國 立 交 通 大 學

應用數學系

碩 士 論 文

耦合微分的緊緻數值方法

解一階 KDV 方程

Coupled Derivatives Compact Schemes

for One-Dimensional KdV Equation

研 究 生：李雅羚

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中 華 民 國 九 十 六 年 六 月

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摘　　要

這篇論文主要之目的是使用耦合微分的緊緻數值方法來解一階KDV方程。首先，我們先回顧一階和二階耦合微分的緊緻數值方法。接著，我們會學習一階和三階耦合微分的緊緻數值方法。再來，我們簡要地介紹Runge-Kutta Methods。最後，我們會給一些例子並且列出數值結果，然後做出結論。

Coupled Derivatives Compact Schemes for One-Dimensional KdV Equation

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ABSTRACT

The primary objective of this thesis is to use coupled derivatives compact schemes (CD) for solving one-dimensional KDV equation. First, we review the coupled first and second derivatives scheme and then we study the coupled first and third derivatives scheme. Next, we introduce roughly the Runge-Kutta methods. Finally, we give some examples and show numerical results, and the conclusion follows.

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目　　　　錄

Coupled Derivatives Compact Schemes for One-Dimensional KdV Equation

Student : Ya-Ling Li   Advisor : Ming-Chih Lai

1 Introduction

The KdV (Korteweg-de Vries) equation is a nonlinear partial differential equation. Two Dutch mathematicians D. J. Korteweg and G. deVries discovered this famous KdV equation

$$u_t + uu_x + u_{xxx} = 0$$

when they derived the shallow water wave, and they only considered dispersion but ignored the dissipation of the energy.

The KdV equation appears in a great number of physical situations. The reason for the ubiquitous incident of KdV equation is at least twofold. First, it associates simple dispersion with weak nonlinearity. Second, using the asymptotic method of manifold scales it can be shown that it describes (on suitable scales) the Riemann invariants of any hyperbolic system with weak nonlinearity and dispersion. The KdV equation is integrable [1], i.e. it can be written as the compatibility condition of a pair of linear eigenvalue equations, called the Lax pair [2]. In many physical situations, KdV appears in the form of an initial-boundary value problem on the semi-infinite line. This is for example the case of a certain laboratory study of water waves [3]. However, the solution of initial-boundary value problems for integrable equations was until recently open.

The KdV equation is the original of integrable equations. Initially presented as an equation with a solitary wave-type solution, it turned out (much) later to hold solutions with an arbitrary number of flexibly scattering solitary waves. The latter were observed numerically by Kruskal and Zabusky, who decided to call this type of solitary waves 'solitons'. In the years that followed this discovery, Kruskal and his collaborators went on to show that the KdV equation held an infinite number of conservation laws and, as the eventual explanation of these properties, they produced a linear differential system the compatibility of which is just the KdV equation. This linear system is traditionally called the Lax pair and allows the efficient linearization of the nonlinear equation. Using techniques developed in the theory of the inverse scattering problems in quantum mechanics (reconstruction of the potential from the scattering data) one can reduce the solution of the KdV equation to that of a linear integrodifferential one. This was the final proof of the integrability of KdV. The discovery of an integrable PDE and the techniques for its integration opened a whole new domain that is still the center of extreme activity a quarter-century later.

This paper presents a family of finite difference schemes for the first and third derivatives of smooth functions. The schemes are Hermitian and symmetric. The objective of this paper is to develop this family of schemes and to assess their potential for computations of the KdV equation. The schemes will be referred to as the “coupled-derivative,” or “C-D” schemes.

2 The Coupled First and Second Derivatives Scheme

First, we review a family of finite schemes for the first and second derivatives of smooth functions [5]. The schemes are Hermitian and symmetric. When defined on a uniform mesh, the schemes are of the form

$$\begin{aligned} & a_1 f'_{i-1} + a_0 f'_i + a_2 f'_{i+1} + h(b_1 f''_{i-1} + b_0 f''_i + b_2 f''_{i+1}) \\ = \; & \frac{1}{h}(c_1 f_{i-2} + c_2 f_{i-1} + c_0 f_i + c_3 f_{i+1} + c_4 f_{i+2}). \end{aligned} \tag{1}$$

Throughout this paper, h denotes the uniform mesh spacing. The interior scheme is of the form given by Eq.(1). Simultaneous solving for f'_i and f''_i implies that the number of unknowns is equal to $2M$. A total of $2M$ equations are therefore needed to close the system. Equation(1) may be used to derive two linearly independent equations at each node. This is done as follow. Both sides of Eq.(1) are first expanded in a Taylor series. The resulting coefficients are then matched, such that Eq.(1) maintains a certain order of accuracy. Note that Eq.(1) has 11 coefficients, of which one is arbitrary; i.e., Eq.(1) may be divided through by one of the constants without loss of generality. A convenient choice of the normalization constant is either of a_0 or b_0. It will be seen that the equation obtained by setting a_0 equal to 1 is linearly independent of the equation obtained when b_0 is set equal to 1. The two equations may therefore be applied at each node, and the resulting system of $2M$ equations solved for the nodal values of the first and second derivative. The process of obtaining the two equations is outlined in Sections 2.1 and 2.2.

TABLE I

Taylor Table for $a_0 = 1$

	LHS	RHS
f_i	0	c_0
f'_i	$1+2a_1$	$2(2c_4+c_3)$
f''_i	b_0	0
f'''_i	$2h^2(a_1/2! + b_2)$	$2h^2(2^3c_4 + c_3)/3!$
f^{iv}_i	0	0
f^{v}_i	$2h^4(a_1/4! + b_2/3!)$	$2h^4(2^5c_4 + c_3)/5!$
f^{vi}_i	0	0
f^{vii}_i	$2h^6(a_1/6! + b_2/5!)$	$2h^6(2^7c_4 + c_3)/7!$
f^{viii}_i	0	0
f^{ix}_i	$2h^8(a_1/8! + b_2/7!)$	$2h^8(2^9c_4 + c_3)/9!$

2.1 First Equation($a_0 = 1$) for First and Second Derivatives

Consider first the case where $a_0 = 1$. The symmetry of the schemes requires that $a_1 = a_2$, $b_1 = -b_2$, $c_1 = -c_4$, and $c_2 = -c_3$. Equation(1) therefore reduces to

$$\begin{aligned} & a_1 f'_{i-1} + f'_i + a_1 f'_{i+1} + h(-b_2 f''_{i-1} + b_0 f''_i + b_2 f''_{i+1}) \\ = & \frac{1}{h}[c_0 f_i + c_3(f_{i+1} - f_{i-1}) + c_4(f_{i+2} - f_{i-2})]. \end{aligned} \tag{2}$$

Expanding both sides of Eq.(2) in a Taylor series and collecting terms of the same order yields Table I. Note that "LHS" and "RHS" denote the coefficients of f_i^k on the left- and right-hand sides, respectively, of Eq.(2).

The Taylor table shows that $b_0 = c_0 = 0$. This leaves four undetermined constants(a_1, b_2, c_3, and c_4). Expressions for these constants may be obtained by matching the terms in the Taylor table.
When $a_0 = 1$, $b_0 = 0$:

Matching terms up to f''_i yields

$$a_1 = -\frac{1}{2} + c_3 + 2c_4,\ \ b_2 \text{ arbitrary }.$$

Matching terms up to f_i^{iv} yields

$$a_1 = -\frac{1}{2} + c_3 + 2c_4,\ \ b_2 = \frac{1}{12}[3 - 4(c_3 - c_4)].$$

Matching terms up to f_i^{vi} yields

$$a_1 = \frac{7}{16} - \frac{15}{4}c_4,\ \ b_2 = \frac{1}{16}(-1 + 36c_4),\ \ c_3 = \frac{15}{16} - \frac{23}{4}c_4.$$

Matching terms up to f_i^{viii} yields

$$a_1 = \frac{17}{36},\ \ b_2 = -\frac{1}{12},\ \ c_3 = \frac{107}{108},\ \ c_4 = -\frac{1}{108}.$$

$$\Rightarrow \frac{17}{36}f'_{i-1} + f'_i + \frac{17}{36}f'_{i+1} + h(\frac{1}{12}f''_{i-1} - \frac{1}{12}f''_{i+1}) = \frac{1}{h}[\frac{107}{108}(f_{i+1} - f_{i-1}) - \frac{1}{108}(f_{i+2} - f_{i-2})].$$

i.e.

$$51f'_{i-1} + 108f'_i + 51f'_{i+1} + 9h(f''_{i-1} - f''_{i+1}) = \frac{107}{h}(f_{i+1} - f_{i-1}) - \frac{f_{i+2} - f_{i-2}}{h}.$$

2.2 Second Equation($b_0 = 1$) for First and Second Derivatives

Consider the case where $b_0 = 1$. Note that a tilde is used above the constants to indicate their difference from the constants obtained when $a_0 = 1$; e.g., b_1 is replaced by $\tilde{b_1}$. Symmetry requires that $\tilde{b_1} = \tilde{b_2}$, $\tilde{c_1} = \tilde{c_4}$, $\tilde{c_2} = \tilde{c_3}$, and $\tilde{a_1} = -\tilde{a_2}$. Equation(1) therefore becomes

$$
\begin{aligned}
& \tilde{a_0} f_i^{'} + \tilde{a_2}(f_{i+1}^{'} - f_{i-1}^{'}) + h(\tilde{b_1} f_{i-1}^{''} + f_i^{''} + \tilde{b_1} f_{i+1}^{''}) \\
= & \frac{1}{h}[\tilde{c_1}(f_{i-2} + f_{i+2}) + \tilde{c_2}(f_{i-1} + f_{i+1}) + \tilde{c_0} f_i]. \qquad (3)
\end{aligned}
$$

Expanding both sides of the above equation in a Taylor series and collecting terms of the same order yields the Taylor Table II.

Table II shows that $\tilde{a_0}$ is required to be zero if $\tilde{b_0}$ is equal to one. The resulting equation may therefore be considered an expression for the second derivative. We have five unknown constants($\tilde{c_0}$, $\tilde{c_1}$, $\tilde{c_2}$, $\tilde{a_2}$, and $\tilde{b_1}$). These constants may be obtained by matching the terms in the above Taylor table and solving the resulting equations.

TABLE II

Taylor Table for $b_0 = 1$

	LHS	RHS
f_i	0	$\tilde{c_0} + 2\tilde{c_1} + 2\tilde{c_2}$
$f_i^{'}$	$\tilde{a_0}$	0
$f_i^{''}$	$h(2\tilde{a_2} + 2\tilde{b_1} + 1)$	$2h(2^2\tilde{c_1} + \tilde{c_2})/2!$
$f_i^{'''}$	0	0
f_i^{iv}	$2h^3(\tilde{a_2}/3! + \tilde{b_1}/2!)$	$2h^3(2^4\tilde{c_1} + \tilde{c_2})/4!$
f_i^{v}	0	0
f_i^{vi}	$2h^5(\tilde{a_2}/5! + \tilde{b_1}/4!)$	$2h^5(2^6\tilde{c_1} + \tilde{c_2})/6!$
f_i^{vii}	0	0
f_i^{viii}	$2h^7(\tilde{a_2}/7! + \tilde{b_1}/6!)$	$2h^7(2^8\tilde{c_1} + \tilde{c_2})/8!$
f_i^{ix}	0	0
f_i^{x}	$2h^9(\tilde{a_2}/9! + \tilde{b_1}/8!)$	$2h^9(2^{10}\tilde{c_1} + \tilde{c_2})/10!$

When $b_0 = 1,\ a_0 = 0$:

Matching terms up to $f_i^{''}$ yields

$$c_0 = -2(c_1 + c_2),\ a_2 = \frac{1}{2}(-1 - 2b_1 + 4c_1 + c_2).$$

Matching terms up to f_i^{iv} yields

$$c_0 = -2(c_1 + c_2),\ a_2 = -\frac{3}{4} + c_1 + \frac{5}{8}c_2,\ b_1 = \frac{1}{4} + c_1 - \frac{c_2}{8}.$$

Matching terms up to f_i^{vi} yields

$$c_0 = -6 + 54c_1,\ c_2 = 3 - 28c_1,\ a_2 = \frac{9}{8} - \frac{33}{2}c_1,\ b_1 = -\frac{1}{8} + \frac{9}{2}c_1.$$

Matching terms up to f_i^{viii} yields

$$c_0 = -\frac{13}{2},\ c_1 = -\frac{1}{108},\ c_2 = \frac{88}{27},\ a_2 = \frac{23}{18},\ b_1 = -\frac{1}{6}.$$

$$\Rightarrow \frac{23}{18}(f_{i+1}^{'} - f_{i-1}^{'}) + h(-\frac{1}{6}f_{i-1}^{''} + f_i^{''} - \frac{1}{6}f_{i+1}^{''}) = \frac{1}{h}[-\frac{1}{108}(f_{i-2} + f_{i+2}) + \frac{88}{27}(f_{i-1} + f_{i+1}) - \frac{13}{2}f_i].$$

i.e.

$$138(f_{i+1}^{'} - f_{i-1}^{'}) - h(18f_{i-1}^{''} - 108f_i^{''} + 18f_{i+1}^{''}) = -\frac{f_{i+2} + f_{i-2}}{h} + \frac{352}{h}(f_{i+1} + f_{i-1}) - \frac{702}{h}f_i.$$

3 The Coupled First and Third Derivatives Scheme

Now, we present a family of finite difference schemes for the first and third derivatives of smooth functions. The schemes are also Hermitian and symmetric. When defined on a uniform mesh, the schemes are of the form

$$\begin{aligned} & a_1 f'_{i-1} + a_0 f'_i + a_2 f'_{i+1} + h^2 (b_1 f'''_{i-1} + b_0 f'''_i + b_2 f'''_{i+1}) \\ = & \frac{1}{h}(c_1 f_{i-2} + c_2 f_{i-1} + c_0 f_i + c_3 f_{i+1} + c_4 f_{i+2}). \end{aligned} \tag{4}$$

The interior scheme is of the form given by Eq.(4). Simultaneous solving for f'_i and f'''_i implies that the number of unknowns is equal to $2M$. A total of $2M$ equations are therefore needed to close the system. Equation(4) may be used to derive two linearly independent equations at each node. This is done as follow. Both sides of Eq.(4) are first expanded in a Taylor series. The resulting coefficients are then matched, such that Eq.(4) maintains a certain order of accuracy. Note that Eq.(4) has 11 coefficients, of which one is arbitrary; i.e., Eq(4) may be divided through by one of the constants without loss of generality. A convenient choice of the normalization constant is either of a_0 or b_0. It will be seen that the equation obtained by setting a_0 equal to 1 is linearly independent of the equation obtained when b_0 is set equal to 1. The two equations may therefore be applied at each node, and the resulting system of $2M$ equations solved for the nodal values of the first and third derivative. The process of obtaining the two equations is outlined in Sections 2.3 and 2.4.

TABLE III

Taylor Table for $a_0 = 1$

	LHS	RHS
f_i	0	c_0
f'_i	a_0+2a_1	$2(2c_4+c_3)$
f''_i	0	0
f'''_i	$2h^2(a_1/2! + b_2)$	$2h^2(2^3 c_4 + c_3)/3!$
f^{iv}_i	0	0
f^{v}_i	$2h^4(a_1/4! + b_2/2!)$	$2h^4(2^5 c_4 + c_3)/5!$
f^{vi}_i	0	0
f^{vii}_i	$2h^6(a_1/6! + b_2/4!)$	$2h^6(2^7 c_4 + c_3)/7!$

3.1 First Equation($a_0 = 1$) for First and Third Derivatives

Consider first the case where $a_0 = 1$. The symmetry of the schemes requires that $a_1 = a_2$, $b_1 = b_2$, $c_1 = -c_4$, and $c_2 = -c_3$. Equation(1) therefore reduces to

$$\begin{aligned} & a_1 f'_{i-1} + f'_i + a_1 f'_{i+1} + h^2(b_2 f'''_{i-1} + b_0 f'''_i + b_2 f'''_{i+1}) \\ = \; & \frac{1}{h}[c_0 f_i + c_3(f_{i+1} - f_{i-1}) + c_4(f_{i+2} - f_{i-2})]. \end{aligned} \tag{5}$$

Expanding both sides of Eq.(5) in a Taylor series and collecting terms of the same order yields Table III. Note that "LHS" and "RHS" denote the coefficients of f_i^k on the left- and right-hand sides, respectively, of Eq.(5).
The Taylor table shows that $c_0 = 0$. This leaves four undetermined constants(a_1, b_2, c_3, and c_4). Expressions for these constants may be obtained by matching the terms in the Taylor table.
When $a_0 = 1$, $b_0 = 0$:

Matching terms up to f'_i yields

$$a_1 = \frac{1}{2}(-1 + 2c_3 + 4c_4), \; b_2 \text{ arbitrary }.$$

Matching terms up to f'''_i yields

$$a_1 = \frac{1}{2}(-1 + 2c_3 + 4c_4), \; b_2 = \frac{1}{12}(3 - 4c_3 + 4c_4).$$

Matching terms up to f^v_i yields

$$a_1 = \frac{1}{32}(9 + 60c_4), \; b_2 = \frac{1}{96}(-1 + 36c_4), \; c_3 = \frac{1}{32}(25 - 4c_4).$$

Matching terms up to f^{vii}_i yields

$$a_1 = \frac{11}{48}, \; b_2 = \frac{-1}{48}, \; c_3 = \frac{113}{144}, \; c_4 = \frac{-1}{36}.$$

$$\Rightarrow \frac{11}{48} f'_{i-1} + f'_i + \frac{11}{48} f'_{i+1} + h^2\left(\frac{-1}{48} f'''_{i-1} - \frac{1}{48} f'''_{i+1}\right) = \frac{1}{h}\left(\frac{1}{36} f_{i-2} - \frac{113}{144} f_{i-1} + \frac{113}{144} f_{i+1} - \frac{1}{36} f_{i+2}\right).$$

i.e.

$$11 f'_{i-1} + 48 f'_i + 11 f'_{i+1} + h^2(-f'''_{i-1} - f'''_{i+1}) = \frac{1}{3h}(4 f_{i-2} - 113 f_{i-1} + 113 f_{i+1} - 4 f_{i+2}).$$

3.2 Third Equation($b_0 = 1$) for First and Third Derivatives

When $b_0 = 1$, $a_0 = 0$:

Matching terms up to $f_i^{'''}$ yields

$$a_1 = c_3 + 2c_4,\ \ b_2 = \frac{1}{6}(-3 - 2c_3 + 2c_4).$$

Matching terms up to f_i^{v} yields

$$a_1 = \frac{-15}{8}(1 - c_4),\ \ b_2 = \frac{1}{8}(1 + 3c_4),\ \ c_3 = \frac{-1}{8}(15 + c_4).$$

Matching terms up to f_i^{vii} yields

$$a_1 = \frac{-35}{32},\ \ b_2 = \frac{9}{32},\ \ c_3 = \frac{-185}{96},\ \ c_4 = \frac{5}{12}.$$

$$\Rightarrow \frac{-35}{32}f_{i-1}^{'} - \frac{35}{32}f_{i+1}^{'} + h^2(\frac{9}{32}f_{i-1}^{'''} + f_i^{'''} + \frac{9}{32}f_{i+1}^{'''}) = \frac{1}{h}(\frac{-5}{12}f_{i-2} + \frac{185}{96}f_{i-1} - \frac{185}{96}f_{i+1} + \frac{5}{12}f_{i+2}).$$

i.e.

$$-35f_{i-1}^{'} - 35f_{i+1}^{'} + h^2(9f_{i-1}^{'''} + 32f_i^{'''} + 9f_{i+1}^{'''}) = \frac{1}{3h}(-40f_{i-2} + 185f_{i-1} - 185f_{i+1} + 40f_{i+2}).$$

3.3 The Scheme

The interior scheme involves applying the equations derived in section 2.3 and 2.4 at each node. The resulting system of $2M$ equations is then solved to obtain $f_i^{'}$ and $f_i^{'''}$.

Schemes:

$$11f_{i-1}^{'} + 48f_i^{'} + 11f_{i+1}^{'} + h^2(-f_{i-1}^{'''} - f_{i+1}^{'''}) = \frac{1}{3h}(4f_{i-2} - 113f_{i-1} + 113f_{i+1} - 4f_{i+2}).$$

$$-35f_{i-1}^{'} - 35f_{i+1}^{'} + h^2(9f_{i-1}^{'''} + 32f_i^{'''} + 9f_{i+1}^{'''}) = \frac{1}{3h}(-40f_{i-2} + 185f_{i-1} - 185f_{i+1} + 40f_{i+2}).$$

Note that the first and third derivatives are coupled in the C-D schemes. The vector of unknowns is therefore equal to $[\cdots, f_i^{'}, \cdots, f_i^{'''}, \cdots]^T$.

We can rewrite the C-D schemes to the form

$$A\mathbf{y} = \mathbf{b},$$

where the vector $\mathbf{y}$ is of length $2M$ and is equal to $[f_1^{'}, f_2{'}, \cdots f_M^{'}, f_1^{'''}, f_2^{'''}, \cdots f_M^{'''}]^T$.

The schemes are presented in matrix from below. Both periodic and nonperiodic domains are considered.

Sixth-Order Scheme:Periodic

The sixth-order scheme on a periodic domain is given by

$$
\left[\begin{array}{ccccccc|ccccccc}
48 & 11 & 0 & \cdots & \cdots & 0 & 11 & 0 & -h^2 & 0 & \cdots & \cdots & 0 & -h^2 \\
11 & 48 & 11 & 0 & \cdots & \cdots & 0 & -h^2 & 0 & -h^2 & 0 & \cdots & \cdots & 0 \\
0 & 11 & 48 & 11 & 0 & \cdots & 0 & 0 & -h^2 & 0 & -h^2 & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & & & \vdots & \vdots & \ddots & \ddots & \ddots & & & \vdots \\
\vdots & & \ddots & \ddots & \ddots & & 0 & \vdots & & \ddots & \ddots & \ddots & & 0 \\
0 & & & \ddots & \ddots & \ddots & 11 & 0 & & & \ddots & \ddots & \ddots & -h^2 \\
11 & 0 & \cdots & \cdots & 0 & 11 & 48 & -h^2 & 0 & \cdots & \cdots & 0 & -h^2 & 0 \\
\hline
0 & -35 & 0 & \cdots & \cdots & 0 & -35 & 32h^2 & 9h^2 & 0 & \cdots & \cdots & 0 & 9h^2 \\
-35 & 0 & -35 & 0 & \cdots & \cdots & 0 & 9h^2 & 32h^2 & 9h^2 & 0 & \cdots & 0 & 0 \\
0 & -35 & 0 & -35 & 0 & \cdots & 0 & 0 & 9h^2 & 32h^2 & 9h^2 & 0 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & & & \vdots & \vdots & \ddots & \ddots & \ddots & & & \vdots \\
\vdots & & \ddots & \ddots & \ddots & & 0 & \vdots & & \ddots & \ddots & \ddots & & 0 \\
0 & & & \ddots & \ddots & \ddots & -35 & 0 & & & \ddots & \ddots & \ddots & 9h^2 \\
-35 & 0 & \cdots & \cdots & 0 & -35 & 0 & 9h^2 & 0 & \cdots & \cdots & 0 & 9h^2 & 32h^2
\end{array}\right]
$$

$$
\left[\begin{array}{c}
f_1' \\ \vdots \\ \vdots \\ f_i' \\ \vdots \\ \vdots \\ f_M' \\ \hline f_1''' \\ \vdots \\ \vdots \\ f_i''' \\ \vdots \\ \vdots \\ f_M'''
\end{array}\right]
= \frac{1}{3h}
\left[\begin{array}{c}
4f_{M-1} - 113f_M + 113f_2 - 4f_3 \\ \vdots \\ \vdots \\ 4f_{i-2} - 113f_{i-1} + 113f_{i+1} - 4f_{i+2} \\ \vdots \\ \vdots \\ 4f_{M-2} - 113f_{M-1} + 113f_1 - 4f_2 \\ \hline -40f_{M-1} + 185f_M - 185f_2 + 40f_3 \\ \vdots \\ \vdots \\ -40f_{i-2} + 185f_{i-1} - 185f_{i+1} + 40f_{i+2} \\ \vdots \\ \vdots \\ -40f_{M-2} + 185f_{M-1} - 185f_1 + 40f_2
\end{array}\right]
$$

Sixth-Order Scheme:Nonperiodic

The sixth-order scheme on a nonperiodic domain is given by

$$
\left[\begin{array}{cccccc|cccccc}
48 & 11 & & & & & 0 & -h^2 & & & & \\
11 & 48 & 11 & & & & -h^2 & 0 & -h^2 & & & \\
 & 11 & 48 & 11 & & & & -h^2 & 0 & -h^2 & & \\
 & & \ddots & \ddots & \ddots & & & & \ddots & \ddots & \ddots & \\
 & & & \ddots & \ddots & 11 & & & & \ddots & \ddots & -h^2 \\
 & & & & 11 & 48 & & & & & -h^2 & 0 \\
\hline
0 & -35 & & & & & 32h^2 & 9h^2 & & & & \\
-35 & 0 & -35 & & & & 9h^2 & 32h^2 & 9h^2 & & & \\
 & -35 & 0 & -35 & & & & 9h^2 & 32h^2 & 9h^2 & & \\
 & & \ddots & \ddots & \ddots & & & & \ddots & \ddots & \ddots & \\
 & & & \ddots & \ddots & -35 & & & & \ddots & \ddots & 9h^2 \\
 & & & & -35 & 0 & & & & & 9h^2 & 32h^2
\end{array}\right]
\left[\begin{array}{c}
f_1' \\ \vdots \\ \vdots \\ f_i' \\ \vdots \\ f_M' \\ \hline f_1''' \\ \vdots \\ \vdots \\ f_i''' \\ \vdots \\ f_M'''
\end{array}\right]
$$

$$
= \frac{1}{3h}
\left[\begin{array}{c}
4f_{-1} - 113f_0 + 113f_2 - 4f_3 \\
\vdots \\
\vdots \\
4f_{i-2} - 113f_{i-1} + 113f_{i+1} - 4f_{i+2} \\
\vdots \\
4f_{M-2} - 113f_{M-1} + 113f_{M+1} - 4f_{M+2} \\
\hline
-40f_{-1} + 185f_0 - 185f_2 + 40f_3 \\
\vdots \\
\vdots \\
-40f_{i-2} + 185f_{i-1} - 185f_{i+1} + 40f_{i+2} \\
\vdots \\
-40f_{M-2} + 185f_{M-1} - 185f_{M+1} + 40f_{M+2}
\end{array}\right]
$$

4 Runge-Kutta Methods

Let us review the Runge-Kutta methods [13].

4.1 Euler's Method

The Taylor-series method with $n = 1$ is called **Euler's method**. It looks like this:

$$x(t+h) = x(t) + hf(t,x).$$

This formula has the obvious advantage of *not* requiring any differentiation of f. This advantage is offset by the necessity of taking small values for h to gain acceptable precision. Still, the method serves as a useful example and is of great importance theoretically because existence theorems can be based on it.

4.2 Second-Order Runge-Kutta Method

Let us begin with the Taylor series for $x(t+h)$:

$$x(t+h) = x(t) + hx'(t) + \frac{h^2}{2!}x''(t) + \frac{h^3}{3!}x'''(t) + \cdots \tag{6}$$

From the differential equation, we have

$$\begin{aligned} x'(t) &= f \\ x''(t) &= f_t + f_x x' = f_t + f_x f \\ x'''(t) &= f_{tt} + f_{tx} f + (f_t + f_x f) f_x + f(f_{xt} + f_{xx} f) \\ &\vdots \end{aligned}$$

Here subscripts denote partial derivatives, and the chain rule of differentiation is used repeatedly. The first three terms in Equation(6) can be written now in the form

$$\begin{aligned} x(t+h) &= x + hf + \frac{1}{2}h^2(f_t + ff_x) + \mathcal{O}(h^3) \\ &= x + \frac{1}{2}hf + \frac{1}{2}h[f + hf_t + hff_x] + \mathcal{O}(h^3). \end{aligned} \tag{7}$$

where x means $x(t)$, f means $f(t,x)$, and so on. We are able to eliminate the partial derivatives with the aid of the first few terms in the Taylor series in two variables:

$$f(t+h, x+hf) = f + hf_t + hff_x + \mathcal{O}(h^2).$$

Equation(7) can be rewritten as

$$x(t+h) = x + \frac{1}{2}hf + \frac{1}{2}hf(t+h, x+hf) + \mathcal{O}(h^3).$$

Hence, the formula for advancing the solution is

$$x(t+h) = x(t) + \frac{h}{2}f(t,x) + \frac{h}{2}f(t+h, x+hf(t,x)),$$

or equivalently,

$$x(t+h) = x(t) + \frac{1}{2}(F_1 + F_2) \tag{8}$$

where

$$\begin{cases} F_1 = hf(t,x) \\ F_2 = hf(t+h, x+F_1) \end{cases}$$

This formula can be used repeatedly to advance the solution one step at a time. It is called a **second-order Runge-Kutta method**. It is also known as **Heun's method**.

In general, second-order Runge-Kutta formulas are of the form

$$x(t+h) = x + w_1 hf + w_2 hf(t+\alpha h, x+\beta hf) + \mathcal{O}(h^3), \tag{9}$$

where w_1, w_2, α, and β are parameters at our disposal. Equation(9) can be rewritten with the aid of the Taylor series in two variables as

$$x(t+h) = x + w_1 hf + w_2 h[f + \alpha hf_t + \beta hff_x] + \mathcal{O}(h^3). \tag{10}$$

Comparing Equations(7) and (10), we see that we should impose these conditions:

$$\begin{cases} w_1 + w_2 &= 1 \\ w_2\alpha &= \frac{1}{2} \\ w_2\beta &= \frac{1}{2} \end{cases} \tag{11}$$

One solution is $w_1 = w_2 = \frac{1}{2}$, $\alpha = \beta = 1$, which is the one corresponding to Heun's method in Equation(8). The system of Equation(11) has solutions other than this one, such as the one obtained by letting $w_1 = 0, w_2 = 1, \alpha = \beta = \frac{1}{2}$. The resulting formula from(9) is called the **modified Euler method** :

$$x(t+h) = x(t) + F_2,$$

where

$$\begin{cases} F_1 = hf(t,x) \\ F_2 = hf(t+\frac{1}{2}h, x+\frac{1}{2}F_1) \end{cases}$$

Compare this to the standard Euler method, described in Section 3.1.

4.3 Fourth-Order Runge-Kutta Method

The higher-order Runge-Kutta formulas are very tedious to derive, and we shall not do so. The formulas are rather elegant, however, and are easily programmed once they have been derived. Here are the formulas for the *classical* **fourth-order Runge-Kutta method** :

$$x(t+h) = x(t) + \frac{1}{6}(F_1 + 2F_2 + 2F_3 + F_4), \tag{12}$$

where

$$\begin{cases} F_1 = hf(t,x) \\ F_2 = hf(t+\frac{1}{2}h, x+\frac{1}{2}F_1) \\ F_3 = hf(t+\frac{1}{2}h, x+\frac{1}{2}F_2) \\ F_4 = hf(t+h, x+F_3) \end{cases}$$

This is called a fourth-order method because it reproduces the terms in the Taylor series up to and including the one involving h^4. The error is therefore $\mathcal{O}(h^5)$. Exact expressions for the h^5 error term are available.

5 The Numerical Examples

5.1 Example 1

Consider the equation,

$$u = \cos 4x,\ \ x \in [0, 2\pi].$$

To compute $u^{'}$ & $u^{'''}$ and compare the absolutely errors with the exact ones,

$$\begin{cases} u^{'} = -4\sin 4x \\ u^{'''} = 64\sin 4x \end{cases}$$

Mesh	**cond(A)**	**Maxnorm-Error**	**order**
16	215.965244021860	3.442540136851857E-003	-
32	799.575261801726	7.867157863383767E-006	8.7734
64	3134.01533292119	2.683871747066746E-008	8.1954
128	12471.7756173990	1.013642503266965E-010	8.0486

Table IV : The error for $u^{'}$.

Mesh	**cond(A)**	**Maxnorm-Error**	**order**
16	215.965244021860	0.356972051819817	-
32	799.575261801726	4.292639448863156E-003	6.3778
64	3134.01533292119	6.327597368027682E-005	6.0841
128	12471.7756173990	9.748273868126489E-007	6.0204

Table V : The error for $u^{'''}$.

Mesh	**cond(A)**	**cond(A)/(Mesh^2)**
16	215.965244021860	0.843614234460390625
32	799.575261801726	0.780835216603248046875
64	3134.01533292119	0.76514046213896240234375
128	12471.7756173990	0.76121677352288818359375

Table VI : The relation between cond(A) and $Mesh$.

From the Table III, we can know that the order of the scheme is equal to ninth order. So the order of the first derivative should be eighth order, and the order of the third derivative should be sixth order.

Note that the condition number is large, so A is **ill conditioned** and any numerical solution of $Ax = b$ must be accepted with a great deal of skepticism.

5.2 Example 2

Consider the linear equation,

$$\begin{cases} u_t + u_x + u_{xxx} = 0 \\ u(x,0) = \sin 2x, \ \ x \in [0, 2\pi] \end{cases}$$

with the exact solution of $u_{exact}(x,t) = \sin(2(x+3t))$ when $T = 1$.

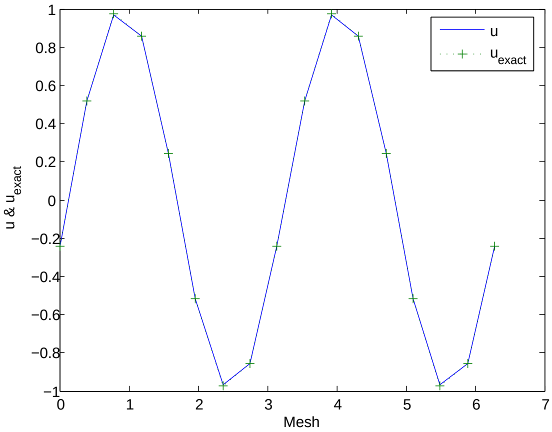

Figure 1: u and u_{exact} for RK3 (when M=16).

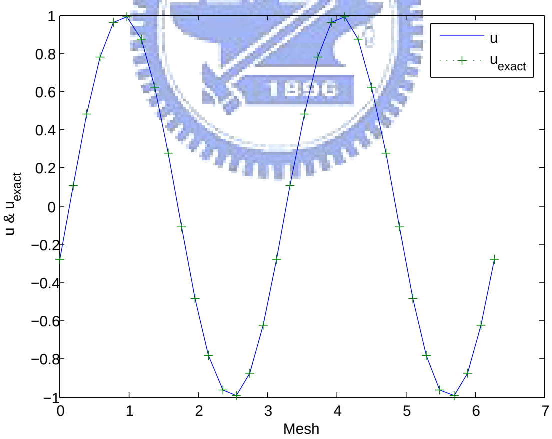

Figure 2: u and u_{exact} for RK3 (when M=32).

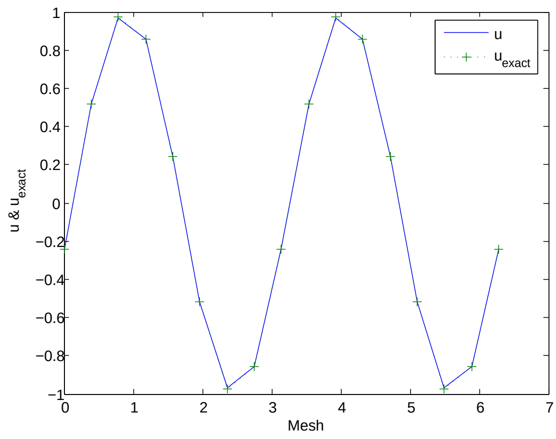

Figure 3: u and u_{exact} for RK4 (when M=16).

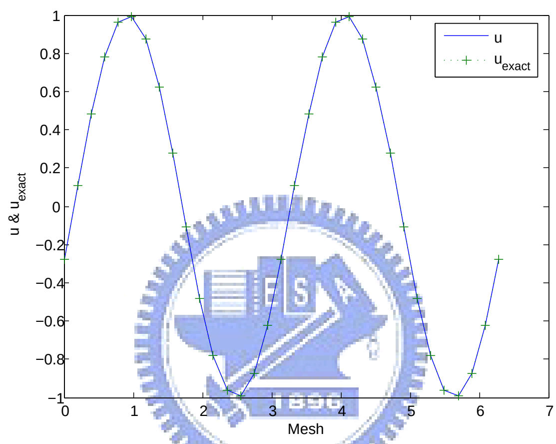

Figure 4: u and u_{exact} for RK4 (when M=32).

Mesh	Time step	Maxnorm-Error	order
16	132	unstable	-
32	1056	unstable	-
64	8454	unstable	-
128	67636	unstable	-

Table VII : The error for RK1(When T=1 ($\Delta t \sim \Delta x^3$)).

Mesh	Time step	Maxnorm-Error	order
16	132	unstable	-
32	1056	unstable	-
64	8454	unstable	-
128	67636	unstable	-

Table VIII : The error for RK2(When T=1 ($\Delta t \sim \Delta x^3$)).

Mesh	Time step	Maxnorm-Error	order
16	132	5.028345551417179E-004	-
32	1056	7.851200683139936E-006	6.0010
64	8454	1.213175020303714E-007	6.0161
128	67636	1.896873163750867E-009	5.9990

Table IX : The error for RK3(When T=1 ($\Delta t \sim \Delta x^3$)).

Mesh	Time step	Maxnorm-Error	order
16	132	5.104998880844369E-004	-
32	1056	7.846674022080058E-006	6.0237
64	8454	1.213253499471323E-007	6.0151
128	67636	1.896881306542864E-009	5.9991

Table X : The error for RK4(When T=1 ($\Delta t \sim \Delta x^3$)).

In order to be **stable**, it is necessary to assume that $\mu = \frac{\Delta t}{(\Delta x)^3} \le \frac{1}{2}$. So we take $\Delta t \approx \frac{(\Delta x)^3}{8}$. Note that $T = n \cdot \Delta t$, where n is the time step, so n depends on Δt when we set $T = 1$. From the above tables, we know that it is about sixth order. This is because it is time dependence, so the order of the error depends on the order of the third derivative.

Mesh	Time step	Maxnorm-Error	order
16	10000	0.1835957083217821E-02	-
32	10000	unstable	-
64	10000	unstable	-
128	10000	unstable	-

Table XI : The error for RK1(When T=1 ($\Delta t = 0.0001$)).

Mesh	Time step	Maxnorm-Error	order
16	10000	0.5110460338352829E-03	-
32	10000	0.7490918246130795E-05	6.0922
64	10000	unstable	-
128	10000	unstable	-

Table XII : The error for RK2(When T=1 ($\Delta t = 0.0001$)).

Mesh	Time step	Maxnorm-Error	order
16	10000	0.5113914889436910E-03	-
32	10000	0.7848784020964006E-05	6.0258
64	10000	0.1213325657306585E-06	6.0154
128	10000	unstable	-

Table XIII : The error for RK3(When T=1 ($\Delta t = 0.0001$)).

Mesh	Time step	Maxnorm-Error	order
16	10000	0.5113915040849681E-03	-
32	10000	0.7848778151214875E-05	6.0258
64	10000	0.1213372820135783E-06	6.0154
128	10000	unstable	-

Table XIV : The error for RK4(When T=1 ($\Delta t = 0.0001$)).

From the previous page, we know that $\Delta t \sim (\Delta x)^3$. Besides, since $\Delta x = \frac{2\pi}{M}$, so $\Delta x \sim \frac{1}{M}$, then we can get $\Delta t \sim (\frac{1}{M})^3$. Since $\Delta t = 0.0001$, so when M is getting larger, the error becomes unstable. From these tables above, we can conclude that $RK4$ is the most stable method and its solution is the most accurate one.

5.3 Example 3

Consider the non-linear equation,

$$\begin{cases} u_t + u \cdot u_x + u_{xxx} = 0 \\ u(x,0) = 3 \cdot (\mathrm{sech}(x/2))^2, \ x \in [0, 2\pi] \end{cases}$$

with the exact solution of $u_{exact}(x,t) = 3 \cdot (\mathrm{sech}((x-t)/2))^2$ when $T = 1$.

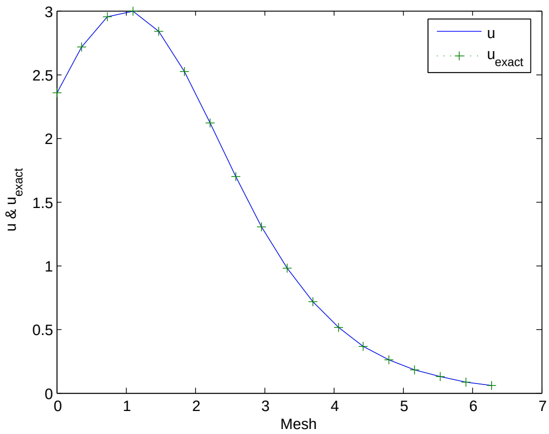

Figure 5: u and u_{exact} for RK3 (when M=16).

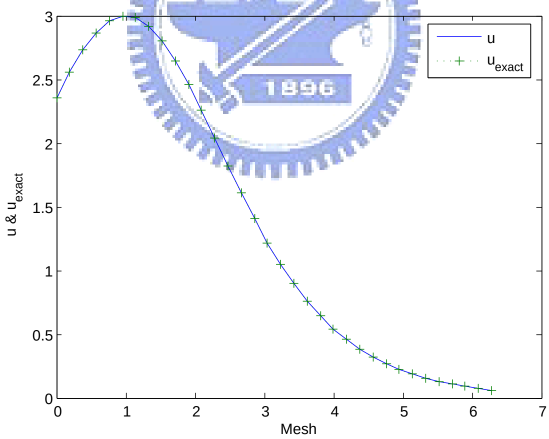

Figure 6: u and u_{exact} for RK3 (when M=32).

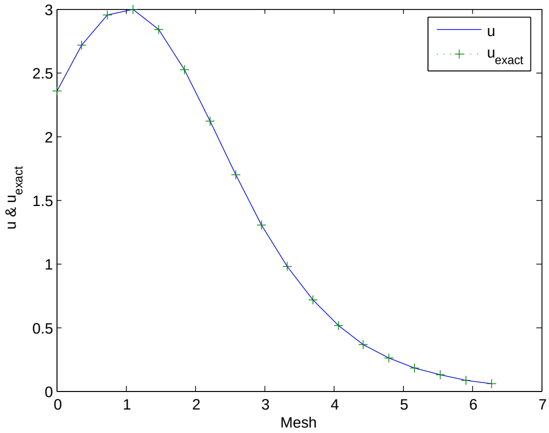

Figure 7: u and u_{exact} for RK4 (when M=16).

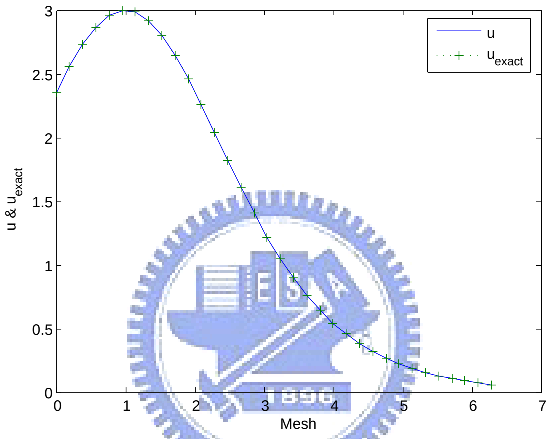

Figure 8: u and u_{exact} for RK4 (when M=32).

Mesh	Time step	Maxnorm-Error	order
16	158	unstable	-
32	1159	unstable	-
64	8857	unstable	-
128	69234	unstable	-

Table XV : The error for RK1(When T=1 ($\Delta t \sim \Delta x^3$)).

Mesh	Time step	Maxnorm-Error	order
16	158	unstable	-
32	1159	unstable	-
64	8857	unstable	-
128	69234	unstable	-

Table XVI : The error for RK2(When T=1 ($\Delta t \sim \Delta x^3$)).

Mesh	Time step	Maxnorm-Error	order
16	158	2.583180630577608E-005	-
32	1159	5.098193027186504E-007	5.6630
64	8857	8.033804399509847E-009	5.9878
128	69234	1.079924483171624E-010	6.2171

Table XVII : The error for RK3(When T=1 ($\Delta t \sim \Delta x^3$)).

Mesh	Time step	Maxnorm-Error	order
16	158	2.524653262514498E-005	-
32	1159	5.132999952306427E-007	5.6201
64	8857	8.047767008356743E-009	5.9951
128	69234	1.079270006698607E-010	6.2205

Table XVIII : The error for RK4(When T=1 ($\Delta t \sim \Delta x^3$)).

Observe this non-linear case, we can get that it is about sixth order. This is because it is time dependence, so the order of the error depends on the order of the third derivative.

6 Conclusions

A family of finite difference schemes for the first and third derivatives of smooth functions were derived. We have extended it to the KdV equation. The schemes are Hermitian and symmetric. They are different from the schemes in that the first and third derivatives are simultaneously evaluated.

Consider that the KdV equation requires both first and third derivatives of the variables, the proposed schemes appear to be attractive alternatives to the schemes which the first and third derivatives are simultaneously evaluated for computations of the KdV equation.

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