AN ABSTRACT OF THE THESIS OF

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The one-dimensional heat equation $u_t = u_{xx}$ is the model problem for this paper. We can solve the heat equation numerically using the method of lines. One example of this method is the Crank-Nicolson scheme, which is second order accurate in both space and time. For many applications, this scheme is impractical because of its low order of accuracy. The purpose of this paper is to investigate higher order discretizations for the space derivative. We consider standard finite differences (explicit) and compact differences (implicit). Techniques for deriving these formulas are discussed in detail. The stability of the standard finite difference approach is examined with the use of eigenvalue analysis. As far as we know, the generation of weights for compact differences of high accuracy have not been attempted before. We propose a strategy which involves computing these weights using the method of undetermined coefficients.

High Order Finite Difference Methods

by

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Table of Contents

List of Figures

Preface

The use of finite difference methods to solve partial differential equations has been actively researched since their introduction in the beginning of this century. Modern studies focus on complicated nonlinear systems, such as those that model the earth's atmosphere or the circulation of the ocean. The complexity of such difference schemes is tremendous. The consideration of linear model problems rather than nonlinear systems provides a way to gain insight into the theoretical behavior of the complex scheme. Familiar examples of linear model problems are the wave equation $u_{tt} = u_{xx}$, the heat equation $u_t = u_{xx}$, and the Laplace equation $u_{xx} + u_{yy} = 0$.

The model problem for this paper is the heat equation

$$u_t = u_{xx}$$

with suitable initial data and boundary conditions, which are given by

$$u(0,t) = u(1,t) = 0, \qquad u(x,0) = f(x).$$

The space and time variables are discretized by $x_j = j\Delta x$ and $t_n = n\Delta t$, respectively. Typically, finite differences are used to approximate the space derivative and a linear multistep or Runge-Kutta formula is used to integrate with respect to time. One common method is the Crank-Nicolson method

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{1}{2}\left(\frac{u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1}}{\Delta x^2} + \frac{u_{j-1}^n - 2u_j^n + u_{j+1}^n}{\Delta x^2}\right), \tag{0.1}$$

where $u_j^n \approx u(x_j, t_n)$. This scheme is second order accurate in both space and time. In other words, if we restrict the step sizes so that $\Delta x = \Delta t$, then the error can be shown to go to zero as $O(\Delta t^2)$ goes to zero as $\Delta t \to 0$ [1]. However, this low order of accuracy is impractical for many applications. This necessitates the use of schemes with a higher convergence rate. The scope of our study is investigating such methods. We shall derive these methods and examine their stability using eigenvalue analysis.

The Crank-Nicolson scheme (0.1) can be derived as follows. The space derivative is approximated by the centered difference

$$u''_j = \frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2}.$$

Thus, the heat equation may be approximated by the semi-discretized system of ordinary differential equations

$$\mathbf{u}_t = D_2 \mathbf{u},$$

where

$$D_2 = \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & & 0 \\ 1 & -2 & 1 & \\ & & \ddots & \\ 0 & & 1 & -2 \end{pmatrix}, \qquad \mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{pmatrix}.$$

Next, we integrate with respect to time. By using the trapezoidal rule, we obtain

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = \frac{1}{2}\left(D_2 \mathbf{u}^{n+1} + D_2 \mathbf{u}^n\right),$$

which is equivalent to the Crank-Nicolson scheme (0.1). The trapezoidal method is second order accurate in time. But improved accuracy in time can be achieved with the use of a higher order method such as a Runge-Kutta or a linear multistep formula. These methods are generally referred to as the method of lines approach for the heat equation.

In terms of the spatial discretization, one can also increase the accuracy. One approach is by merely increasing the stencil width, i.e., by including more grid points in the difference formula. Complications may arise at the boundaries, which requires the implementation of boundary formulas. Another approach is using implicit differences, which are also referred to as compact difference formulas or "Mehrstellenverfahren" by Collatz [3]. With the compact difference formulas, we can increase the accuracy without increasing the stencil width, but the disadvantage is the introduction of implicit calculations for the derivative.

Chapter 1 provides relevant background information to this paper. We define notation of difference methods (Section 1.1). We also review features of the one-dimensional heat equation which pertain to our study (Section 1.2). The theory behind the eigenvalue analysis in regards to the heat equation is also discussed (Section 1.3).

Chapter 2 deals with standard finite difference approximations of the space derivative u_{xx} of high accuracy. There are various methods for deriving such formulas. In Section 2.1, we review the construction of these differences using Taylor series, the method of undetermined coefficients, and the Lagrange interpolation polynomial. Fornberg devised an efficient algorithm for generating these formulas, which we discuss in Section 2.2. Differentiation matrices are constructed (Section 2.3), which incorporate the boundary conditions alluded to above. A numerical experiment is conducted in order to contrast the accuracy of the Crank-Nicolson method with a high order finite difference scheme (Section 2.4). Section 2.5 is one of the main sections of this thesis. We analyze the stability of high order spatial discretizations by studying the behavior of the eigenvalues of the second derivative operators D_2. The behavior is summarized in a conjecture. Briefly stated, we conjecture that for stencil widths less than or equal to five, the eigenvalues are real and negative, but for larger stencil widths complex eigenvalues are introduced.

Chapter 3 presents another means for generating high order approximations to u_{xx}. More specifically, the compact difference approach referred to above is discussed. There does not appear to be an efficient way to calculate the weights for compact difference methods of high accuracy. We outline an approach that involves the method of undetermined coefficients. The results are summarized in the table in Section 3.2.

In summary, we highlight what we believe to be the original research of this thesis: (i) the eigenvalue analysis of high order discretizations of the second derivative operators D_2, and (ii) the computation of compact difference weights for formulas of high accuracy.

High Order Finite Difference Methods

Chapter 1

Introduction

1.1 Difference Methods

Differential equations model several natural phenomena, such as diffusion and convection. Ideally, we want exact solutions to these mathematical models. However, nonlinearities and equations with non-constant coefficients are obstacles that are not easily overcome. An alternative is constructing approximate solutions. This is where finite difference methods come into play.

1.1.1 Notation

Let $x_0, x_1, \ldots, x_{N+1}$ be equispaced grid points on an interval $[a, b]$ of the real line. Then $x_j = x_0 + j\Delta x$, where $\Delta x = (b-a)/(N+1)$. Let $u_j = u(x_j)$, for $j = 0, 1, 2, \ldots, N+1$, which are components of the column vector $\mathbf{u}$, i.e., $\mathbf{u} = [\ u_1,\ \ u_2,\ \ \ldots,\ \ u_N\ ]^T$. Let $\mathbf{u}^{(m)}$ denote the approximation of the mth derivative. In other words, $\mathbf{u}^{(m)} = [\ u_1^{(m)},\ \ u_2^{(m)},\ \ \ldots,\ \ u_N^{(m)}\ ]^T$. We will distinguish between $u^{(m)}(x_j)$, the exact value at x_j, and $u_j^{(m)}$, the approximate value at x_j. If D_m is a matrix which approximates the mth derivative, then

$$D_m \mathbf{u} = \mathbf{u}^{(m)}.$$

We refer to D_m as a differentiation matrix; examples will be given below. We will often assume the boundary conditions $u_0 = u_{N+1} = 0$.

1.1.2 Examples

We shall discretize the first derivative. A familiar example is the forward difference quotient

$$u_j' = \frac{u_{j+1} - u_j}{\Delta x}, \quad j = 1, 2, \ldots, N.$$

If the boundary condition $u_{N+1} = 0$ is assumed, then the corresponding differentiation matrix is represented by

$$D_1 = \frac{1}{\Delta x}\begin{pmatrix} -1 & 1 & & 0 \\ & -1 & 1 & \\ & & \ddots & \\ 0 & & & -1 \end{pmatrix}.$$

Thus, $D_1\mathbf{u} = \mathbf{u}'$.

Similarly, we can approximate the second derivative with

$$u_j'' = \frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2}, \quad j = 1, 2, \ldots, N. \tag{1.2}$$

If zero boundary conditions are assumed, the differentiation matrix is represented by

$$D_2 = \frac{1}{\Delta x^2}\begin{pmatrix} -2 & 1 & & 0 \\ 1 & -2 & 1 & \\ & & \ddots & \\ 0 & & 1 & -2 \end{pmatrix}, \tag{1.3}$$

where

$$D_2\mathbf{u} = \mathbf{u}''.$$

In this study, we shall focus our attention on discretizations of the second derivative, such as (1.3). One practical reason for this is that operators such as these often model diffusive properties in partial differential equations. The heat equation and reaction-diffusion equations, defined respectively by

$$\begin{aligned} u_t &= u_{xx} \\ u_t &= u_{xx} + u(1-u), \end{aligned} \tag{1.4}$$

are examples. In the next section, the heat equation will be discussed in more detail.

1.2 The One-Dimensional Heat Equation

Let the unknown function $u(x,t)$ be the temperature at a given point x at time t of a thin laterally insulated rod of length 1. Then the one-dimensional heat equation can be described by the partial differential equation

$$u_t = u_{xx}, \quad 0 < x < 1, \quad t > 0. \tag{1.5}$$

Assume we are given the initial data,

$$u(x,0) = f(x), \quad 0 < x < 1,$$

and boundary conditions

$$u(0,t) = u(1,t) = 0, \quad t > 0. \tag{1.6}$$

Using separation of variables, we will solve equation (1.5).

Assume $u(x,t)$ is separable, i.e., $u(x,t) = X(x)T(t)$. Then equation (1.5) implies that

$$X(x)T'(t) = X''(x)T(t)$$

and so

$$\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)} \tag{1.7}$$

for all $0 < x < 1$ and every $t > 0$. Equation (1.7) holds if and only if (1.7) is constant. Therefore, we have the following equations

$$\frac{T'(t)}{T(t)} = \lambda, \tag{1.8}$$

$$\frac{X''(x)}{X(x)} = \lambda, \tag{1.9}$$

where λ is a constant. The boundary conditions imply that $X(0) = X(1) = 0$. Equation (1.9) and the boundary conditions imply that the solution is of the form

$$X(x) = b_1 \cos(\sqrt{-\lambda}\, x) + b_2 \sin(\sqrt{-\lambda}\, x).$$

Using the boundary conditions, we find that the eigenvalues are

$$\lambda_k = -k^2\pi^2, \quad k = 1, 2, \ldots, \tag{1.10}$$

with corresponding eigenfunctions

$$X_k(x) = \sin(k\pi x), \quad k = 1, 2, \ldots. \tag{1.11}$$

Equation (1.8) becomes

$$\frac{T_k'(t)}{T_k(t)} = \lambda_k.$$

A solution of this equation is $T_k(t) = e^{\lambda_k t}$. Each $u_k(x,t) = e^{\lambda_k t}\sin(k\pi x)$ satisfies the boundary conditions and (1.5). By the principle of superposition and assuming sufficient smoothness of the solution

$$u(x,t) = \sum_{k=1}^{\infty} c_k e^{\lambda_k t}\sin(k\pi x). \tag{1.12}$$

The initial condition is satisfied if

$$f(x) = \sum_{k=1}^{\infty} c_k \sin(k\pi x), \quad \text{where} \quad c_k = 2\int_0^1 f(x)\sin(k\pi x)\,dx.$$

Formula (1.12) represents an explicit solution to the heat equation, but it is often not very practical for computational purposes. When high accuracy is required it is more advantageous to use a numerical method with a high order of accuracy rather than a series expression (1.12). Once nonlinearities are added, such as the reaction-diffusion equation in (1.4), general closed form expressions are unavailable and a numerical method is the only recourse.

We shall consider the *method of lines* for solving for u. Let $x_0, x_1, \ldots, x_{N+1}$ be equispaced grid points, where

$$x_j = x_0 + j\Delta x, \qquad u_j(t) = u(x_j,t), \quad j = 0,1,2,\ldots,N+1.$$

At this point we semi-discretize the heat equation, i.e., we discretize the space leaving the time as a continuous variable

$$\mathbf{u}_t = D_2\mathbf{u}, \tag{1.13}$$

where

$$\mathbf{u}(t) = \begin{pmatrix} u_1(t) \\ u_2(t) \\ \vdots \\ u_N(t) \end{pmatrix}, \qquad \mathbf{u}(0) = \begin{pmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_N) \end{pmatrix}, \qquad \mathbf{u}_t(t) = \begin{pmatrix} u_1'(t) \\ u_2'(t) \\ \vdots \\ u_N'(t) \end{pmatrix},$$

and D_2 is an $N \times N$ matrix which approximates the second derivative, such as the matrix (1.3). The standard approach for solving a linear system of ordinary differential equations, like (1.13), is integrating with respect to t using a Runge-Kutta or linear multistep formula, such as Euler's method or the Crank-Nicolson (trapezoidal) method, defined respectively by

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t D_2 \mathbf{u}^n \tag{1.14}$$

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \frac{1}{2}\Delta t(D_2\mathbf{u}^{n+1} + D_2\mathbf{u}^n). \tag{1.15}$$

Here $\mathbf{u}^n$ denotes the approximate solution at time level $n\Delta t$, where Δt is the step size. Other linear multistep formulas will be discussed in Section 1.3. However, sometimes one is primarily concerned with the characteristics displayed by the spatial discretization operator D_2. In these cases, we will choose to eliminate the errors associated with time integration by solving (1.13) analytically rather than numerically. This can be accomplished by

$$\mathbf{u}(t) = e^{D_2 \cdot t}\mathbf{u}(0).$$

Now we calculate $\mathbf{u}(t+\Delta t)$ in terms of $\mathbf{u}(t)$:

$$\begin{aligned}
\mathbf{u}(t+\Delta t) &= e^{D_2 \cdot (t+\Delta t)}\mathbf{u}(0) \\
&= e^{D_2 \cdot \Delta t}\left[e^{D_2 \cdot t}\mathbf{u}(0)\right] \\
&= e^{D_2 \cdot \Delta t}\mathbf{u}(t) \\
&= E\mathbf{u}(t),
\end{aligned} \tag{1.16}$$

where E is defined by $E = e^{D_2 \cdot \Delta t}$.

Applying formula (1.16), the solution at time intervals $\Delta t, 2\Delta t, 3\Delta t, \ldots$ can be computed. One drawback to this method is the cost of computing E. This requires the numerical diagonalization of D_2 (discussed further in Section 1.3), which can be very costly if N is large. We stress the fact that we will consider this method when we are solely interested in the effects of the spatial discretization.

1.3 Asymptotic Stability

Let D_2 be the matrix defined in (1.3). Assuming zero boundary conditions, it can be shown that the eigenvalues of $D_2\mathbf{u} = \lambda\mathbf{u}$ are (see [1])

$$\lambda_k = -4(N+1)^2 \sin^2\left(\frac{k\pi}{2(N+1)}\right), \quad k = 1, 2, \ldots, N, \tag{1.17}$$

with corresponding eigenvectors

$$\mathbf{v}_k = \begin{pmatrix} \sin(k\pi x_1) \\ \sin(k\pi x_2) \\ \vdots \\ \sin(k\pi x_N) \end{pmatrix}, \quad k = 1, 2, \ldots, N. \tag{1.18}$$

Observe that the eigenvalues of the discretized case (1.17) are similar to the eigenvalues of the continuous case (1.10) in that they are both real and negative and the corresponding eigenfunctions (1.18) and (1.11) evaluated at $x_1, x_2, \ldots, x_N$, respectively, are equivalent.

Let D_2 be any $N \times N$ matrix approximation of the second derivative. If D_2 is diagonalizable, then the matrix can be expressed as

$$D_2 = V\Lambda V^{-1}, \quad \text{where} \quad V = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N], \quad \Lambda = \begin{pmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_N \end{pmatrix},$$

where each λ_k corresponds to the eigenvector $\mathbf{v}_k$ and $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$ are linearly independent.

The exact solution of the semi-discretized heat equation (1.13) can be expressed as a unique linear combination of the eigenvectors, i.e., there exists scalars $c_j \in \mathbb{R}$ such that

$$\mathbf{u}(t) = c_1 e^{\lambda_1 t}\mathbf{v}_1 + c_2 e^{\lambda_2 t}\mathbf{v}_2 + \cdots + c_N e^{\lambda_N t}\mathbf{v}_N. \tag{1.19}$$

Notice the similarity between (1.19) and (1.12). Each solution can be viewed as an eigenfunction (or eigenvector) expansion, where each eigenfunction is multiplied by the exponential of the corresponding eigenvalue. The eigenvalues defined in (1.10) are real and negative, which means each term of the exact solution consists of purely decaying exponentials. Naturally, we desire the same behavior for the approximate solution (1.19). In particular, we want (1.19) to have real and negative eigenvalues. In general, this condition cannot be guaranteed. The focus of this paper is to investigate the qualitative properties of several differentiation matrices to determine which ones possess the desired properties and which ones do not.

A case in which we are guaranteed real and negative eigenvalues is if D_2 is negative symmetric definite.[1] For example, the matrix

$$D_2 = \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & & 0 \\ 1 & -2 & 1 & \\ & & \ddots & \\ 0 & & 1 & -2 \end{pmatrix}$$

is negative symmetric definite as may be seen from (1.17). For other differentiation matrices the eigenvalues may be complex, but lie in the left half-plane. This introduces temporal oscillations in the solution. When $\lambda_k \in \mathbb{C}$, then $\lambda_k = a_k + ib_k$, for some $a_k, b_k \in \mathbb{R}$, and so

$$e^{\lambda_k t} = e^{a_k t}[\cos(b_k t) + i\sin(b_k t)].$$

Worse yet, if D_2 possesses complex eigenvalues in the right half-plane, the solution contains growing modes, which means the numerical solution is not asymptotically stable.

Formulas such as Euler's method (1.14) and the Crank-Nicolson method (1.15) are called *linear multistep formulas.* The general representation of these formulas is

$$\mathbf{u}^{n+1} = \sum_{i=0}^{p} a_i \mathbf{u}^{n-i} + \Delta t \sum_{i=-1}^{p} b_i D_2 \mathbf{u}^{n-i}, \tag{1.20}$$

when applied to the heat equation, i.e., $\mathbf{u}_t = D_2\mathbf{u}$. We have

$$(1-b_{-1}\Delta t D_2)\mathbf{u}^{n+1} - (a_0+b_0\Delta t D_2)\mathbf{u}^n - (a_1+b_1\Delta t D_2)\mathbf{u}^{n-1} - \cdots - (a_p+b_p\Delta t D_2)\mathbf{u}^{n-p} = 0.$$

Now recall our assumption that D_2 is diagonalizable, i.e., $D_2 = V\Lambda V^{-1}$. It follows that

$$(1-b_{-1}\Delta t\lambda_j)w_j^{n+1} - (a_0+b_0\Delta t\lambda_j)w_j^n - (a_1+b_1\Delta t\lambda_j)w_j^{n-1} - \cdots - (a_p+b_p\Delta t\lambda_j)w_j^{n-p} = 0,$$

[1] A real symmetric matrix is negative definite if and only if all its eigenvalues are negative.

where $\mathbf{w}^n = V^{-1}\mathbf{u}^n$. We can solve this difference equation by letting $w_j^i = r^i$. Thus

$$(1 - b_{-1}\Delta t\lambda_j)r^p - (a_0 + b_0\Delta t\lambda_j)r^{p-1} - (a_1 + b_1\Delta t\lambda_j)r^{p-2} - \cdots - (a_p + b_p\Delta t\lambda_j) = 0.$$

There are $p+1$ roots, say $r_0(\Delta t\lambda_j)$, $r_1(\Delta t\lambda_j)$, ..., $r_p(\Delta t\lambda_j)$. Thus the general solution is

$$w_j^n = \alpha_0[r_0(\Delta t\lambda_j)]^n + \alpha_1[r_1(\Delta t\lambda_j)]^n + \cdots + \alpha_p[r_p(\Delta t\lambda_j)]^n,$$

by the principle of superposition. If $r_i(\Delta t\lambda_j)$ is a root of multiplicity greater than one, then α_i may be a polynomial in n. We can guarantee asymptotic stability [2] if and only if for all $|r_i(\Delta t\lambda_j)| \leq 1$, for $i = 0, 1, \ldots, p$. The stability region is defined by

$$\{\Delta t\lambda_j \in \mathbb{C} \ : \ |r_i(\Delta t\lambda_j)| \leq 1, \quad n = 0, 1, \ldots, p\}. \tag{1.21}$$

Example

We will determine the stability region for Euler's method. By equation (1.20), we have

$$\mathbf{u}^{n+1} = (1 + \Delta t D_2)\mathbf{u}^n.$$

Since we are assuming that D_2 is diagonalizable, $D_2 = V\Lambda V^{-1}$. Thus,

$$w_j^{n+1} = (1 + \Delta t\lambda_j)w_j^n,$$

where $\mathbf{w}^n = V^{-1}\mathbf{u}^n$. Let $w_j^i = r^i$. Then

$$r^{n+1} = (1 + \Delta t\lambda_j)r^n$$

and so $r_0(\Delta t\lambda_j) = 1 + \Delta t\lambda_j$. In order to satisfy (1.21), we must have

$$|1 + \Delta t\lambda_j| \leq 1,$$

which can be represented by the region shown in Figure 1.3. The graph shows the complex z-plane, where $z = \Delta t\lambda_j$.

[2] We call a numerical solution to $\mathbf{u}_t = D_2\mathbf{u}$ asymptotically stable if the solution u_j^n remains bounded for a fixed step size Δt as $n \to \infty$.

Recall that the eigenvalues (1.17) of the approximation matrix (1.3) are all real and negative. To guarantee that these eigenvalues lie within the stability region, we must have $\Delta t|\lambda_j| \leq 2$, for all j. By equation (1.17) this inequality holds if

$$\Delta t \leq \frac{\Delta x^2}{2},$$

which is the well-known stability restriction for solving the heat equation using Euler's method and centered differences for the spatial discretization.

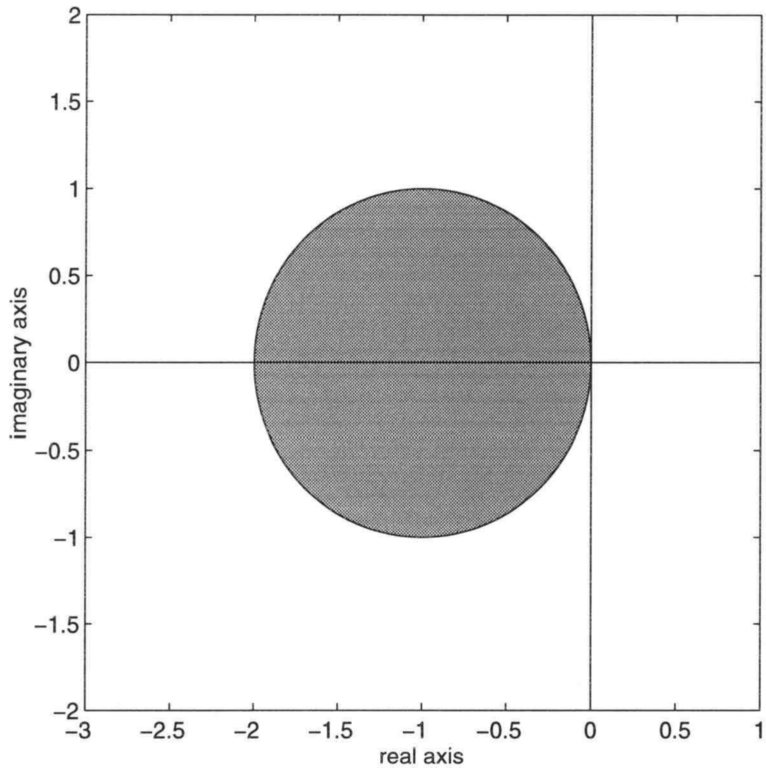

Figure 1: Stability region of Euler's method

Chapter 2

Finite Difference Methods

Recall the formula for the approximation of the second derivative discussed in Section 1.1

$$u_j'' = \frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2}, \quad j = 1, 2, \ldots, N, \tag{2.22}$$

which has stencil width[3] $W = 3$ and order of accuracy two. Also recall that

$$D_2 = \frac{1}{\Delta x^2}\begin{pmatrix} -2 & 1 & & 0 \\ 1 & -2 & 1 & \\ & & \ddots & \\ 0 & & 1 & -2 \end{pmatrix}, \tag{2.23}$$

and

$$D_2\mathbf{u} = \mathbf{u}''.$$

The eigenvalues of D_2 are given by (1.17). In this chapter we construct finite difference formulas of higher accuracy for the second derivative, and we examine numerically the eigenvalues of the corresponding differentiation matrices.

2.1 Methods for Deriving Finite Difference Formulas

There are various methods used to derive finite differences. As an illustration, we shall derive equation (2.22) using three of these methods. For simplicity, let $j = 0$.

2.1.1 Taylor Series

We can rewrite u_{-1} and u_1 as a Taylor series expansion. Since $x_{\pm 1} = x_0 \pm \Delta x$, then assuming that $u(x)$ has four continuous derivatives gives

$$u(x_{-1}) = u(x_0 - \Delta x) = u(x_0) - \Delta x u'(x_0) + \frac{1}{2}\Delta x^2 u''(x_0) - \frac{1}{6}\Delta x^3 u'''(x_0) + O(\Delta x^4),$$
$$u(x_1) = u(x_0 + \Delta x) = u(x_0) + \Delta x u'(x_0) + \frac{1}{2}\Delta x^2 u''(x_0) + \frac{1}{6}\Delta x^3 u'''(x_0) + O(\Delta x^4).$$

[3]The number of grid points used in the difference formula is referred to as the stencil width.

Notice that

$$u(x_{-1}) + u(x_1) = 2u(x_0) + \Delta x^2 u''(x_0) + O(\Delta x^4),$$

or

$$u''(x_0) = \frac{u(x_1) - 2u(x_0) + u(x_1)}{\Delta x^2} + O(\Delta x^2).$$

Thus,

$$u_0'' = \frac{u_{-1} - 2u_0 + u_1}{\Delta x^2} \tag{2.24}$$

is a second order approximation to $u''(x_0)$.

2.1.2 Method of Undetermined Coefficients

We propose a difference formula of the form

$$u_0'' = a_{-1}u_{-1} + a_0 u_0 + a_1 u_1, \tag{2.25}$$

where the coefficients are to be determined. We want to maximize the accuracy, so the approximation must be exact for polynomials of degree less than or equal to two. When formula (2.25) is applied to $u = 1$, $u = x$, and $u = x^2$, the three equations

$$\begin{aligned} 0 &= a_{-1} + a_0 + a_1 \\ 0 &= -a_{-1} + a_1 \\ 2 &= \Delta x^2 (a_{-1} + a_1) \end{aligned}$$

are obtained. Solving this system gives $a_{-1} = \frac{1}{\Delta x^2}$, $a_0 = -\frac{2}{\Delta x^2}$, $a_1 = \frac{1}{\Delta x^2}$, and thus (2.24) is recovered.

2.1.3 Interpolation Polynomial

Finally, we look at a method involving an interpolation polynomial. Let $p(x)$ be the polynomial of degree two that interpolates the points (x_{-1}, u_{-1}), (x_0, u_0), and (x_1, u_1). Also, let

$$p(x) = \sum_{j=-1}^{1} L_j(x) u_j,$$

where the $L_j(x)$ are the usual Lagrange interpolation polynomials of degree two defined by

$$\begin{aligned} L_{-1}(x) &= \frac{(x-x_0)(x-x_1)}{(x_{-1}-x_0)(x_{-1}-x_1)}, \\ L_0(x) &= \frac{(x-x_{-1})(x-x_1)}{(x_0-x_{-1})(x_0-x_1)}, \\ L_1(x) &= \frac{(x-x_{-1})(x-x_0)}{(x_1-x_{-1})(x_1-x_0)}. \end{aligned}$$

By differentiating the interpolation polynomial twice and evaluating the result at $x = x_0$ one gets

$$u''(x_0) \approx p''(x_0) = \sum_{j=-1}^{1} L_j''(x_0)u_j.$$

Because of the equidistant points, it follows that

$$L_{-1}(x) = \frac{1}{2\Delta x^2}(x - x_{-1})(x - x_0),$$

and so

$$L_{-1}''(x_0) = \frac{1}{\Delta x^2}.$$

Similarly, we observe that $L_0''(x_0) = -\frac{2}{\Delta x^2}$ and $L_1''(x_0) = \frac{1}{\Delta x^2}$. Once again, we arrive at (2.24).

In order to obtain a formula of higher accuracy, additional grid points must be included. For example, for $W = 5$ it can be shown that

$$u_j'' = \frac{-u_{j-2} + 16u_{j-1} - 30u_j + 16u_{j+1} - u_{j+2}}{12\Delta x^2}, \quad j = 2, 3, \ldots, N-1, \tag{2.26}$$

has order of accuracy four.

Generating difference formulas of higher accuracy involves formulas with larger stencil widths. With the introduction of more grid points, the derivation of difference formulas increases in complexity. Each of the methods discussed here can be used to find these high accuracy formulas. However, the method involving the interpolation polynomial appears to be the most efficient, especially for arbitrarily spaced points.

2.2 Fornberg's Algorithm

In the previous section, we used Lagrange's interpolation polynomial to determine the weights of the finite difference formula for $W = 3$. Fornberg [4] generalizes this idea to find the mth derivative weights recursively. He considered using arbitrary grid points, but we will restrict ourselves to the use of equispaced points.

Let $p(x)$ be Lagrange's interpolation polynomial and $M \geq 0$ be the highest order of the derivative we wish to approximate. Let $x_0, x_1, ..., x_N$ be $N+1$ distinct grid points, where $N \geq 0$ and $N \geq M$. (Note: In Fornberg's algorithm, he uses the points $x_0, x_1, ..., x_N$, rather than $x_0, x_1, .., x_{N+1}$.) Also let ξ be the point $x = \xi$, where the derivative is to be approximated. Then

$$p(x) = \sum_{i=0}^{j} L_{i,j}(x) u_i, \quad j = 0, 1, \ldots, N, \tag{2.27}$$

where the Lagrangian interpolation polynomials are given by

$$L_{i,j}(x) = \frac{(x - x_0) \cdots (x - x_{i-1})(x - x_{i+1}) \cdots (x - x_j)}{(x_i - x_0) \cdots (x_i - x_{i-1})(x_i - x_{i+1}) \cdots (x_i - x_j)}. \tag{2.28}$$

For simplicity, assume $\xi = 0$. Applying the mth derivative to (2.27) and evaluating it at $\xi = 0$, we have

$$\begin{aligned} \left.\frac{d^m p(x)}{dx^m}\right|_{x=0} &\approx \sum_{i=0}^{j} \left.\frac{d^m L_{i,j}(x)}{dx^m}\right|_{x=0} u_i, \\ &= \sum_{i=0}^{j} l_{i,j}^m u_i, \quad m = 0, 1, \ldots, M; \quad j = m, m+1, \ldots, N, \end{aligned}$$

where $l_{i,j}^m$ is defined by

$$l_{i,j}^m = \left[\frac{d^m L_{i,j}(x)}{dx^m}\right]_{x=0}.$$

By Taylor's formula, we know that

$$L_{i,j}(x) = \sum_{m=0}^{j} \frac{l_{i,j}^m}{m!} x^m.$$

The recursion relations

$$L_{i,j}(x) = \frac{(x - x_j)}{(x_i - x_j)} L_{i,j-1}(x),$$

$$L_{j,j}(x) = \frac{\prod_{k=0}^{j-2}(x_{j-1} - x_k)}{\prod_{k=0}^{j-1}(x_j - x_k)} (x - x_{j-1}) L_{j-1,j-1}(x)$$

follow from (2.28). The weights are obtained by substituting the Taylor series of $L_{i,j}(x)$ in the recursion relations above and then equating coefficients. This yields

$$\begin{aligned} l_{i,j}^m &= \frac{1}{x_j - x_i}(x_j l_{i,j-1}^m - m l_{i,j-1}^{m-1}) \\ l_{j,j}^m &= \frac{(x_{j-1} - x_0)(x_{j-1} - x_1) \cdots (x_{j-1} - x_{j-2})}{(x_j - x_0)(x_j - x_1) \cdots (x_j - x_{j-1})} (m l_{j-1,j-1}^{m-1} - x_{j-1} l_{j-1,j-1}^m). \end{aligned}$$

These approximations have an optimal order of accuracy.[4] The following algorithm computes the $l_{i,j}^{m}$'s, i.e., the weights for the mth derivative finite difference formula.

Given $M, N, \xi, x_0, x_1, x_2, \ldots, x_N$

$l_{0,0}^{0} := 1$

$c1 := 1$

for $j := 1$ to N do

  $c2 := 1$

  for $i := 0$ to $j-1$ do

    $c3 := x_j - x_i$

    $c2 := c2 \cdot c3$

    if $j \leq M$ then $l_{i,j-1}^{j} := 0$

    for $m := 0$ to $\min(j, M)$ do

      $l_{i,j}^{m} := ((x_j - \xi) l_{i,j-1}^{m} - m l_{i,j-1}^{m-1})/c3$

      next m

    next i

  for $m := 0$ to $\min(j, M)$ do

    $l_{j,j}^{m} := \frac{c1}{c2}(m l_{j-1,j-1}^{m-1} - (x_{j-1} - \xi) l_{j-1,j-1}^{m})$

    next m

  $c1 := c2$

  next j

2.3 Implementation

For $W = 3$, we have a symmetric Toeplitz[5] matrix (see (2.22)). However, for $W \geq 5$, we encounter a problem at the boundaries. We overcome this obstacle by using one-sided differences (of the same order of accuracy) at the boundaries. Because we desire the same order of accuracy, we use a stencil width of $W+1$. Both one-sided

[4]The maximum order of accuracy for a given stencil width W.

[5]A Toeplitz matrix has constant entries along the diagonals.

and centered differences are calculated with Fornberg's algorithm. Suppose there are k points, which lie outside the domain. Then we must have one-sided difference formulas for $u_1'', u_2'', \ldots, u_k''$, where each u_i'' includes the points $u_0, u_1, \ldots, u_W$, for the left boundary. Likewise, we must have one-sided difference formulas for $u_{N-k+1}'', u_{N-k+2}'', \ldots, u_N''$, where each u_j'' includes the points $u_{N-W+1}, u_{N-W+2}, \ldots, u_{N+1}$, for the right boundary. Our differentiation matrix D_2 is no longer symmetric. Therefore, we are no longer guaranteed that D_2 has real eigenvalues and that all eigenvalues are in the left half-plane.

Example

Consider the case $W = 5$. If $j = 1$ in equation (2.26), then our formula contains u_{-1}, which lies outside the domain. We resolve the problem as described above, by using one-sided differences. In order to maintain an order of accuracy of four, the stencil for the one-sided difference is of width $W = 6$. Using Fornberg's algorithm, we find that

$$u_1'' = \frac{10u_0 - 15u_1 - 4u_2 + 14u_3 - 6u_4 + u_5}{12\Delta x^2}.$$

Similarly, the one-sided difference for u_N is

$$u_N'' = \frac{u_{N-4} - 6u_{N-3} + 14u_{N-2} - 4u_{N-1} - 15u_N + 10u_{N+1}}{12\Delta x^2},$$

and so,

$$D_2 = \frac{1}{12\Delta x^2}\begin{pmatrix} -15 & -4 & 14 & -6 & 1 & & 0 \\ 16 & -30 & 16 & -1 & & & \\ -1 & 16 & -30 & 16 & -1 & & \\ & & & \ddots & & & \\ & & & & \ddots & & \\ & & & -1 & 16 & -30 & 16 \\ 0 & & 1 & -6 & 14 & -4 & -15 \end{pmatrix}. \tag{2.29}$$

2.4 Numerical Experiment

In this section, we solve the heat equation with the Crank-Nicolson method and a high order finite difference scheme. First, observe that one can easily verify that

$$u(x,t) = e^{-\pi^2 t}\sin(\pi x)$$

is a solution of the heat equation (1.5), which satisfies the boundary conditions (1.6) and initial data

$$u(x,0) = \sin(\pi x). \tag{2.30}$$

An equivalent form of the second order accurate Crank-Nicolson scheme (1.15) is

$$\left(I - \frac{1}{2}\Delta t D_2\right)\mathbf{u}^{n+1} = \left(I + \frac{1}{2}\Delta t D_2\right)\mathbf{u}^n, \tag{2.31}$$

where I is the identity matrix and D_2 is the second derivative operator given by (2.23). Next, consider the following high order finite difference scheme. For the space derivative we shall use the differentiation matrix D_2 (2.29) presented in the previous section for $W = 5$. For the time integration we shall use the third order backward differentiation formula

$$\mathbf{u}^{n+1} = \frac{18}{11}\mathbf{u}^n - \frac{9}{11}\mathbf{u}^{n-1} + \frac{2}{11}\mathbf{u}^{n-2} + \frac{6}{11}\Delta t D_2 \mathbf{u}^{n+1}$$

or equivalently

$$\left(I - \frac{6}{11}\Delta t D_2\right)\mathbf{u}^{n+1} = \frac{18}{11}\mathbf{u}^n - \frac{9}{11}\mathbf{u}^{n-1} + \frac{2}{11}\mathbf{u}^{n-2}.$$

The starting values will be calculated with the Crank-Nicolson method (2.31). The magnitude of the maximum error at the grid points is computed. We plot the logarithm of the error as a function of the logarithm of the step size Δx (Figure 2.4). We refine the grid to $\Delta x = \frac{1}{2}\Delta t$. The slope of these lines represent the order of accuracy. The graph clearly demonstrates the superiority of the high order method.

2.5 Eigenvalues of Second Derivative Matrices

The eigenvalues of the differentiation matrices of various stencil widths ($W = 3$ to $W = 101$) and various matrix sizes ($N = 5$ to $N = 800$) were investigated numerically. Let us consider matrices of size $N \times N$, where $N = 50$. After constructing D_2, as described in the preceding section, the eigenvalues were calculated using Matlab's `eig`

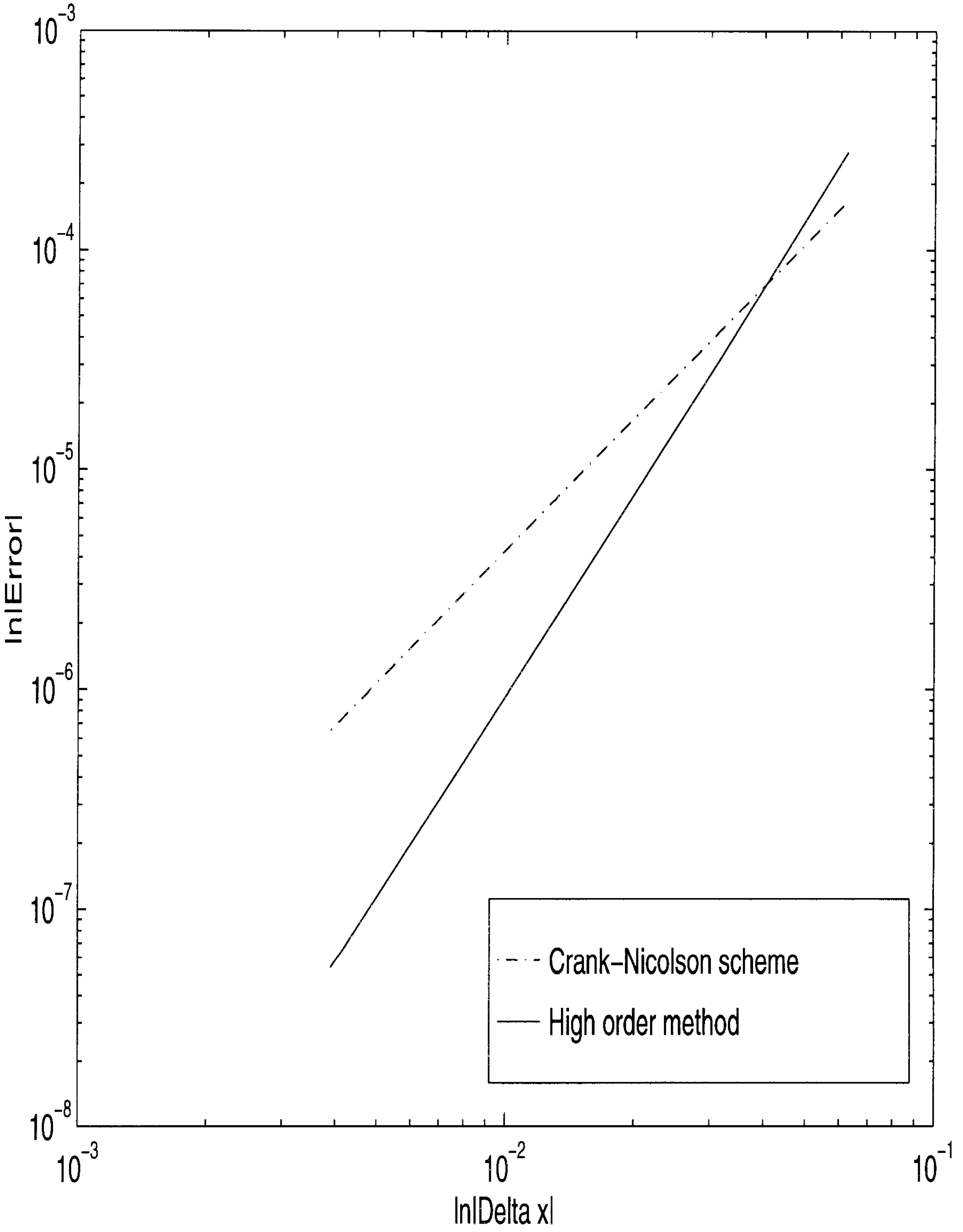

Figure 2: Logarithm of the error of the Crank-Nicolson scheme and a high order method as a function of the step size Δx, where $\Delta x = \frac{1}{2}\Delta t$

function, for $W = 5, 11, 17, \ldots, 47$ (Figure 2.5(a)–(h)). These computations lead us to the following conjecture.

Conjecture *Let W be the stencil width and let the size of the differentiation matrix be $N \times N$, where $N \geq W$. Then, if*

1. *$W \leq 5$, all of the eigenvalues are real and negative*
2. *$7 \leq W \leq 33$, at least two of the eigenvalues are complex, but all eigenvalues are in the left half-plane, with the exception that if $W = N = 33$, two of the complex eigenvalues lie in the right half-plane*
3. *$W \geq 35$, at least two of the complex eigenvalues lie in the right half-plane.*

Observe that if $W = N$, then the finite difference method is precisely the spectral method for equidistant points and the eigenvalues are the same as those seen in Weideman and Trefethen's paper [10], Figure 3, when $W = N = 50$.

For the centered difference approximations with a stencil width W for the second derivative, the order of accuracy is $W-1$. We achieve a higher order of accuracy with a larger stencil width. However, for $W \geq 7$, there are at least two complex eigenvalues, which introduces temporal oscillations in the solution. In order to illustrate these oscillations, we will consider the following example.

Example

Once again, we assume the initial condition (2.30). We shall use the sixth order backward differentiation formula

$$\mathbf{u}^{n+1} = \frac{120}{49}\mathbf{u}^{n} - \frac{150}{49}\mathbf{u}^{n-1} + \frac{400}{147}\mathbf{u}^{n-2} - \frac{75}{49}\mathbf{u}^{n-3} + \frac{24}{49}\mathbf{u}^{n-4} - \frac{10}{147}\mathbf{u}^{n-5} + \frac{60}{147}\Delta t D_2\mathbf{u}^{n+1}$$

or equivalently

$$(I - \frac{60}{147}\Delta t D_2)\mathbf{u}^{n+1} = \frac{120}{49}\mathbf{u}^{n} - \frac{150}{49}\mathbf{u}^{n-1} + \frac{400}{147}\mathbf{u}^{n-2} - \frac{75}{49}\mathbf{u}^{n-3} + \frac{24}{49}\mathbf{u}^{n-4} - \frac{10}{147}\mathbf{u}^{n-5}.$$

Since we desire to illustrate the effects of the complex eigenvalues, rather than obtaining the actual solution, we will use the exact solution for the starting values.

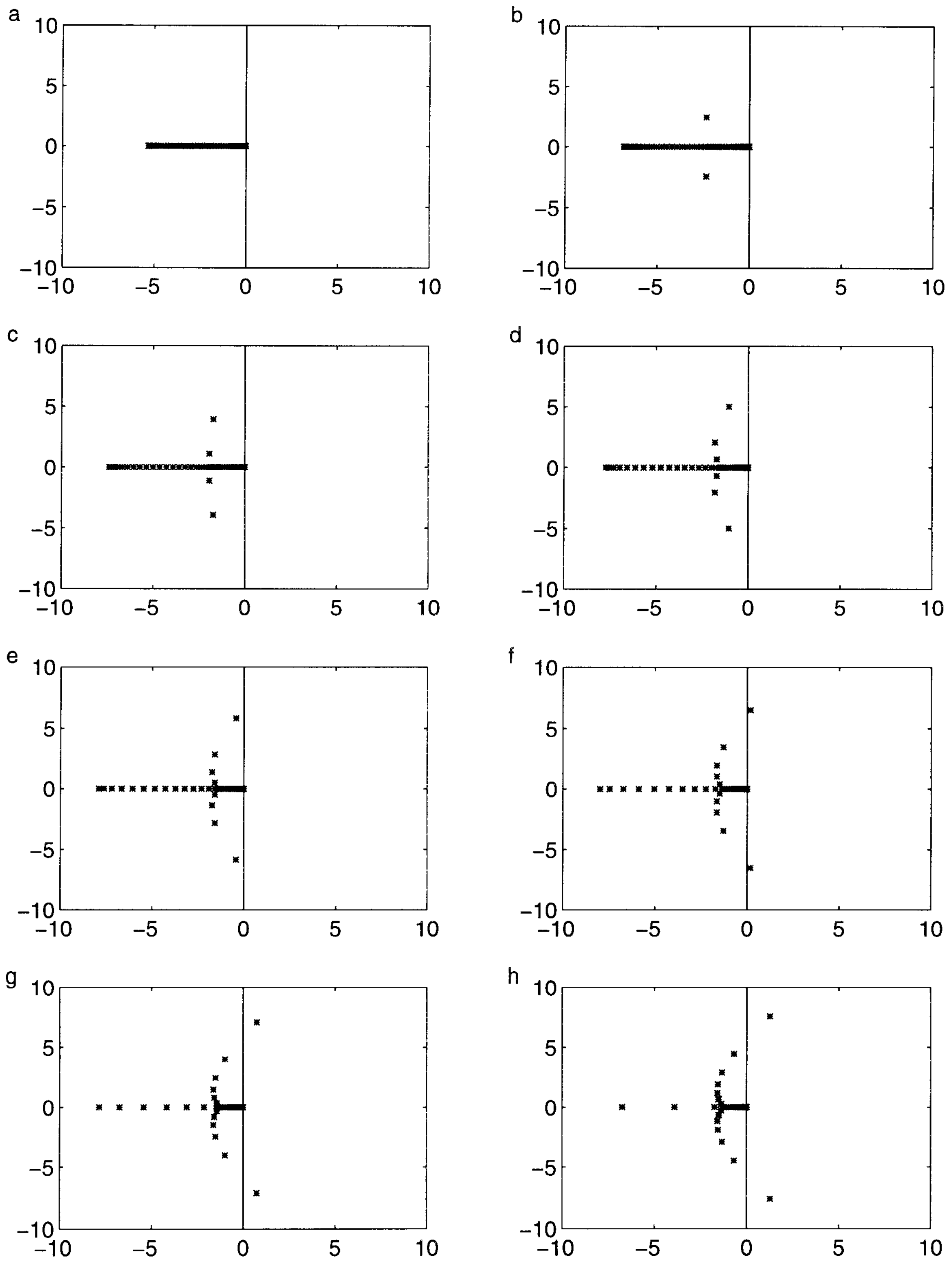

Figure 3: Eigenvalues of 50×50 finite differentiation matrices with stencil widths (a) 5, (b) 11, (c) 17, (d) 23, (e) 29, (f) 35, (g) 41, (h) 47. NOTE: The eigenvalues are scaled by $(N+1)^2 = 2601$.

The eigenvalues of D_2 scaled by Δt and the corresponding solution are graphed in Figures 2.5 and 2.5 along with the stability region (shaded) for the six-step backward difference formula. As discussed in Section 1.3, when all the eigenvalues lie within the stability region, the solution decays. However, if any of the eigenvalues lie outside our region of stability, then growing oscillations are introduced into the solution.

First, let $N = 20$ and $\Delta t = .005$. Next, we vary the stencil width. When $W = 7$ and $W = 9$, all the scaled eigenvalues lie within the stability region and the solution decays as desired (Figure 2.5). However, if $W = 11$, two of the eigenvalues lie outside the region of stability (Figure 2.5a). As predicted, the solution oscillates (Figure 2.5b). Now, let $\Delta t = .01$. This increase in the time step size results in a decaying solution (Figure 2.5d) along with eigenvalues that lie in the stability region (Figure 2.5c).

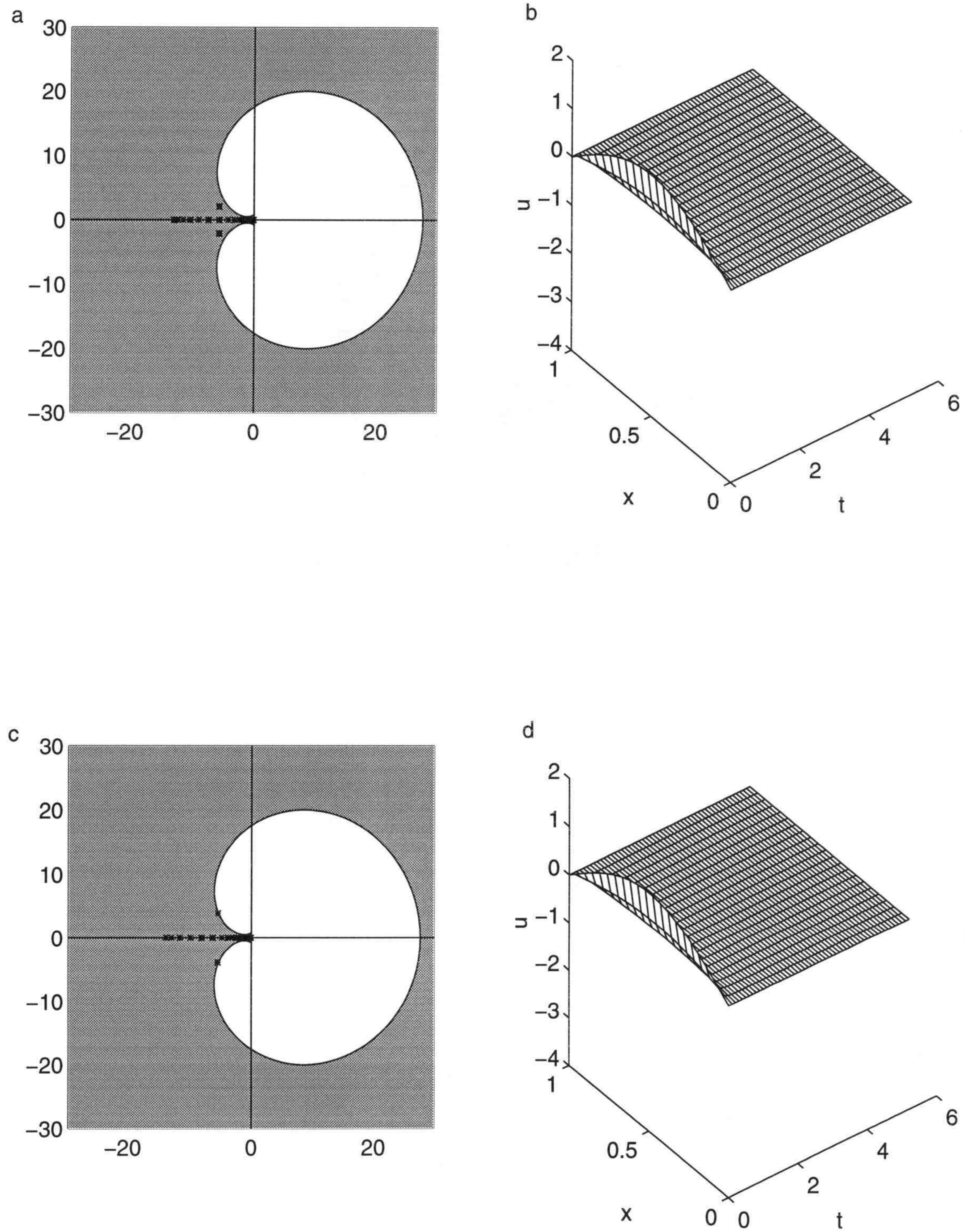

Figure 4: Scaled eigenvalues and solutions of the six-step backward differentiation formula with $N = 20$ and $\Delta t = .005$. (a) Eigenvalues, $W = 7$ (b) Solution $u(x,t)$ versus x and t, $W = 7$ (c) Eigenvalues, $W = 9$ (d) Solution $u(x,t)$ versus x and t, $W = 9$.

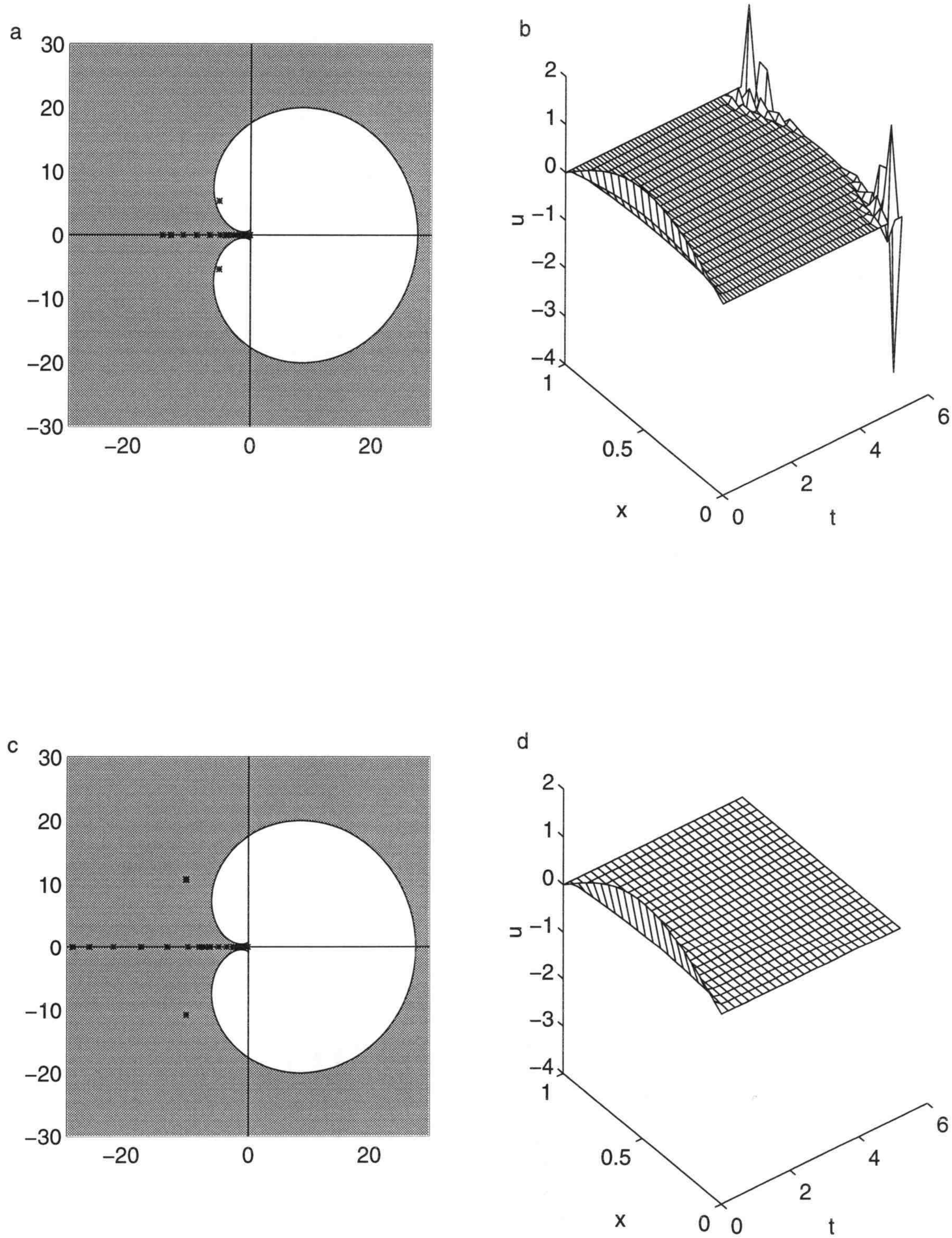

Figure 5: Scaled eigenvalues and solutions of the six-step backward differentiation formula with $N = 20$ and $W = 11$. (a) Eigenvalues, $\Delta t = .005$ (b) Solution $u(x,t)$ versus x and t, $\Delta t = .005$ (c) Eigenvalues, $\Delta t = .01$ (d) Solution $u(x,t)$ versus x and t, $\Delta t = .01$.

Chapter 3

Compact Difference Methods

3.1 Example

Another method for approximating derivatives is the *compact difference method.* A familiar example of this implicit method is

$$\frac{u''_{j-1} + 10u''_j + u''_{j+1}}{12} = \frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2}, \quad j = 1, 2, \ldots, N.$$

Assume that $u_0 = u_{N+1} = 0$ and $u''_0 = u''_{N+1} = 0$. Recall for the heat equation, we assumed that $u(0,t) = u(1,t) = 0$ and so $u_{xx}(0,t) = u_{xx}(1,t) = 0$. Thus, $u''_0 = u''_{N+1} = 0$ is a valid assumption in reference to the heat equation.

Now let

$$B = \frac{1}{12}\begin{pmatrix} 10 & 1 & & 0 \\ 1 & 10 & 1 & \\ & & \ddots & \\ 0 & & 1 & 10 \end{pmatrix}, \quad A = \frac{1}{\Delta x^2}\begin{pmatrix} -2 & 1 & & 0 \\ 1 & -2 & 1 & \\ & & \ddots & \\ 0 & & 1 & -2 \end{pmatrix}.$$

Then

$$B\mathbf{u}'' = A\mathbf{u},$$

which implies that

$$\begin{aligned} \mathbf{u}'' &= B^{-1}A\mathbf{u} \\ &= D_2\mathbf{u}, \end{aligned}$$

where $D_2 = B^{-1}A$. Note that diagonal dominance ensures that B is non-singular.

By using the compact difference method, we have preserved a stencil width of three and yet at the same time increased the order of accuracy to four. By solving

$$D_2\mathbf{u} = \lambda\mathbf{u}, \tag{3.32}$$

we can find the eigenvalues of D_2 explicitly. Let $M = N + 1$. Then from (3.32), we find that

$$12M^2(u_{j-1} - 2u_j + u_{j+1}) = \lambda(u_{j-1} + 10u_j + u_{j+1})$$

and so

$$(12M^2 - \lambda)u_{j-1} - (24M^2 + 10\lambda)u_j + (12M^2 - \lambda)u_{j+1} = 0.$$

Let

$$2A = \frac{24M^2 + 10\lambda}{12M^2 - \lambda}. \tag{3.33}$$

Then

$$u_{j-1} - 2Au_j + u_{j+1} = 0.$$

Now let $u_i = r^i$. Thus, we have

$$r^{j-1} - 2Ar^j + r^{j+1} = 0$$

and so

$$r^2 - 2Ar + 1 = 0. \tag{3.34}$$

The two roots of equation (3.34), which we shall call r_+ and r_-, satisfy $r_+r_- = 1$. The general solution is of the form

$$u_j = \alpha r_+^j + \beta r_-^j = \alpha r_+^j + \beta r_+^{-j}.$$

Using the boundary conditions, we find that

$$\begin{aligned} u_0 &= \alpha + \beta = 0 \\ u_M &= \alpha r_+^M + \beta r_+^{-M} = 0. \end{aligned}$$

From the above equations, we have $r_+^{2M} = 1$ and so the $2M$th roots of unity are

$$r_+ = e^{\frac{k\pi i}{M}}, \quad k = 1, 2, \ldots, M.$$

Now the solution is of the form

$$u_j = \alpha\left(e^{\frac{k\pi ij}{M}} - e^{-\frac{k\pi ij}{M}}\right) = \tilde{\alpha}\sin\left(\frac{k\pi j}{M}\right) = \tilde{\alpha}\sin\left(k\pi x_j\right).$$

From equation (3.34), we know that

$$A = \frac{1}{2}(r_+ + r_+^{-1}) = \cos\left(\frac{\pi k}{M}\right)$$

and so we find that

$$\cos\left(\frac{k\pi}{M}\right) = \frac{24M^2 + 10\lambda_k}{24M^2 - 2\lambda_k},$$

by using (3.33). Solving for λ_k and using trigonometric identities yields

$$\lambda_k = \frac{-12M^2(1 - \cos\left(\frac{k\pi}{M}\right))}{5 + \cos\left(\frac{k\pi}{M}\right)} = \frac{3}{3 - \sin^2\left(\frac{k\pi}{2M}\right)}\eta_k$$

where $\eta_k = \left[-4M^2\sin^2\left(\frac{k\pi}{2M}\right)\right]$. Notice that η_k's are the eigenvalues of the finite difference formula for $W = 3$ (see (1.17)). The corresponding eigenfunctions are equivalent to that of the continuous problem (1.11) evaluated at $x_1, x_2, \ldots, x_N$ and to that of the finite difference (1.18).

Now let us verify algebraically that the eigenvalues of the finite and compact difference methods are of order $O\left(\frac{1}{M^2}\right)$ and $O\left(\frac{1}{M^4}\right)$, respectively, for $W = 3$. Using the Taylor series of $\sin(x)$, we find that

$$\begin{aligned} \sin^2(x) &= \left(x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5 - \frac{1}{7!}x^7 + O(x^7)\right)^2 \\ &= x^2 - \frac{1}{3}x^4 + \frac{2}{45}x^6 + O(x^8). \end{aligned}$$

Recall from Section 1.2 that the eigenvalues of the continuous problem are

$$\lambda_k = -k^2\pi^2, \quad k = 1, 2, \ldots.$$

3.1.1 <u>Finite Difference Method</u>

$$\begin{aligned} \lambda_k &= -4M^2\sin^2\left(\frac{k\pi}{2M}\right) \\ &= -k^2\pi^2 + O\left(\frac{1}{M^2}\right), \quad \text{for any fixed } k, \text{ as } M \to \infty \end{aligned}$$

3.1.2 Compact Difference Method

Note that

$$\begin{aligned}
\frac{3}{3-\sin^2\left(\frac{k\pi}{2M}\right)} &= \frac{1}{1-\frac{1}{3}\sin^2\left(\frac{k\pi}{2M}\right)} = 1+\frac{1}{3}\sin^2\left(\frac{k\pi}{2M}\right)+\frac{1}{9}\sin^4\left(\frac{k\pi}{2M}\right)+O\left(\frac{1}{M^6}\right) \\
&= 1+\frac{k^2\pi^2}{12M^2}+O\left(\frac{1}{M^4}\right). \qquad (3.35)
\end{aligned}$$

Using (3.35), we have

$$\begin{aligned}
\lambda_k &= \frac{3}{3-\sin^2\left(\frac{k\pi}{2M}\right)}\left[-4M^2\sin^2\left(\frac{k\pi}{2M}\right)\right] \\
&= \left(1+\frac{k^2\pi^2}{12M^2}+O(\frac{1}{M^4})\right)\left[-k^2\pi^2+\frac{k^4\pi^4}{12M^2}-\frac{k^6\pi^6}{360M^4}+O\left(\frac{1}{M^6}\right)\right] \\
&= -k^2\pi^2+O\left(\frac{1}{M^4}\right), \quad \text{for any fixed } k, \text{ as } M\to\infty.
\end{aligned}$$

Figure 3.1 illustrates the improved accuracy achieved by using the compact difference method rather than the finite difference method.

Demanding a higher order of accuracy requires an increased number of grid points in the compact difference formula. Unlike the standard finite difference method, there does not appear to be an "efficient" way to generate weights for a compact difference formula with an optimal order of accuracy. However, we can determine the weights using the method of undetermined coefficients, which will be discussed in the next section.

3.2 Constructing Compact Difference Formulas

The construction of compact difference formulas has been discussed in various studies [3], [5], and [7], but there does not appear to be any general theory for computing compact difference formulas of high order. However, we will sketch an approach using the method of undetermined coefficients.

We propose an equation of the form

$$0=\sum_{i=-n}^{n}a_iu_i+\Delta x^2\sum_{i=-n}^{n}b_iu_i'', \qquad (3.36)$$

where the coefficients are to be determined. Note that one coefficient is undetermined. We can normalize the scheme by setting $b_n=1$. In order to maximize the order of

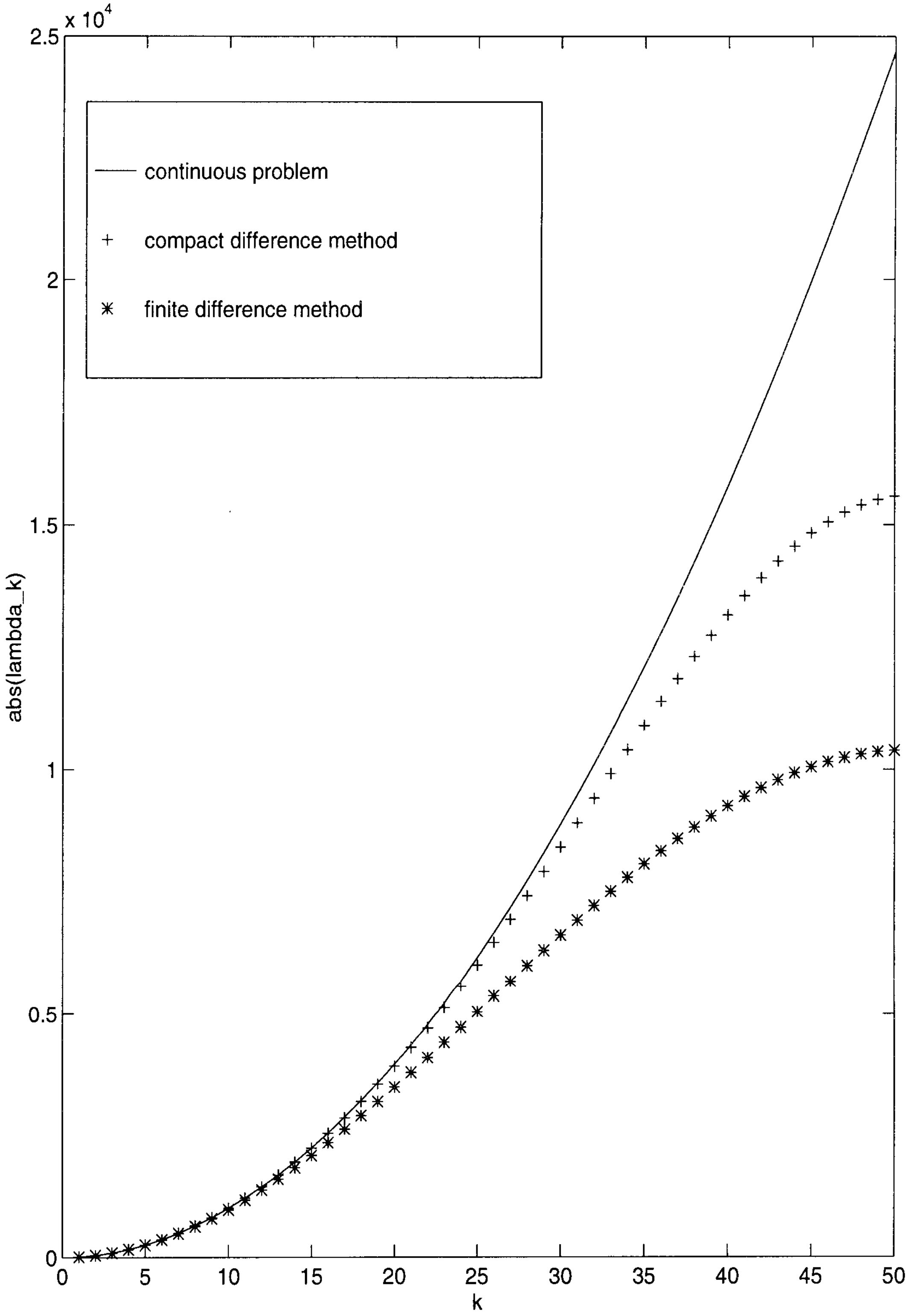

Figure 6: Eigenvalues of the continuous problem compared with the finite difference method and the compact difference method of stencil width $W = 3$

accuracy, the approximation must be exact for polynomials of degree less than or equal to $4n$. To find the remaining $4n+1$ unknowns, we apply formula (3.36) to $u=1$, $u=x$, $u=x^2$, $u=x^3$, ..., $u=x^{4n}$. We will solve this system of $4n+1$ equations using Matlab's symbolic environment. This method is illustrated with the following example.

Example

Let $n=1$. Then we have the equation

$$0 = a_{-1}u_{-1} + a_0u_0 + a_1u_1 + \Delta x^2(b_{-1}u''_{-1} + b_0u''_0 + b_1u''_1).$$

Since one coefficient is undetermined, let $b_1 = 1$. We apply the above formula to $u=1$, $u=x$, $u=x^2$, $u=x^3$, and $u=x^4$. The five equations

$$\begin{aligned}
0 &= a_{-1} + a_0 + a_1 \\
0 &= -a_{-1} + a_1 \\
0 &= \Delta x^2(a_{-1} + a_1) + 2(b_{-1} + b_0 + b_1) \\
0 &= -b_{-1} + b_1 \\
0 &= \Delta x^2(a_{-1} + a_1) + 12(b_{-1} + b_1)
\end{aligned}$$

are obtained. The normalized solution of this system is $a_{-1} = -12 = a_1$, $a_0 = 24$, $b_{-1} = 1 = b_1$, and $b_0 = 10$ and so

$$\frac{u''_{-1} + 10u''_0 + u''_1}{12} = \frac{u_{-1} - 2u_0 + u_1}{\Delta x^2}.$$

Using this method for $n = 1, 2, 3, 4$, we generate the following table.

Compact Difference Weights						
	Order of accuracy	a_0	$a_{\pm 1}$	$a_{\pm 2}$	$a_{\pm 3}$	$a_{\pm 4}$
weights for u_i	4	24	-12			
	8	$\frac{4770}{23}$	$-\frac{1920}{23}$	$-\frac{465}{23}$		
	12	$\frac{3252620}{1857}$	$-\frac{263655}{619}$	$-\frac{261954}{619}$	$-\frac{49483}{1857}$	
	16	$\frac{32213407975}{1985442}$	$-\frac{1152538240}{992721}$	$-\frac{5809420960}{992721}$	$-\frac{1059629440}{992721}$	$-\frac{127053415}{3970884}$
		b_0	$b_{\pm 1}$	$b_{\pm 2}$	$b_{\pm 3}$	$b_{\pm 4}$
weights for u_i''	4	10	1			
	8	$\frac{2358}{23}$	$\frac{688}{23}$	1		
	12	$\frac{725308}{619}$	$\frac{329913}{619}$	$\frac{36774}{619}$	1	
	16	$\frac{4824096670}{330907}$	$\frac{2750389888}{330907}$	$\frac{543878896}{330907}$	$\frac{32535424}{330907}$	1

Like the standard finite difference method, we cannot use a centered difference at the boundaries for $W \geq 5$ and so we would need to use one-sided differences. We have not examined the eigenvalues numerically, but we expect the eigenvalues to display characteristics similar to those of the standard finite differentiation matrices.

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