysis procedures have led to important results in the study of the stability properties of both linear and nonlinear partial differential equations. A major need is to generalize these methods so that nonlinear stability can be studied. Model equations that should be considered include the following equations.

\begin{align}
(3.8) \quad & \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u(1-u), \\
(3.9) \quad & \frac{\partial u}{\partial t} = i \frac{\partial^2 u}{\partial x^2} + |u|^2 u, \quad i = \sqrt{-1} \\
(3.10) \quad & \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = A \frac{\partial^2 u}{\partial x^2}, \quad A = \text{constant}.
\end{align}
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