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CONSTRUCTION OF A THREE-STAGE DIFFERENCE SCHEME FOR ORDINARY DIFFERENTIAL EQUATIONS*

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Abstract

In this paper, we construct a three-stage difference scheme of 4th order for ordinary differential equations by the method of composing 2nd order schemes symmetrically.

1. Introduction

We know that the difference scheme $Z_{k+1} = Z_k + \frac{h}{2}(f(Z_k) + f(Z_{k+1}))$ with h the step length, is of order two for ordinary differential equations $Z' = f(Z)$, where $Z = Z(t)$. We hope that the three-stage method of the form

$$\begin{cases} Z_1 = Z_0 + c_1 h(f(Z_0) + f(Z_1)) \\ Z_2 = Z_1 + c_2 h(f(Z_1) + f(Z_2)) \\ Z_3 = Z_2 + c_3 h(f(Z_2) + f(Z_3)) \end{cases} \tag{1}$$

would be of order 4 (i.e., $Z_3 - Z(t+h) = O(h^5)$, $Z(t+h)$ is the exact solution at $t+h$ and Z_3 the numerical one) when the parameters c_1, c_2 and c_3 are chosen properly.

We will use the method of Taylor expansion to deal with the simple case when there is only one ordinary differential equation(ODE). When we deal with the case of systems of ODE's, the Taylor expansions become very complex, although it surely can be applied and the same conclusion as in the former case can be got. We introduce another method[2] known as "trees and elementary differentials" to deal with the latter case. In fact, the essence of the two methods are the same, they are just two different ways of expression.

2. Construction for Single Equation

In this section, without specific statements, the values of all functions are calculated at Z_0, and we consider only the terms up to $o(h^4)$ in the following calculations, the higher order terms of h are omitted.

First we calculate the Taylor expansion of the exact solution. Since

$$\dot{Z} = f,\ \ddot{Z} = f'\dot{Z} = f'f,\ Z^{(3)} = f''f^2 + f'^2 f,\ Z^{(4)} = f'''f^3 + 4f''f'f^2 + f'^3 f, \tag{2}$$

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we have, with $Z_0 = Z(t)$,

$$Z(t+h) = Z_0+hf+\frac{h^2}{2!}f'f+\frac{h^3}{3!}(f''f^2+f'^2f)+\frac{h^4}{4!}(f'''f^3+4f''f'f^2+f'^3f)+O(h^5). \quad (3)$$

Now we turn to the Taylor expansion of the numerical solution. We can rewrite (3) as

$$Z_3 = Z_0 + h[c_1 f + (c_1 + c_2)f_1 + (c_2 + c_3)f_2 + c_3 f_3], \quad (4)$$

where for simplicity, we denote $f_i = f(Z_i),\ i = 1, 2, 3$. We need figure out the Taylor expansions of f_1, f_2, f_3. Noticing (4), we just have to expand them up to the terms of order 3 of h.

$$f_i = f + f'(Z_i - Z_0) + \frac{f''}{2!}(Z_i - Z_0)^2 + \frac{f'''}{3!}(Z_i - Z_0)^3 + O(h^4). \quad (5)$$

Since $Z_1 = Z_0 + c_1 h(f_1 + f)$, we then have

$$\begin{aligned} f_1 =& f + (c_1h)2f'f + (c_1h)^2(2f'^2f + 2f''f^2) \\ &+ (c_1h)^3(2f'^3f + 6f''f'f^2 + 4/3f'''f^3) + O(h^4). \end{aligned} \quad (6)$$

We use the same technique to expand the Taylor expansions of f_2, f_3. Since $Z_2 - Z_0 = c_1h(f_1 + f) + c_2h(f_2 + f_1) = c_1hf + (c_1 + c_2)hf_1 + c_2hf_2$, we have

$$\begin{aligned} f_2 =& f + h[2(c_1 + c_2)f'f] + h^2[(c_1 + c_2)^2[2f'^2f + 2f''f^2]] \\ &+ h^3[(c_1 + c_2)(c_1^2 + c_1c_2 + c_2^2)2f'^3f + [(c_1 + c_2)2c_1^2 \\ &+ 2c_2(c_1 + c_2)^2 + 4(c_1 + c_2)^3]f''f'f^2 + 4/3(c_1 + c_2)^3f'''f^3] + O(h^4). \end{aligned} \quad (8)$$

Similarly, we can get

$$\begin{aligned} f_3 =& f + h[2(c_1 + c_2 + c_3)f'f] + h^2[(c_1 + c_2 + c_3)^2 2f'^2f + (c_1 + c_2 + c_3)^2 2f''f^2] \\ &+ h^3[[(c_1 + c_2)c_1^2 + (c_2 + c_3)(c_1 + c_2)^2 + c_3(c_1 + c_2 + c_3)^2]2f'^3f \\ &+ [(c_1 + c_2)c_1^2 + (c_2 + c_3)(c_1 + c_2)^2 + c_3(c_1 + c_2 + c_3)^2 + 2(c_1 + c_2 + c_3)^3]2f''f'f^2 \\ &+ 4/3(c_2 + c_2 + c_3)^3f'''f^3] + O(h^4). \end{aligned} \quad (9)$$

Inserting the Taylor expansions of $f_i (i = 1, 2, 3)$ into (4), we get the Taylor expansion of the numerical solution

$$\begin{aligned} Z_3 =& Z_0 + [c_1 + (c_1 + c_2) + (c_2 + c_3) + c_3]hf \\ &+ [(c_1 + c_2)2c_1 + (c_2 + c_3)2(c_1 + c_2) + c_3 2(c_1 + c_2 + c_3)]h^2f'f \\ &+ [(c_1 + c_2)2c_1^2 + (c_2 + c_3)2(c_1 + c_2)^2 + c_3 2(c_1 + c_2 + c_3)^2]h^3(f''f^2 + f'^2f) \\ &+ [(c_1 + c_2)4/3c_1^3 + (c_2 + c_3)4/3(c_1 + c_2)^3 + c_3 4/3(c_1 + c_2 + c_3)^3]h^4f'''f^3 \\ &+ [(c_1 + c_2)2c_1^3 + (c_1 + c_2)2(c_1^2 + c_2^2 + c_1c_2)(c_2 + c_3) \\ &+ c_3 2[(c_1 + c_2)c_1^2 + (c_2 + c_3)(c_1 + c_2)^2 + c_3(c_1 + c_2 + c_3)^2]]h^4f'^3f \\ &+ [(c_1 + c_2)6c_1^3 + (c_2 + c_3)[4(c_1 + c_2)^3 + 2c_1^2(c_1 + c_2) + 2c_2(c_1 + c_2)^2) + c_3 2(c_1^2(c_1 + c_2) \\ &+ (c_2 + c_3)(c_1 + c_2)^2 + c_3(c_1 + c_2 + c_3)^2 + 2(c_1 + c_2 + c_3)^3]]h^4f''f'f^2 + O(h^5). \end{aligned}$$

Let $c_1 = c_3 = w_1/2, c_2 = w_0/2$ and compare the Taylor expansion (3) of the exact solution with the above one, we get the following equations

$$hf : c_1 + (c_1 + c_2) + (c_2 + c_3) + c_3 = 1 \Longleftrightarrow 2w_1 + w_0 = 1 \tag{10}$$

$$h^2 f'f : (c_1 + c_2)2c_1 + (c_2 + c_3)2(c_1 + c_2) + c_3 2(c_1 + c_2 + c_3) = 1/2 \tag{11}$$

$$h^3 f'' f^2, h^3 f'^2 f : (c_1 + c_2)2c_1^2 + (c_2 + c_3)2(c_1 + c_2)^2 + c_3 2(c_1 + c_2 + c_3)^2 = 1/6 \tag{12}$$

$$h^4 f''' f^3 : (c_1 + c_2)4/3c_1^3 + (c_2 + c_3)4/3(c_1 + c_2)^3 + c_3 4/3(c_1 + c_2 + c_3)^3 = 1/24 \tag{13}$$

$$\begin{aligned} h^4 f'^3 f : (c_1 + c_2)2c_1^3 &+ (c_1 + c_2)2(c_1^2 + c_2^2 + c_1c_2)(c_2 + c_3) + c_3 2[(c_1 + c_2)c_1^2 \\ &+ (c_2 + c_3)(c_1 + c_2)^2 + c_3(c_1 + c_2 + c_3)^2] = 1/24 \end{aligned} \tag{14}$$

$$\begin{aligned} &h^4 f'' f' f^2 : (c_1 + c_2)6c_1^3 + (c_2 + c_3)[4(c_1 + c_2)^3 + 2c_1^2(c_1 + c_2) + 2c_2(c_1 + c_2)^2] \\ &+ c_3 2[c_1^2(c_1 + c_2) + (c_2 + c_3)(c_1 + c_2)^2 + c_3(c_1 + c_2 + c_3)^2 + 2(c_1 + c_2 + c_3)^3] = 1/24\ . \end{aligned} \tag{15}$$

When $2w_1 + w_0 = 1$ holds, the equation (11) becomes identity, and the equations (12),(13), (14) and (15) become the same, that is $6w_1^3 - 12w_1^2 + 6w_1 - 1 = 0$. So we get the conditions for the difference scheme (3) to be of order 4

$$2w_1 + w_0 = 1, \quad 6w_1^3 - 12w_1^2 + 6w_1 - 1 = 0.$$

Thus we get $w_0 = -2^{1/3}/(2 - 2^{1/3}), w_1 = 1/(2 - 2^{1/3})$. So the scheme (1) with $c_1 = c_3 = w_1/2$, $c_2 = w_0/2$ is the 4th order scheme.

3. Construction for Systems of ODE's

In this section, we use the method of "trees and elementary differentials" given in [2]. We first rewrite the scheme (3) in the form of Runge-Kutta methods.

$$\begin{cases} g_1 = Z_0 \\ g_2 = Z_0 + c_1 hf(g_1) + c_1 hf(g_2) \\ g_3 = Z_0 + c_1 hf(g_1) + (c_1 + c_2)hf(g_2) + c_2 hf(g_3) \\ g_4 = Z_0 + c_1 hf(g_1) + (c_1 + c_2)hf(g_2) + (c_2 + c_3)hf(g_3) + c_3 hf(g_4) \\ Z = Z_0 + h(c_1 f(g_1) + (c_1 + c_2)f(g_2) + (c_2 + c_3)f(g_3) + c_3 f(g_4)) \end{cases} \tag{16}$$

where $g_2 = Z_1, g_3 = Z_2, g_4 = Z_3$, and $Z = Z_3$. So the Butcher tableau is

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 2c_1 & c_1 & c_1 & 0 & 0 \\ 2(c_1 + c_2) & c_1 & c_1 + c_2 & c_2 & 0 \\ 2(c_1 + c_2 + c_3) & c_1 & c_1 + c_2 & c_2 + c_3 & c_3 \\ \hline & c_1 & c_1 + c_2 & c_2 + c_3 & c_3 \end{array}$$

Using the order conditions for the scheme (16) of order 4, we get

$$\begin{cases} \sum_{j=1}^{4} b_j = 1 & \sum_{j=1}^{4} b_j \sum_{k,l,m=1}^{4} a_{jk}a_{jl}a_{jm} = \frac{1}{4} \\ \sum_{j=1}^{4} b_j \sum_{k=1}^{4} a_{jk} = \frac{1}{2} & \sum_{j=1}^{4} b_j \sum_{k,l,m=1}^{4} a_{jk}a_{kl}a_{jm} = \frac{1}{8} \\ \sum_{j=1}^{4} b_j \sum_{k,l=1}^{4} a_{jk}a_{jl} = \frac{1}{3} & \sum_{j=1}^{4} b_j \sum_{k,l,m=1}^{4} a_{jk}a_{kl}a_{km} = \frac{1}{12} \\ \sum_{j=1}^{4} b_j \sum_{k,l=1}^{4} a_{jk}a_{kl} = \frac{1}{6} & \sum_{j=1}^{4} b_j \sum_{k,l,m=1}^{4} a_{jk}a_{kl}a_{lm} = \frac{1}{24}. \end{cases} \tag{17}$$

Where b_j, a_{ij} are the elements of the vector b^T and the matrix A, respectively. As in section 1, let $c_1 = c_3 = w_1/2,\ c_2 = w_0/2$, from the first two equations of (17), we get an equivalent condition $2w_1 + w_0 = 1$. Using this condition, we can simplify the remaining equations of (17) and get a single equivalent condition $2w_1^3 + w_0^3 = 0$. These conditions are just the same as we got in section 1. (For details of Runge-Kutta methods and their order conditions, see [2] [3]).

4. Some Notes On The Construction

From [1], we know that the centered Euler scheme is symplectic and the scheme (18) is non-symplectic.

$$Z_{k+1} - Z_k = \frac{h}{2}(f(Z_k) + f(Z_{k+1})). \tag{18}$$

However, in this section we will see that through a non-linear transformation, $\xi_k = \rho(Z_k) = Z_k + h/2f(Z_k)$, $\xi_{k+1} = \rho(Z_{k+1}) = Z_{k+1} + h/2f(Z_{k+1})$. we can change (18) into the centered Euler scheme. So

$$\xi_k + \xi_{k+1} = Z_k + Z_{k+1} + h/2(f(Z_k) + f(Z_{k+1})).$$

Replace the last term by the right side of (18) hence $\xi_k+\xi_{k+1} = Z_k+Z_{k+1}+Z_{k+1}-Z_k = 2Z_{k+1}$, then $Z_{k+1} = \frac{\xi_k + \xi_{k+1}}{2}$. Noticing the second equation of transformation, we get $\xi_{k+1} = \frac{\xi_k + \xi_{k+1}}{2} + \frac{h}{2}f(\frac{\xi_k + \xi_{k+1}}{2}) \Longrightarrow \xi_{k+1} = \xi_k + hf(\frac{\xi_k + \xi_{k+1}}{2})$ and this is just the centered Euler scheme.

We can apply the "composing" method used in sections 1 and 2 to the centered Euler scheme since the scheme is equivalent to the RK method which has the Butcher-tableau

$$\begin{array}{r|ccc} d_1/2 & d_1/2 & 0 & 0 \\ d_1 + d_2/2 & d_1 & d_2/2 & 0 \\ d_1 + d_2 + d_3/2 & d_1 & d_2 & d_3/2 \\ \hline & d_1 & d_2 & d_3 \end{array}$$

Using the same method as in section 2, we can prove

$$\begin{cases} Z_1 = Z_0 + 1/(2-2^{1/3})hf((Z_0+Z_1)/2) \\ Z_2 = Z_1 + -2^{1/3}/(2-2^{1/3})hf((Z_1+Z_2)/2) \\ Z_3 = Z_2 + 1/(2-2^{1/3})hf((Z_2+Z_3)/2) \end{cases} \tag{19}$$

is a three-stage scheme of order 4.

In [5], schemes like (19) are got with the coefficients $d_1 = d_2 = 1/(2-2^{1/3}), \quad d_3 = -2^{1/3}/(2-2^{1/3})$. However, their schemes are of order 3. J.M. Sanz-Serna pointed out in [6] that, if the coefficients d_1, d_2, d_3 are symmetrically ordered with: $d_1 = d_3 = 1/(2-2^{1/3}), \quad d_2 = -2^{1/3}/(2-2^{1/3})$, the scheme can be of order 4, and we get the same conclusion here.

We have proved a general theorem on the construction of higher order schemes by composing lower order ones in [7]. The conclusion here serves as an example in that paper. At last, we should mention that our work is motivated by Haruo Yosida[4], he used the "composing" method to construct explicit symplectic integrators of higher order.

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