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Runge-Kutta Type Integration Formulas Including the Evaluation of the Second Derivative

Part I

By

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Introduction

We are concerning with theoretical study of numerical integration procedure for the initial-value problem of ordinary differential equation:

$$\text{(E)} \qquad \frac{dy}{dx}=f(x, y),$$

$$\text{(IV)} \qquad y(x_I)=y_I.$$

Many numerical analysts have been investigating the discrete variable methods for the problem. Consequently everyone can enjoy to solve numerically ordinary differential equation in almost all computing centers. It seems as if we got the *numerical integrator* through the use of the computer. But the study is yet continued for "better" numerical procedure.

Among the one-step methods, *Runge-Kutta methods* (RK methods, in short) are popular because of the high accuracy and the feasibility of changing step-size. In general the methods are expressed as follows. The solution of (E) at x_0+h is approximated by

$$y_1=y_0+h\sum_{i=1}^{p}\mu_i k_i,$$

where

$$(*) \qquad \begin{aligned} &k_1=f(x_0, y_0),\\ &k_i=f(x_0+\alpha_i h,\ y_0+h\sum_{j=1}^{i-1}\beta_{ij}k_j), \quad i=2,\dots, p, \end{aligned}$$

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h is the step-size and y_0 is the approximated value at x_0. This type of the method is called (explicit) p-stage Runge-Kutta algorithm. According to the choice of the stage number p and the parameters α_i, β_{ij}, μ_i we have many variations, among which the classical Runge-Kutta method or the Runge-Kutta-Fehlberg method is famous. A distinguished contribution for the study of the Runge-Kutta methods has been made by J. C. BUTCHER ([1] ~ [4]). He determined the attainable order of the RK methods up to 10-stage formula. On the other hand he introduced the semi-explicit (the summation is up to i instead of $i-1$ in (*)) or implicit (the summation is up to p in (*)) formula.

RK methods (and perhaps many other quadrature formulas for the initial-value problem) are constructed on the principle that the required function evaluation is only for $f(x, y)$, i.e. the first derivative of the solution. It is quite natural because we are acquainted with the functional form of the first derivative in the ordinary differential equation. Recently, however, some propositions have been made to employ the function evaluation of the *second derivative* of the solution. Functional form of it is given by

$$g(x, y)=f_x(x, y)+f_y(x, y)f(x, y).$$

M. URABE [15] made a first attempt to employ $g(x, y)$ by presenting an implicit one-step method with step-size control strategy. Let y_0 and y_{-1} be approximations of $y(x)$ at x_0 and x_0-h, respectively. His algorithm employs the predictor given by

$$\hat{y}_1=-31y_{-1}+32y_0-h(14f_{-1}+16f_0)+h^2(-2g_{-1}+4g_0)$$

and the corrector given by

$$\begin{aligned} y_0=y_{-1}&+\frac{h}{240}(101f_{-1}+128f_0+11\hat{f}_1) \\ &+\frac{h^2}{240}(13g_{-1}-40g_0-3\hat{g}_1), \end{aligned}$$

where $f_i=f(x_0+ih, y_i)$, $g_i=f(x_0+ih, y_i)$, $\hat{f}_1=f(x_0+h, \hat{y}_1)$ and $\hat{g}_1=g(x_0+h, \hat{y}_1)$. Succeeding his result, J. R. CASH [5] has considered this type of formula more generally and made some stability analysis. On the other hand H. SHINTANI [12], [13] has proposed some formulas analogous to RK formula employing one evaluation for $f(x, y)$ and some for $g(x, y)$. He has given the values of the parameters appearing in the formulas up to the order 7. His results, closely related to the present work, will be mentioned afterward.

In this context another type of integration formula, for the origination of which H. H. ROSENBROCK [11] is given credit, is now being developed. It employs the partial derivative $f_y(x, y)$ and is reported to have good stability for stiff systems of ordinary differential equations ([7], [9]).

Here we shall examine an explicit (p, q)-stage Runge-Kutta type formula including the second derivative. It requires p times evaluations for the first derivative and q times for the second derivative in a similar manner for RK methods. We are interested in the following problems.

(1) What is the attainable order of the (p, q)-stage formula from the viewpoint of its local accuracy?

(2) How are the parameters in the formula determined?

(3) What formula is good for practical use?

These problems will be solved in the following sections and the forthcoming paper by the author. The present paper is especially devoted to investigate the $(1, q)$-stage formulas.

First, we shall define explicit (p, q)-stage formula. Next, some algebraic computations are carried out to investigate (p, q)-stage formulas. Here SAM software is used as a powerful tool. Then, the attainable order of $(1, q)$-stage formula is determined up to $q=4$.

Remark. In the case of very complicated functional form of $f(x, y)$ in higher dimension, the calculation of the second derivative $g(x, y)$ requires a laborious work. It is the main reason why the methods employing $g(x, y)$ have not been considered. But the recent development of the symbolic and algebraic manipulation (SAM) software brings the change of the situation. SAM software, for example, REDUCE-2 or MACSYMA, is now a helpful tool for mathematical sciences. In fact, some SAM program may print expressions in a FORTRAN notation so that one can carry out the calculation of the second derivative from $f(x, y)$ in an automatic way. Once after algebraic computation we may call $g(x, y)$ as a FUNCTION subprogram.

Moreover, SAM software is very useful for the theoretical study of the RK and its analogous methods. For example, H. TODA [14] has considered 5-stage RK limiting formula of order 5. He has utilized MACSYMA essentially. We shall also attempt to apply SAM for our study.

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§ 1.1. Explicit (*p*, *q*)-Stage Formula

We shall discuss numerical integration procedure for the initial-value problem of ordinary differential equation:

$$\frac{dy}{dx}=f(x, y), \tag{1.1.1}$$

$$y(x_I)=y_I. \tag{1.1.2}$$

Here f is sufficiently smooth with respect to x and y. Let us define an explicit (p, q)-stage Runge-Kutta type formula including the second derivative of the solution. Let g stand for the second derivative of $y(x)$,

$$g(x, y)=f_x(x, y)+f_y(x, y)f(x, y). \tag{1.1.3}$$

Explicit (p, q)-stage formula is given as follows.

$$y_{n+1}=y_n+h\sum_{i=1}^{p}\mu_i k_i+h^2\sum_{i=1}^{q}\nu_i K_i, \qquad n=0, 1, 2,\dots, \tag{1.1.4}$$

where

$$\begin{cases} k_1=f(x_n+\alpha_1 h,\ y_n), \\ k_i=f(x_n+\alpha_i h,\ y_n+h\sum_{j=1}^{i-1}\beta_{ij}k_j+h^2\sum_{j=1}^{i-1}\gamma_{ij}K_j), \qquad i=2,\dots, p, \end{cases} \tag{1.1.5}$$

$$\begin{cases} K_1=g(x_n+\rho_1 h,\ y_n+h\sigma_{11}k_1), \\ K_i=g(x_n+\rho_i h,\ y_n+h\sum_{j=1}^{i}\sigma_{ij}k_j+h^2\sum_{j=1}^{i-1}\tau_{ij}K_j), \qquad i=2,\dots, q. \end{cases} \tag{1.1.6}$$

Remark 1. The parameters μ_i, ν_i, α_i, β_{ij}, γ_{ij}, ρ_i, σ_{ij} and τ_{ij} are, of course, real numbers.

Remark 2. In the case of simultaneous equations in (1), y and f are considered vectors of the same dimension. Then $f_y(x, y)$, the Jacobian matrix of f, is given in the matrix form. For example, assume that

$$f(x, y)=\begin{pmatrix} f_1(y_1, y_2) \\ f_2(y_1, y_2) \end{pmatrix}=\begin{pmatrix} (a_1-b_1y_2)y_1 \\ (a_2-b_2y_1)y_2 \end{pmatrix}$$

where a_i and b_i are constants, then

$$f_y(x, y)=\begin{pmatrix} a_1-b_1y_2 & -b_1y_1 \\ -b_2y_2 & a_2-b_2y_1 \end{pmatrix}$$

and

$$g(x, y)=\begin{pmatrix} a_1^2y_1+(b_2y_1+b_1y_2-2a_1-a_2)b_1y_1y_2 \\ a_2^2y_2+(b_2y_1+b_1y_2-a_1-2a_2)b_2y_1y_2 \end{pmatrix}.$$

Similar to the RK formulas, the determining equations and the parameters are possible to be slightly different between the single differential equation and the systems of equations. For convenience sake we shall investigate the single case. The attainable order of the formula is not depend on whether (1) is single or system.

§ 1.2. The Taylor Series Expansion of the Solution

To investigate Runge-Kutta type methods of higher order, we are required to represent the solution $y(x_0+h)$ for (E) and (IV) in Section 1.1 into the power series of the stepsize h. For our quadrature formula it is preferable to represent the solution into the power series utilizing the second derivative g.

Twice integration after differentiation for the equation

$$\frac{dy}{dx}=f(x, y), \qquad x\geqq x_0$$

implies the formula

$$\text{(1.2.1)} \qquad \int_{x_0}^{x_0+h}\left\{\int_{x_0}^{t}\frac{d^2y(x)}{dx^2}\,dx\right\}dt=\int_{x_0}^{x_0+h}\left\{\int_{x_0}^{t}g(x, y(x))dx\right\}dt\,.$$

The left-hand side of the above formula is equal to

$$\begin{aligned} &y(x_0+h)-y(x_0)-hf(x_0, y(x_0)) \\ &=y(x_0+h)-y_0-hf_0\,. \end{aligned}$$

Hereafter the subscript 0 stands for the evaluation at $x=x_0$ and $y=y_0$.

The right-hand side of (1) becomes

$$\int_0^h\left\{\int_{x_0}^{x_0+\xi}g(x, y(x))dx\right\}d\xi=\int_0^h\left\{\int_0^{\xi}g(x_0+\zeta, y(x_0+\zeta))d\zeta\right\}d\xi.$$

Then, assume that for $0 \leqq \zeta \leqq h$, $y(x_0+\zeta)$ can be expanded in the power series of ζ by

$$(1.2.2) \qquad y(x_0+\zeta)=y_0+\zeta f_0+\sum_{r=2}^{m}\frac{\kappa_{r-2}}{r!}\zeta^r+O(\zeta^{m+1}),$$

where κ_j $(j=1, 2,\dots, m)$ is the coefficient to be determined later. Substitution (2) into the integrand implies

$$\begin{aligned} g(x_0+\zeta, y(x_0+\zeta)) &= g(x_0+\zeta, y_0+\zeta f_0+\sum_{r=0}^{m}\frac{\kappa_{r-2}}{r!}\zeta^r+O(\zeta^{m+1})) \\ &= \sum_{l=0}^{m}\frac{1}{l!}\left[\left(\zeta\frac{\partial}{\partial x}+\left(\zeta f_0+\sum_{r=0}^{m}\frac{\kappa_{r-2}}{r!}\zeta^r\right)\frac{\partial}{\partial y}\right)^l g\right]_0+O(\zeta^{m+1}) \\ &= \sum_{l=0}^{m}\frac{\zeta^l}{l!}\left[\left(D_0+\left(\sum_{r=2}^{m}\frac{\kappa_{r-2}}{r!}\zeta^{r-1}\right)\frac{\partial}{\partial y}\right)^l g\right]_0+O(\zeta^{m+1}) \\ &= \sum_{l=0}^{m}\frac{\zeta^l}{l!}\left\{\sum_{k=0}^{l}\binom{l}{k}\left(\sum_{r=1}^{m-1}\frac{\kappa_{r-1}}{(r+1)!}\zeta^r\right)^k \right. \\ &\qquad \left. \times\left[D_0^{l-k}\left(\frac{\partial}{\partial y}\right)^k g\right]_0\right\}+O(\zeta^{m+1}). \end{aligned}$$

Here D_0 is a differential operator defined by

$$D_0=\frac{\partial}{\partial x}+f_0\frac{\partial}{\partial y}.$$

Therefore we have the following equation:

$$\begin{aligned} (1.2.3) \quad & y_0+hf_0+\sum_{r=2}^{m+2}\frac{\kappa_{r-2}}{r!}\zeta^r=y_0+hf_0+ \\ & +\int_0^h\left(\int_0^\xi\sum_{l=0}^{m}\frac{\zeta^l}{l!}\left\{\sum_{k=0}^{l}\binom{l}{k}\left(\sum_{r=1}^{m-1}\frac{\kappa_{r-1}}{(r+1)!}\zeta^r\right)^k\left[D_0^{l-k}\left(\frac{\partial}{\partial y}\right)g\right]_0\right\}d\zeta\right)d\xi, \end{aligned}$$

which determines κ_j recurrently.

Twice differentiation for (3) with respect to h implies

$$(1.2.4) \quad \sum_{l=0}^{m}\frac{\kappa_l}{l!}h^l=\sum_{l=0}^{m}\frac{h^l}{l!}\left\{\sum_{k=0}^{l}\binom{l}{k}\left(\sum_{r=1}^{m-1}\frac{\kappa_{r-1}}{(r+1)!}h^r\right)^k\left[D_0^{l-k}\left(\frac{\partial}{\partial y}\right)^k g\right]_0\right\}.$$

Then, we have the following important result.

Theorem 1. *The coefficient κ_l $(l=0, 1,\dots, m)$ is determined by the following way*:

$$(1.2.5) \quad \begin{cases} \kappa_0=g_0. \\ \kappa_l=[D_0^l g]_0+\displaystyle\sum_{s=1}^{l-1}\left\{\sum_{t=1}^{m(l,s)}\frac{l!}{s!(l-s-t)!}\right. \\ \qquad \left.\times B_{s,t}\left(\dfrac{\kappa_0}{2}, \dfrac{\kappa_1}{3},\dots, \dfrac{\kappa_{s-1}}{s+1}\right)\left[D_0^{l-s-t}\left(\dfrac{\partial}{\partial y}\right)^t g\right]_0\right\}, \\ \qquad\qquad\qquad \textit{for} \quad l=1, 2,\dots, m. \end{cases}$$

Here $B_{s,t}(x_1, x_2,\dots, x_s)$ *is the multivariable polynomial of E. T. Bell of the order* (s, t) *and*

$$\mathrm{m}(l, s)\equiv\min(s, l-s).$$

Note. κ_j appeared in the summation of the right-hand side of (5) is for j less than or equal to $l-2$ so that we can determine κ_l recurrently by the formula.

Proof. $\kappa_0=g_0$ is clear. Let us introduce two functions $G(h)$ and $A(h;\, l)$ as follows:

$$(1.2.6)\qquad G(h)=\sum_{r=1}^{m-1}\frac{\kappa_{r-1}}{(r+1)!}h^r,$$

$$(1.2.7)\qquad A(h;l)=\sum_{k=0}^{l}\binom{l}{k}\{G(h)\}^k\left[D_0^{l-k}\left(\frac{\partial}{\partial y}\right)^k g\right]_0,\ l=0, 1,\dots, m.$$

Note that $G(h)$ is of the order h and $G(0)=0$ holds. Then, the right-hand side of (4) is equal to $\sum_{s=0}^{m}\frac{A(h;\, s)}{s!}h^s$.

Hence, we have the equation

$$(1.2.8)\qquad \sum_{l=0}^{m}\frac{\kappa_l}{l!}h^l=\sum_{s=0}^{m}\frac{A(h;s)}{s!}h^s.$$

For an integer l such that $1\leqq l\leqq m$, l-times differentiation to (8) with respect to h implies

$$(1.2.9)\qquad \kappa_l=\sum_{s=0}^{l-1}\binom{l}{s}A^{(s)}(0;\, l-s).$$

By (7), the equation

$$A(0;\, l)=[D_0^l g]_0$$

is clear. For $s\geqq 1$, we have from (7)

$$\begin{aligned}A^{(s)}(h;\, l-s)=&\binom{l-s}{1}G^{(s)}(h)[D_0^{l-s-1}g_y]_0\\&+\binom{l-s}{2}\frac{d^s}{dh^s}\{G(h)\}^2[D_0^{l-s-2}g_{yy}]_0+\cdots\\&+\binom{l-s}{k}\frac{d^s}{dh^s}\{G(h)\}^k\left[D_0^{l-s-k}\left(\frac{\partial}{\partial y}\right)^k g\right]_0+\cdots\\&+\frac{d^s}{dh^s}\{G(h)\}^{l-s}\left[\left(\frac{\partial}{\partial y}\right)^{l-s}g\right]_0.\end{aligned}$$

For higher derivatives of composite functions, the formula employing the Bell polynomial is known (J. RIORDAN [10]). Hence, applying the formula, we have for $k=1, 2, \ldots, l-s$

$$\frac{d^s}{dh^s}\{G(h)\}^k = \sum_{t=1}^{\min(s,k)} \frac{k!}{(k-t)!} B_{s,t}(G'(h), G''(h), \ldots, G^{(s)}(h)) \times \{G(h)\}^{k-t},$$

which implies

$$\left[\frac{d^s}{dh^s}\{G(h)\}^k\right]_{h=0} = \begin{cases} k!B_{s,k}(G'(0), G''(0), \ldots, G^{(s)}(0)) & \text{for } s \geqq k, \\ 0 & \text{for } s < k. \end{cases}$$

From (6), the equation

$$G^{(s)}(h) = \sum_{r=s}^{m-1} \frac{r!}{(r-s)!} \frac{\kappa_{r-1}}{(r+1)!} h^{r-s} = \sum_{r=s}^{m-1} \frac{\kappa_{r-1}}{(r+1)!(r-s)!} h^{r-s}$$

holds. Hence we have

$$G^{(s)}(0) = \frac{\kappa_{s-1}}{s+1}, \qquad s=1, 2, \ldots, m-1.$$

Then $A^{(s)}(0; l-s)$ is given by

$$\begin{aligned} A^{(s)}(0, l-s) &= \sum_{k=1}^{\mathrm{m}(l,s)} \binom{l-s}{k} k!B_{s,t}(G'(0), \ldots, G^{(s)}(0)) \left[D_0^{l-s-k}\left(\frac{\partial}{\partial y}\right)^k g\right]_0 \\ &= \sum_{t=1}^{\mathrm{m}(l,s)} \frac{(l-s)!}{(l-s-t)!} B_{s,t}\left(\frac{\kappa_0}{2}, \frac{\kappa_1}{3}, \ldots, \frac{\kappa_{s-1}}{s+1}\right)\left[D_0^{l-s-t}\left(\frac{\partial}{\partial y}\right)^t g\right]_0, \end{aligned}$$

which implies from (9)

$$\begin{aligned} \kappa_l &= [D_0^l g]_0 + \sum_{s=1}^{l-1} \binom{l}{s} \left\{ \sum_{t=1}^{\mathrm{m}(l,s)} \frac{(l-s)!}{(l-s-t)!} B_{s,t}\left(\frac{\kappa_0}{2}, \frac{\kappa_1}{3}, \ldots, \frac{\kappa_{s-1}}{s+1}\right) \right. \\ &\qquad \left. \times \left[D_0^{l-s-t}\left(\frac{\partial}{\partial y}\right)^t g\right]_0 \right\} \\ &= [D_0^l g]_0 + \sum_{s=1}^{l-1} \left\{ \sum_{t=1}^{\mathrm{m}(l,s)} \frac{l!}{s!(l-s-t)!} B_{s,t}\left(\frac{\kappa_0}{2}, \frac{\kappa_1}{3}, \ldots, \frac{\kappa_{s-1}}{s+1}\right) \right. \\ &\qquad \left. \times \left[D_0^{l-s-t}\left(\frac{\partial}{\partial y}\right)^t g\right]_0 \right\}. \end{aligned}$$

This is the desired result. □

The multivariable polynomial $B_{s,t}(x_1, x_2, \ldots, x_s)$ has a recurrence formula to calculate it conveniently by the application of any SAM software. That is,

$$\sum_{t=1}^{s} x_1 B_{s,t}(x_1,\dots, x_s)a^{t+1} + \sum_{t=1}^{s}\left(\sum_{k=1}^{s} x_{k+1}\frac{\partial B_{s,t}}{\partial x_k}\right)a^t$$
$$= \sum_{t=1}^{s+1} B_{s+1,t}(x_1,\dots, x_{s+1})a^t .$$

Here, the both sides of the formula is considered as a polynomial of a. The recurrence formula for $B_{s,t}$ will be employed during the calculations of κ_l by REDUCE-2.

Theorem 1 tells us a concrete method to determine the Taylor series expansion (2) employing the second derivative. For example,

$$\kappa_1 = [D_0 g]_0 ,$$
$$\kappa_2 = [D_0^2 g]_0 + 2!B_{1,1}\left(\frac{\kappa_0}{2}\right)g_{y,0} = [D_0^2 g]_0 + \kappa_0 g_{y,0} = [D_0^2 g]_0 + g_0 g_{y,0} ,$$
$$\kappa_3 = [D_0^3 g]_0 + 3!B_{1,1}\left(\frac{\kappa_0}{2}\right)[D_0 g_y]_0 + \frac{3!}{2!}B_{2,1}\left(\frac{\kappa_0}{2}, \frac{\kappa_1}{3}\right)g_{y,0}$$
$$= [D_0^3 g]_0 + 3\kappa_0[D_0 g_y]_0 + \kappa_1 g_{y,0}$$
$$= [D_0^3 g]_0 + 3g_0[D_0 g_y]_0 + [D_0 g]_0 g_{y,0} .$$

We may also carry out the process by the SAM software up to the desired order. The result by REDUCE-2 is shown in Table 1.

Note that because of Remark 2 in the preceding section we do not care the order of the higher partial derivatives.

Another important result from Theorem 1 is that any κ_j is a summation of an integer multiple of some product of $[D_0^p(\partial/\partial y)^q g]_0$. Hence, we shall call any product of $[D_0^p(\partial/\partial y)^q g]_0$ an *elementary differential* of g. J. C. BUTCHER [1] has used the terminology of elementary differential in a different sense. However, our study of the expression of the coefficient of Taylor series in the elementary differentials is on the similar point of view.

In fact, the way of the proof of Theorem 1 is applicable to the Taylor series expansion of $y(x_0+h)$ employing the first derivative.

Theorem 2. *Assume that*

$$y(x_0+h) = y_0 + \sum_{r=1}^{m}\frac{\lambda_{r-1}}{r!}h^r + O(h^{m+1}) . \tag{1.2.10}$$

Then, the coefficient λ_l $(l=0, 1,\dots, m-1)$ *is determined by*

$$(1.2.11)\qquad \begin{cases} \lambda_0 = f_0 \\ \lambda_l = [D_0^l f]_0 + \sum_{s=1}^{l-1} \left\{ \sum_{t=1}^{m(l,s)} \frac{l!}{(l-s-t)!s!} \right. \\ \qquad \left. \times B_{s,t}\left(\frac{\lambda_1}{2}, \frac{\lambda_2}{3}, \dots, \frac{\lambda_s}{s+1}\right)\left[D_0^{l-s-t}\left(\frac{\partial}{\partial y}\right)^t f\right]_0 \right\}, \\ \qquad l = 1, 2, \dots, m. \end{cases}$$

We shall call (10) the first type power series expansion in contrast with (2) which will be mentioned as the second type expansion.

Table 1.

$\kappa_0 = g_0$

$\kappa_1 = [D_0 g]_0$

$\kappa_2 = [D_0^2 g]_0 + g_0 \cdot g_{y,0}$

$\kappa_3 = [D_0^3 g]_0 + [D_0 g]_0 \cdot g_{y,0} + 3g_0 \cdot [D_0 g_y]_0$

$\kappa_4 = [D_0^4 g]_0 + [D_0^2 g]_0 \cdot g_{y,0} + 4[D_0 g]_0 \cdot [D_0 g_y]_0 + 6g_0 \cdot [D_0^2 g_y]_0 + g_0 \cdot g_{y,0}^2$
$\quad + 3g_0^2 \cdot g_{yy,0}$

$\kappa_5 = [D_0^5 g]_0 + [D_0^3 g]_0 \cdot g_{y,0} + 5[D_0^2 g]_0 \cdot [D_0 g_y]_0 + 10[D_0 g]_0 \cdot [D_0^2 g_y]_0$
$\quad + 10g_0 \cdot [D_0^3 g_y]_0 + [D_0 g]_0 \cdot g_{y,0}^2 + 8g_0 \cdot g_{y,0} \cdot [D_0 g_y]_0 + 10g_0 \cdot [D_0 g]_0 \cdot g_{yy,0}$
$\quad + 15g_0^2 \cdot [D_0 g_{yy}]_0$

$\kappa_6 = [D_0^6 g]_0 + [D_0^4 g]_0 \cdot g_{y,0} + 6[D_0^3 g]_0 \cdot [D_0 g_y]_0 + 15[D_0^2 g]_0 \cdot [D_0^2 g_y]_0$
$\quad + 20[D_0 g]_0 \cdot [D_0^3 g_y]_0 + 15g_0 \cdot [D_0^4 g_y]_0 + [D_0^2 g]_0 \cdot g_{y,0}^2 + 18g_0 \cdot [D_0 g_y]_0^2$
$\quad + 10[D_0 g]_0 \cdot g_{y,0} \cdot [D_0 g_y]_0 + 21g_0 \cdot g_{y,0} \cdot [D_0^2 g_y]_0 + 10[D_0 g]_0^2 \cdot g_{yy,0}$
$\quad + 15g_0 \cdot [D_0^2 g]_0 \cdot g_{yy,0} + 60g_0 \cdot [D_0 g]_0 \cdot [D_0 g_{yy}]_0 + 45g_0^2 \cdot [D_0^2 g_{yy}]_0$
$\quad + g_0 \cdot g_{y,0}^3 + 18g_0^2 \cdot g_{y,0} \cdot g_{yy,0} + 15g_0^3 \cdot g_{yyy,0}$

$\kappa_7 = [D_0^7 g]_0 + [D_0^5 g] \cdot g_{y,0} + 7[D_0^4 g]_0 \cdot [D_0 g_y]_0 + 21[D_0^3 g]_0 \cdot [D_0^2 g_y]_0$
$\quad + [D_0^3 g]_0 \cdot g_{y,0}^2 + 35[D_0^2 g]_0 \cdot [D_0^3 g_y]_0 + 12[D_0^2 g]_0 \cdot g_{y,0} \cdot [D_0 g_y]_0$
$\quad + 35[D_0 g]_0 \cdot [D_0^4 g_y]_0 + 28[D_0 g]_0 \cdot [D_0 g_y]_0^2 + 31[D_0 g]_0 \cdot g_{y,0} \cdot [D_0^2 g_y]_0$
$\quad + [D_0 g]_0 \cdot g_{y,0}^3 + 35[D_0 g]_0 \cdot [D_0^2 g]_0 \cdot g_{yy,0} + 70[D_0 g]_0^2 \cdot [D_0 g_{yy}]_0$
$\quad + 21g_0 \cdot [D_0^5 g_y]_0 + 105g_0 \cdot [D_0 g_y]_0 \cdot [D_0^2 g_y]_0 + 45g_0 \cdot g_{y,0} \cdot [D_0^3 g_y]_0$
$\quad + 15g_0 \cdot g_{y,0}^2 \cdot [D_0 g_y]_0 + 21g_0 \cdot [D_0^3 g]_0 \cdot g_{yy,0} + 105g_0 \cdot [D_0^2 g]_0 \cdot [D_0 g_{yy}]_0$
$\quad + 210g_0 \cdot [D_0 g]_0 \cdot [D_0^2 g_{yy}]_0 + 66g_0 \cdot [D_0 g]_0 \cdot g_{y,0} \cdot g_{yy,0} + 105g_0^2 \cdot [D_0^3 g_{yy}]_0$
$\quad + 84g_0^2 \cdot [D_0 g_y]_0 \cdot g_{yy,0} + 120g_0^2 \cdot g_{y,0} \cdot [D_0 g_{yy}]_0 + 105g_0^2 \cdot [D_0 g]_0 \cdot g_{yyy,0}$
$\quad + 105g_0^3 \cdot [D_0 g_{yyy}]_0$

$\kappa_8 = [D_0^8 g]_0 + [D_0^6 g]_0 \cdot g_{y,0} + 8[D_0^5 g]_0 \cdot [D_0 g_y]_0 + 28[D_0^4 g]_0 \cdot [D_0^2 g_y]_0$
$\quad + [D_0^4 g]_0 \cdot g_{y,0}^2 + 56[D_0^3 g]_0 \cdot [D_0^3 g_y]_0 + 14[D_0^3 g]_0 \cdot g_{y,0} \cdot [D_0 g_y]_0$

$$
\begin{aligned}
&+70[D_0^2g]_0\cdot[D_0^4g_y]_0+40[D_0^2g]_0\cdot[D_0g_y]_0^2+43[D_0^2g]_0\cdot g_{y,0}\cdot[D_0^2g_y]_0\\
&+[D_0^2g]\cdot g_{y,0}^3+35[D_0^2g]_0^2\cdot g_{yy,0}+56[D_0g]_0\cdot[D_0^5g_y]_0\\
&+192[D_0g]_0\cdot[D_0g_y]_0\cdot[D_0^2g_y]_0+76[D_0g]_0\cdot g_{y,0}\cdot[D_0^3g_y]_0\\
&+18[D_0g]_0\cdot g_{y,0}^2\cdot[D_0g_y]_0+56[D_0g]_0\cdot[D_0^3g]_0\cdot g_{yy,0}\\
&+280[D_0g]_0\cdot[D_0^2g]_0\cdot[D_0g_{yy}]_0+280[D_0g]_0^2\cdot[D_0^2g_{yy}]_0\\
&+66[D_0g]_0^2\cdot g_{y,0}\cdot g_{yy,0}+28g_0\cdot[D_0^6g_y]_0+168g_0\cdot[D_0^2g_y]_0^2\\
&+248g_0\cdot[D_0g_y]_0\cdot[D_0^3g_y]_0+85g_0\cdot g_{y,0}\cdot[D_0^4g_y]_0+82g_0\cdot g_{y,0}\cdot[D_0g_y]_0^2\\
&+49g_0\cdot g_{y,0}^2\cdot[D_0^2g_y]_0+g_0,\ g_{y,0}^4+28g_0\cdot[D_0^4g]_0\cdot g_{yy,0}\\
&+168g_0\cdot[D_0^3g]_0\cdot[D_0g_{yy}]_0+420g_0\cdot[D_0^2g]_0\cdot[D_0^2g_{yy}]_0\\
&+113g_0\cdot[D_0^2g]_0\cdot g_{y,0}\cdot g_{yy,0}+560g_0\cdot[D_0g]_0\cdot[D_0^3g_{yy}]_0\\
&+360g_0\cdot[D_0g]_0\cdot[D_0g_y]_0\cdot g_{yy,0}+508g_0\cdot[D_0g]_0\cdot g_{y,0}\cdot[D_0g_{yy}]_0\\
&+280g_0\cdot[D_0g]_0^2\cdot g_{yyy,0}+210g_0^2\cdot[D_0^4g_{yy}]_0\\
&+252g_0^2\cdot[D_0^2g_y]_0\cdot g_{yy,0}+624g_0^2\cdot[D_0g_y]_0\cdot[D_0g_{yy}]_0\\
&+465g_0^2\cdot g_{y,0}\cdot[D_0^2g_{yy}]_0+81g_0^2\cdot g_{y,0}^2\cdot g_{yy,0}+210g_0^2\cdot[D_0^2g]_0\cdot g_{yyy,0}\\
&+840g_0^2\cdot[D_0g]_0\cdot[D_0g_{yyy}]_0+420g_0^3\cdot[D_0^2g_{yyy}]_0+84g_0^3\cdot g_{yy,0}^2\\
&+225g_0^3\cdot g_{y,0}\cdot g_{yyy,0}+105g_0^4\cdot g_{yyyy,0}
\end{aligned}
$$

§ 1.3. Implicit (1, q)-Stage Formula

For the study of the general (1, q)-stage formula, it is convenient to analyse the corresponding implicit (1, q)-stage formula, because we gain an insight into its algebraic relations by them.

Consider an implicit (1, q)-stage formula as follows:

$$y_{n+1}=y_n+\mu_1 hk_1+\sum_{i=1}^{q}\nu_i h^2K_i, \qquad n=0,\ 1,\ 2,\dots, \tag{1.3.1}$$

$$\begin{cases} k_1=f(x_n+\alpha_1 h,\ y_0), \\ K_i=g(x_n+\rho_i h,\ y_n+\sigma_{i1}hk_1+\sum_{j=1}^{q}\tau_{ij}h^2K_j), \qquad i=1,\dots,q\,. \end{cases} \tag{1.3.2}$$

We need to analyse one-step integration by (1) and (2), so we may substitute $n=0$, i.e.

$$\begin{cases} y_1=y_0+\mu_1 hk_1+\sum_{i=1}^{q}\nu_i h^2K_i, \\ k_1=f(x_0+\alpha_1 h,\ y_0), \\ K_i=g(x_0+\rho_i h,\ y_0+\sigma_{i1}hk_1+\sum_{j}\tau_{ij}h^2K_j), \qquad i=1,\dots,q. \end{cases} \tag{1.3.3}$$

For k_1, we have the following expansion:

$$k_1=f_0+\alpha_1 hf_{x,0}+\frac{1}{2}\alpha_1^2h^2f_{xx,0}+O(h^3).$$

On the other hand, K_i has the expansion

$$K_i=g_0+O(h).$$

Hence, the equation

$$y_1=y_0+\mu_1 hf_0+h^2(\mu_1\alpha_1 f_{x,0}+\sum_{i=1}^{q}\nu_i g_0)+O(h^3) \tag{1.3.4}$$

holds. The solution $y(x_0+h)$ has the power series of h as follows:

$$y(x_0+h)=y_0+hf_0+\frac{1}{2}h^2g_0+O(h^3). \tag{1.3.5}$$

Comparison of the terms having the same power of h in (4) and (5) yields the following equations.

$$\mu_1=1,$$
$$\mu_1\alpha_1 f_{x,0}+\sum_{i=1}^{q}\nu_i g_0=\frac{1}{2}g_0.$$

Thus, $\mu_1=1$, $\alpha_1=0$ and $\sum_{i=1}^{q}\nu_i=1/2$ must hold in the implicit $(1, q)$-stage formula.

Next, since K_i has the expansion

$$K_i=g_0+\left[\left(\rho_i\frac{\partial}{\partial x}+\sigma_{i1}f_0\frac{\partial}{\partial y}\right)g\right]_0\cdot h+O(h^2),$$

the comparison of the third order term of y_1 and $y(x_0+h)$ implies the equation

$$\frac{1}{2}[D_0g]_0=\frac{1}{2}(g_{x,0}+f_0\cdot g_{y,0})=\sum_{i=1}^{q}\nu_i[(\rho_i g_{x,0}+\sigma_{i1}f_0\cdot g_{y,0})].$$

From the viewpoint of homogenuity of differential operation, $\rho_i=\sigma_{i1}$ must hold for $i=1, 2,\dots, q$.

Hence, let us rewrite (3) by

$$\begin{cases} y_1=y_0+hf_0+\sum_{i=1}^{q}\nu_i h^2K_i, \\ K_i=g(x_0+\rho_i h,\ y_0+\rho_i hf_0+\sum_j \tau_{ij}h^2K_j), \qquad i=1,\dots, q. \end{cases} \tag{1.3.6}$$

We shall assume the Taylor series expansion for K_i by

$$K_i=\sum_{l=0}^{m}\frac{\kappa_{il}}{l!}h^l+O(h^{m+1}), \tag{1.3.7}$$

where κ_{il} will be determined by the similar manner for Theorem 1.

Theorem 3. *For each i, κ_{il} in (1.3.7) is determined by the following:*

$$(1.3.8)\quad \begin{cases} \kappa_{i0}=g_0, \\ \kappa_{il}=\rho_i^l[D_0^l g]_0+\sum_{s=1}^{l-1}\left\{\sum_{t=1}^{m(l,s)}\frac{l!}{s!(l-s-t)!}\rho_i^{l-s-t}\right. \end{cases}$$

$$\left.\times B_{s,t}\Big(\sum_{j=1}^{q}\tau_{ij}\kappa_{j0},\dots,s\sum_j\tau_{ij}\kappa_{j,s-1}\Big)\left[D_0^{l-s-t}\left(\frac{\partial}{\partial y}\right)^t g\right]_0\right\},$$
$$l=1,2,\dots,m.$$

Note. By the above formula, κ_{il} can be determined in the ascending order of the second subscript, i.e., κ_{i2} $(i=1,\dots,q)$ after κ_{i1}, κ_{i3} $(i=1,\dots,q)$ after κ_{i2}, and so on.

Proof. Two-variable Taylor series expansion for K_i gives

$$K_i=\sum_{l=0}^{m}\frac{1}{l!}\left[\left\{\rho_i h\frac{\partial}{\partial x}+(\rho_i hf_0+\sum\tau_{ij}h^2K_j)\frac{\partial}{\partial y}\right\}^l g\right]_0+O(h^{m+1})$$
$$=\sum_{l=0}^{m}\frac{h^l}{l!}\left[\left\{\rho_i D_0+(\sum\tau_{ij}hK_j)\frac{\partial}{\partial y}\right\}^l g\right]_0+O(h^{m+1})$$
$$=\sum_{l=0}^{m}\frac{h^l}{l!}\left[\left\{\rho_i D_0+\left(\sum_{r=0}^{m-1}\left(\sum_{j=1}^{q}\frac{\tau_{ij}\kappa_{jr}}{r!}\right)h^{r+1}\right)\frac{\partial}{\partial y}\right\}^l g\right]_0+O(h^{m+1})$$
$$=\sum_{l=0}^{m}\frac{h^l}{l!}\left\{\sum_{k=0}^{l}\binom{l}{k}\rho_i^{l-k}\left(\sum_{r=0}^{m-1}\left(\sum_j\frac{\tau_{ij}\kappa_{jr}}{r!}\right)h^{r+1}\right)^k\left[D_0^{l-k}\left(\frac{\partial}{\partial y}\right)^k g\right]_0\right\}$$
$$+O(h^{m+1}).$$

Thus, putting $G_i(h)$ as

$$(1.3.9)\qquad G_i(h)=\sum_{r=0}^{m-1}\left(\sum_{j=1}^{q}\frac{\tau_{ij}\kappa_{jr}}{r!}\right)h^{r+1}$$

and noting that $G_i(h)$ is of the order h and $G_i(0)=0$, we have the equation

$$\sum_{l=0}^{m}\frac{\kappa_{il}}{l!}h^l=\sum_{l=0}^{m}\frac{h^l}{l!}\left\{\sum_{k=0}^{l}\binom{l}{k}\rho_i^{l-k}(G_i(h))^k\left[D_0^{l-k}\left(\frac{\partial}{\partial y}\right)^k g\right]_0\right\},$$

which is similar to (1.2.4). Hence, following after the proof of Theorem 1, we have

$$\kappa_{il}=\rho_i^l[D_0^l g]_0+\sum_{s=1}^{l-1}\binom{l}{s}\left\{\sum_{t=1}^{m(l,s)}\frac{(l-s)!}{(l-s-t)!}\rho_i^{l-s-t}B_{s,t}(G_i'(0),\dots,G_i^{(s)}(0))\right.$$
$$\left.\times\left[D_0^{l-s-t}\left(\frac{\partial}{\partial y}\right)^t g\right]_0\right\}.$$

From (9), for $k=1,2,\dots,s$

$$G_i^{(k)}(h)=\sum_{r=k-1}^{m-1}\frac{(r+1)!}{(r-k+1)!}\left(\sum_j\frac{\tau_{ij}\kappa_{jr}}{r!}\right)h^{r-k+1}$$

holds, which implies

$$G_i^{(k)}(0)=k!\left(\sum_j \frac{\tau_{ij}\kappa_{j,k-1}}{(k-1)!}\right)=k\sum_j \tau_{ij}\kappa_{j,k-1}\,.$$

Thus we have the desired result. □

By Theorem 3, κ_{il} is given as follows:

$$\begin{aligned}
\kappa_{i1}&=\rho_i[D_0g]_0\,,\\
\kappa_{i2}&=\rho_i^2[D_0^2g]_0+2!B_{1,1}(\sum_j \tau_{ij}\kappa_{j0})\cdot g_{y,0}\\
&=\rho_i^2[D_0^2g]_0+2(\sum_j \tau_{ij})g_0\cdot g_{y,0}\,,\\
\kappa_{i3}&=\rho_i^3[D_0^3g]_0+3!\rho_i\cdot B_{1,1}(\sum \tau_{ij}\kappa_{j0})\,[D_0g_y]_0+3B_{2,1}(\sum \tau_{ij}\kappa_{j0},\, 2\sum \tau_{ij}\kappa_{j1})\cdot g_{y,0}\\
&=\rho_i^3[D_0^3g]_0+6\rho_i(\sum_j \tau_{ij})g_0\cdot[D_0g_y]_0+6(\sum_j \tau_{ij}\rho_j)\,[D_0g]_0\cdot g_{y,0}\,.
\end{aligned}$$

The result with the help of REDUCE-2 is shown in Table 2. Here we employ the notation

$$T_{ik}=\sum_{j=1}^{q}\rho_j^k\tau_{ij},\qquad i=1,2,\dots,q,\quad k=0,1,2,\dots\,.$$

From (6) and (7), the Taylor series expansion for y_1 is given by

$$\begin{aligned}
(1.3.10)\qquad y_1&=y_0+hf_0+\sum_{i=1}^{q}v_ih^2\left(\sum_{l=0}^{m}\frac{\kappa_{il}}{l!}h^l\right)+O(h^{m+3})\\
&=y_0+hf_0+\sum_{l=0}^{m}(\sum_{i=1}^{q}v_i\kappa_{il})\frac{h^{l+2}}{l!}+O(h^{m+3})\\
&=y_0+hf_0+\sum_{r=2}^{m}(\sum_{i=1}^{q}v_i\kappa_{i,r-2})\frac{h^r}{(r-2)!}+O(h^{m+1})\,.
\end{aligned}$$

On the other hand, from (1.2.2), the (second type) Taylor series expansion of the solution $y(x_0+h)$ is given by

$$(1.3.11)\qquad y(x_0+h)=y_0+hf_0+\sum_{r=2}^{m}\frac{\kappa_{r-2}}{r!}h^r+O(h^{m+1})\,,$$

where κ_l is represented by (1.2.5). The comparison of (10) and (11) brings the determining equation of the implicit $(1, q)$-stage formula, for which we have the following

Theorem 4. *Each κ_{il} in* (10) *is constructed with the all elementary differentials included in the corresponding κ_l in* (11). *Hence the determining equation of the implicit* $(1, q)$*-stage formula is of the form such as*

$$(\textit{an integer})\times(\textit{a polynomial of } v_i,\ \rho_i,\ \tau_{ij})=(\textit{an integer})\,.$$

Proof. From (10) and (11), κ_l and $\kappa_{i,l}$ must satisfy

$$\frac{1}{l!}\sum_{i=1}^{q} v_i\kappa_{il}=\frac{\kappa_l}{(l+2)!}, \quad l=0, 1, 2, \ldots, m-2,$$

which implies

$$(l+1)(l+2)\sum_i v_i\kappa_{il}=\kappa_l.$$

From (1.2.5) and (1.3.8) the conclusion follows. □

Table 2.

$$\kappa_{i0}=g_0$$

$$\kappa_{i1}=\rho_i[D_0g]_0$$

$$\kappa_{i2}=\rho_i^2[D_0^2g]_0+2T_{i0}\cdot g_0\cdot g_{y,0}$$

$$\kappa_{i3}=\rho_i^3[D_0^3g]_0+6T_{i1}\cdot[D_0g]_0\cdot g_{y,0}+6\rho_iT_{i0}\cdot g_0\cdot[D_0g_y]_0$$

$$\begin{aligned}\kappa_{i4}=&\rho_i^4[D_0^4g]_0+12T_{i2}[D_0^2g]_0\cdot g_{y,0}+24\rho_iT_{i1}[D_0g]_0\cdot[D_0g_y]_0\\&+12\rho_i^2T_{i0}\cdot g_0\cdot[D_0^2g_y]_0+24(\sum_j\tau_{ij}T_{j0})g_0\cdot g_{y,0}^2+12T_{i0}^2\cdot g_0^2\cdot g_{yy,0}\end{aligned}$$

$$\begin{aligned}\kappa_{i5}=&\rho_i^5\cdot[D_0^5g]_0+20T_{i3}\cdot[D_0^3g]_0\cdot g_{y,0}+60\rho_iT_{i2}\cdot[D_0^2g]_0[D_0g_y]_0\\&+60\rho_i^2T_{i1}[D_0g]_0[D_0^2g_y]_0+120(\sum_j\tau_{ij}T_{j1})\cdot[D_0g]_0\cdot g_{y,0}^2\\&+20\rho_i^3T_{i0}\cdot g_0\cdot[D_0^3g_y]_0+120\{\sum_j(\rho_i+\rho_j)\tau_{ij}T_{j0}\}g_0\cdot g_{y,0}\cdot[D_0g_y]_0\\&+120T_{i0}T_{i1}\cdot g_0\cdot[D_0g]_0\cdot g_{yy,0}+60\rho_iT_{i0}^2\cdot g_0^2\cdot[D_0g_{yy}]_0\end{aligned}$$

$$\begin{aligned}\kappa_{i6}=&\rho_i^6[D_0^6g]_0+30T_{i4}[D_0^4g]_0\cdot g_{y,0}+120\rho_iT_{i3}[D_0^3g]\cdot[D_0g_y]_0\\&+180\rho_i^2T_{i2}[D_0^2g]_0[D_0^2g_y]_0+360(\sum_j\tau_{ij}T_{j2})[D_0^2g]_0\cdot g_{y,0}^2\\&+120\rho_i^3T_{i1}[D_0g]_0\cdot[D_0^3g_y]_0+720\{\sum_j(\rho_i+\rho_j)\tau_{ij}T_{j1}\}[D_0g]_0\cdot g_{y,0}\cdot[D_0g_y]_0\\&+360T_{i1}^2[D_0g]_0^2\cdot g_{yy,0}+30\rho_i^4T_{i0}\cdot g_0\cdot[D_0^4g_y]_0\\&+720(\sum_j\rho_i\rho_j\tau_{ij}T_{j0})\cdot g_0\cdot[D_0g_y]_0^2+360\{\sum_j(\rho_i^2+\rho_j^2)\tau_{ij}T_{j0}\}g_0\cdot g_{y,0}\cdot[D_0^2g_y]_0\\&+720(\sum_j\sum_k\tau_{ij}\tau_{jk}T_{k0})g_0\cdot g_{y,0}^3+360T_{i0}T_{i2}\cdot g_0\cdot[D_0^2g]_0\cdot g_{yy,0}\\&+720\rho_iT_{i0}T_{i1}\cdot g_0\cdot[D_0g]_0\cdot[D_0g_{yy}]_0+180\rho_i^2T_{i0}^2g_0^2\cdot[D_0^2g_{yy}]_0\\&+360\{\sum_j\tau_{ij}(T_{j0}^2+2T_{i0}T_{j0})\}g_0^2\cdot g_{y,0}\cdot g_{yy,0}+120T_{i0}^3\cdot g_0^3\cdot g_{yyy,0}\end{aligned}$$

$$\begin{aligned}\kappa_{i7}=&\rho_i^7\cdot[D_0^7g]_0+42T_{i5}[D_0^5g]_0\cdot g_{y,0}+210\rho_iT_{i4}[D_0^4g]_0\cdot[D_0g_y]_0\\&+420\rho_i^2T_{i3}[D_0^3g]_0\cdot[D_0^2g_y]_0+840(\sum_j\tau_{ij}T_{j3})[D_0^3g]_0\cdot g_{y,0}^2\\&+420\rho_i^3T_{i2}[D_0^2g]_0\cdot[D_0^3g_y]_0+2520(\sum_j(\rho_i+\rho_j)\tau_{ij}T_{j2})[D_0^2g]_0\cdot g_{y,0}\cdot[D_0g_y]_0\\&+210\rho_i^4T_{i1}[D_0g]_0\cdot[D_0^4g_y]_0+5040(\sum_j\rho_i\rho_j\tau_{ij}T_{j1})[D_0g]_0\cdot[D_0g_y]_0^2\\&+2520(\sum_j(\rho_i^2+\rho_j^2)\tau_{ij}T_{j1})[D_0g]_0\cdot g_{y,0}\cdot[D_0^2g_y]_0\end{aligned}$$

$$
\begin{aligned}
&+5040\Big(\sum_j \sum_k \tau_{ij}\tau_{jk}T_{k1}\Big)[D_0g]_0\cdot g_{y,0}^3+2520T_{i1}T_{i2}[D_0g]_0\cdot[D_0^2g]_0\cdot g_{yy,0}\\
&+2520\rho_iT_{i1}^2[D_0g]_0^2\cdot[D_0g_{yy}]_0+42\rho_i^5T_{i0}g_0\cdot[D_0^5g_y]_0\\
&+2520\Big(\sum_j \rho_i\rho_j(\rho_i+\rho_j)\tau_{ij}T_{j0}\Big)g_0\cdot[D_0g_y]_0\cdot[D_0^2g_y]_0\\
&+840\Big(\sum_j)\rho_i^3+\rho_j^3)\tau_{ij}T_{j0}\Big)g_0\cdot g_{y,0}\cdot[D_0^3g_y]_0\\
&+5040\Big(\sum_j \sum_k (\rho_i+\rho_j+\rho_k)\tau_{ij}\tau_{jk}T_{k0}\Big)g_0\cdot g_{y,0}^2\cdot[D_0g_y]_0\\
&+840T_{i0}T_{i3}g_0\cdot[D_0^3g]_0\cdot g_{yy,0}+2520\rho_iT_{i0}T_{i2}g_0\cdot[D_0^2g]_0\cdot[D_0g_{yy}]_0\\
&+2520\rho_i^2T_{i0}T_{i1}g_0\cdot[D_0g]_0\cdot[D_0^2g_{yy}]_0\\
&+5040\Big(\sum_j \tau_{ij}(T_{i0}T_{j1}+T_{j0}T_{j1}+T_{j0}T_{i1})\Big)g_0\cdot[D_0g]_0\cdot g_{y,0}\cdot g_{yy,0}\\
&+420\rho_i^3T_{i0}^2g_0^2\cdot[D_0^3g_{yy}]_0\\
&+2520\Big(\sum_j (2\rho_iT_{i0}+\rho_jT_{j0})\tau_{ij}T_{j0}\Big)g_0^2\cdot[D_0g_y]_0\cdot g_{yy,0}\\
&+2520\Big(\sum_j (\rho_iT_{j0}+2\rho_jT_{i0})\tau_{ij}T_{j0}\Big)g_0^2\cdot g_{y,0}\cdot[D_0g_{yy}]_0\\
&+2520T_{i0}^2T_{i1}g_0^2\cdot[D_0g]_0\cdot g_{yyy,0}+840\rho_iT_{i0}^3g_0^3\cdot[D_0g_{yyy}]_0
\end{aligned}
$$

$$
\begin{aligned}
\kappa_{i8}=&\ \rho_i^8[D_0^8g]_0+56T_{i6}\cdot[D_0^6g]_0\cdot g_{y,0}+336\rho_iT_{i5}[D_0^5g]_0\cdot[D_0g_y]_0\\
&+840\rho_i^2T_{i4}[D_0^4g]_0\cdot[D_0^2g_y]_0+1680\Big(\sum_j \tau_{ij}T_{j4}\Big)[D_0^4g]_0\cdot g_{y,0}^2\\
&+1120\rho_i^3T_{i3}[D_0^3g]_0\cdot[D_0^3g_y]_0+6720\Big(\sum_j (\rho_i+\rho_j)\tau_{ij}T_{j3}\Big)[D_0^3g]_0\cdot g_{y,0}\cdot[D_0g_y]_0\\
&+840\rho_i^4T_{i2}[D_0^2g]_0\cdot[D_0^4g_y]_0+20160\Big(\sum_j \rho_i\rho_j\tau_{ij}T_{j2}\Big)[D_0^2g]_0\cdot[D_0g_y]_0^2\\
&+10080\Big(\sum_j (\rho_i^2+\rho_j^2)\tau_{ij}T_{j2}\Big)[D_0^2g]_0\cdot g_{y,0}\cdot[D_0^2g_y]_0\\
&+20160\Big(\sum_j \sum_k \tau_{ij}\tau_{jk}T_{k2}\Big)[D_0^2g]_0\cdot g_{y,0}^3+5040T_{i2}^2[D_0^2g]_0^2\cdot g_{yy,0}\\
&+336\rho_i^5T_{i1}[D_0g]_0\cdot[D_0^5g_y]_0\\
&+20160\Big(\sum_j \rho_i\rho_j(\rho_i+\rho_j)\tau_{ij}T_{j1}\Big)[D_0g]_0\cdot[D_0g_y]_0\cdot[D_0^2g_y]_0\\
&+6720\Big(\sum_j (\rho_i^3+\rho_j^3)\tau_{ij}T_{j1}\Big)[D_0g]_0\cdot g_{y,0}\cdot[D_0^3g_y]_0\\
&+40320\Big(\sum_j \sum_k (\rho_i+\rho_j+\rho_k)\tau_{ij}\tau_{jk}T_{k1}\Big)[D_0g]_0\cdot g_{y,0}^2\cdot[D_0g_y]_0\\
&+6720T_{i1}T_{i3}[D_0g]_0\cdot[D_0^3g]_0\cdot g_{yy,0}+20160\rho_iT_{i1}T_{i2}[D_0g]_0\cdot[D_0^2g]_0\cdot[D_0g_{yy}]_0\\
&+10080\rho_i^2T_{i1}^2[D_0g]_0^2\cdot[D_0^2g_{yy}]_0\\
&+20160\Big(\sum_j \tau_{ij}T_{j1}(2T_{i1}+T_{j1})\Big)[D_0g]_0^2\cdot g_{y,0}\cdot g_{yy,0}\\
&+56\rho_i^6T_{i0}g_0\cdot[D_0^6g_y]_0+10080\Big(\sum_j \rho_i^2\rho_j^2\tau_{ij}T_{j0}\Big)g_0\cdot[D_0^2g_y]_0^2\\
&+6720\Big(\sum_j \rho_i\rho_j(\rho_i^2+\rho_j^2)\tau_{ij}T_{j0}\Big)g_0\cdot[D_0g_y]_0\cdot[D_0^3g_y]_0\\
&+1680\Big(\sum_j (\rho_i^4+\rho_j^4)\tau_{ij}T_{j0}\Big)g_0\cdot g_{y,0}\cdot[D_0^4g_y]_0\\
&+40320\Big(\sum_j \sum_k (\rho_i\rho_j+\rho_j\rho_k+\rho_i\rho_k)\tau_{ij}\tau_{jk}T_{k0}\Big)g_0\cdot g_{y,0}\cdot[D_0g_y]_0^2\\
&+20160\Big(\sum_j \sum_k (\rho_i^2+\rho_j^2+\rho_k^2)\tau_{ij}\tau_{jk}T_{k0}\Big)g_0\cdot g_{y,0}^2\cdot[D_0^2g_y]_0\\
&+40320\Big(\sum_j \sum_k \sum_l \tau_{ij}\tau_{jk}\tau_{kl}T_{l0}\Big)g_0\cdot g_{y,0}^4+1680T_{i0}T_{i4}g_0\cdot[D_0^4g]_0\cdot g_{yy,0}
\end{aligned}
$$

$$+6720\rho_i T_{i0} T_{i3} g_0 \cdot [D_0^3 g]_0 \cdot [D_0 g_{yy}]_0$$
$$+10080\rho_i^2 T_{i0} T_{i2} g_0 \cdot [D_0^2 g]_0 \cdot [D_0^2 g_{yy}]_0$$
$$+20160(\sum_j \tau_{ij}(T_{i2}T_{j0}+T_{i0}T_{j2}+T_{j0}T_{j2}))g_0 \cdot [D_0^2 g]_0 \cdot g_{y,0} \cdot g_{yy,0}$$
$$+6720\rho_i^3 T_{i0} T_{i1} g_0 \cdot [D_0 g]_0 \cdot [D_0^3 g_{yy}]_0$$
$$+40320(\sum_j \tau_{ij}(\rho_j T_{i0}T_{j1}+\rho_j T_{i1}T_{j0}+\rho_i T_{j0}T_{j1}))g_0 \cdot [D_0 g]_0 \cdot [D_0 g_y]_0 \cdot g_{yy,0}$$
$$+40320(\sum_j \tau_{ij}(\rho_i T_{i0}T_{j1}+\rho_i T_{i1}T_{j0}+\rho_j T_{j0}T_{j1}))g_0 \cdot [D_0 g]_0 \cdot g_{y,0} \cdot [D_0 g_{yy}]_0$$
$$+20160 T_{i0} T_{i1}^2 g_0 \cdot [D_0 g]_0^2 \cdot g_{yyy,0}+840\rho_i^4 T_{i0}^2 g_0^2 \cdot [D_0^4 g_{yy}]_0$$
$$+10080(\sum_j \tau_{ij}(\rho_i^2 T_{j0}+2\rho_j^2 T_{i0})T_{j0})g_0^2 \cdot [D_0^2 g_y]_0 \cdot g_{yy,0}$$
$$+20160(\sum_j \rho_i\rho_j\tau_{ij}(2T_{i0}+T_{j0})T_{j0})g_0^2 \cdot [D_0 g_y]_0 \cdot [D_0 g_{yy}]_0$$
$$+10080(\sum_j \tau_{ij}(\rho_j^2 T_{j0}+2\rho_i^2 T_{i0})T_{j0})g_0^2 \cdot g_{y,0} \cdot [D_0^2 g_{yy}]_0$$
$$+20160(\sum_j \sum_k \tau_{ij}(2\tau_{jk}T_{i0}T_{k0}+2\tau_{jk}T_{j0}T_{k0}+\tau_{ik}T_{j0}T_{k0}+\tau_{jk}T_{k0}^2))g_0^2 \cdot g_{y,0}^2 \cdot g_{yy,0}$$
$$+10080 T_{i0}^2 T_{i2} g_0^2 \cdot [D_0^2 g]_0 \cdot g_{yyy,0}+20160\rho_i T_{i0}^2 T_{i1} g_0^2 \cdot [D_0 g]_0 \cdot [D_0 g_{yyy}]_0$$
$$+3360\rho_i^2 T_{i0}^3 g_0^3 \cdot [D_0^2 g_{yyy}]_0+20160(\sum_j \tau_{ij} T_{i0} T_{j0}^2)g_0^3 \cdot g_{yy,0}^2$$
$$+6720(\sum_j \tau_{ij}(3T_{i0}^2+T_{j0}^2)T_{j0})g_0^3 \cdot g_{y,0} \cdot g_{yyy,0}$$
$$+1680 T_{i0}^4 g_0^4 \cdot g_{yyyy,0}$$

§ 1.4. Determining Equation for (1, q)-Stage Formula

An algebraic computation according to Theorem 1 gives the number of elementary differentials including in each κ_l. Let m_l be the number of elementary differentials in κ_l and define the integer M_l by

$$M_l = \sum_{j=0}^{l} m_j .$$

Each m_l and M_l are given in Table 3 up to $l=8$.

Thus, we have M_l restrictions for the parameters v_i, ρ_i, τ_{ij} of the formula. In the implicit (1, q)-stage formula the number of the parameters to be determined, say $N_q^{(I)}$, can be given as a simple function of q

$$N_q^{(I)} = q(q+2) .$$

It implies that the implicit (1, q)-stage formula can attain at least the order $(\bar{l}+2)$ where $\bar{l}$ is the largest integer satisfying the inequality $M_l \leqq N_q^{(I)}$. These relations are shown in Table 4.

However, the above argument based on merely counting the number of the equations that must be satisfied, ignores the relationship between them.

In fact, it may happen that M_l restrictions are satisfied with fewer than M_l variables. But, since we are interested in the explicit formula rather than implicit one, we shall not come into more investigation for the attainable order of the implicit formula.

An explicit (1, q)-stage formula, which is defined by the parameters ν_i, ρ_i and τ_{ij} ($\tau_{ij}=0$ for $j \geqq i$) in (1.3.6), has $N_q^{(E)}$ parameters to be determined. Here $N_q^{(E)}$ is given by

$$N_q^{(E)} = q(q+3)/2.$$

Hence, similar consideration for the implicit case gives the largest integer l^* satisfying the inequality $M_l \leqq N_q^{(E)}$. Table 4 includes the relations between q, the number of stages, and l^*.

Table 3.

l	m_l	M_l
0	1	1
1	1	2
2	2	4
3	3	7
4	6	13
5	9	22
6	17	39
7	26	65
8	46	111

Table 4.

q	$N_q^{(I)}$	$\bar{l}$	$N_q^{(E)}$	l^*
1	3	1	2	1
2	8	3	5	2
3	15	4	9	3
4	24	5	14	4
5	35	5	20	4
6	48	6	27	5
7	63	6	35	5
8	80	7	44	6
9	99	7	54	6
10	120	8	65	7

SHINTANI has given some explicit one-step methods utilizing the second derivative [12], whose formulation coincides with our explicit (1, q)-stage formula. He has determined the parameters for $q=1$, 2, 3, 4 and 5 which give the formula obtaining the order 3, 4, 5, 6 and 7 respectively. His results attain the orders that we have argued as the least number l^* for each stage formula. Hence, it is a question whether Shintani's results can be improved.

We shall consider the determining equation for the explicit (1, q)-stage formula. Tables 1 and 2 give the equation as follows. We employ the notation for summation symbol such that the upper limit of summation can not exceed the variable of the preceding summation symbols, i.e. $\sum_i \cdots (\sum_j \cdots)$ means $\sum_{i=1}^q \cdots (\sum_{j=1}^{i-1} \cdots)$. Moreover, the symbol T_{ik} means

$$T_{1k}=0 \quad \text{and} \quad T_{ik}=\sum_{j=1}^{i-1} \rho_i^k \tau_{ij}, \qquad i=2, 3, \ldots, q.$$

Determining equations.

$l=0$: (E–0) $2\sum_i v_i=1$

$l=1$: (E–1) $6\sum_i v_i\rho_i=1$

$l=2$: (E–21) $12\sum_i v_i\rho_i^2=1$

(E–22) $24\sum_i v_iT_{i0}=1$

$l=3$: (E–31) $20\sum_i v_i\rho_i^3=1$

(E–32) $120\sum_i v_iT_{i1}=1$

(E–33) $120\sum_i v_i\rho_iT_{i0}=3$

$l=4$: (E–41) $30\sum_i v_i\rho_i^4=1$

(E–42) $360\sum_i v_iT_{i2}=1$

(E–43) $720\sum_i v_i\rho_iT_{i1}=4$

(E–44) $360\sum_i v_i\rho_i^2T_{i0}=6$

(E–45) $720\sum_i\sum_j v_i\tau_{ij}T_{j0}=1$

(E–46) $360\sum_i v_iT_{i0}^2=3$

$l=5$: (E–51) $42\sum_i v_i\rho_i^5=1$

(E–52) $840\sum_i v_iT_{i3}=1$

(E–53) $2520\sum_i v_i\rho_iT_{i2}=5$

(E–54) $2520\sum_i v_i\rho_i^2T_{i1}=10$

(E–55) $5040\sum_i\sum_j v_i\tau_{ij}T_{j1}=1$

(E–56) $840\sum_i v_i\rho_i^3T_{i0}=10$

(E–57) $5040 \sum_i \sum_j v_i(\rho_i+\rho_j)\tau_{ij}T_{j0}=8$

(E–58) $5040 \sum_i v_i T_{i0} T_{i1}=10$

(E–59) $2520 \sum_i v_i \rho_i T_{i0}^2=15$

$l=6$: (E–601) $56 \sum_i v_i \rho_i^6=1$

(E–602) $1680 \sum_i v_i T_{i4}=1$

(E–603) $6720 \sum_i v_i \rho_i T_{i3}=6$

(E–604) $10080 \sum_i v_i \rho_i^2 T_{i2}=15$

(E–605) $20160 \sum_i \sum_j v_i \tau_{ij} T_{j2}=1$

(E–606) $6720 \sum_i v_i \rho_i^3 T_{i1}=20$

(E–607) $40320 \sum_i \sum_j v_i(\rho_i+\rho_j)\tau_{ij}T_{j1}=10$

(E–608) $20160 \sum_i v_i T_{i1}^2=10$

(E–609) $1680 \sum_i v_i \rho_i^4 T_{i0}=15$

(E–610) $40320 \sum_i \sum_j v_i \rho_i \rho_j \tau_{ij} T_{j0}=18$

(E–611) $20160 \sum_i \sum_j v_i(\rho_i^2+\rho_j^2)\tau_{ij}T_{j0}=21$

(E–612) $40320 \sum_i \sum_j \sum_k v_i \tau_{ij}\tau_{jk} T_{k0}=1$

(E–613) $20160 \sum_i v_i T_{i0} T_{i2}=15$

(E–614) $40320 \sum_i v_i \rho_i T_{i0} T_{i1}=60$

(E–615) $10080 \sum_i v_i \rho_i^2 T_{i0}^2=45$

(E–616) $20160 \sum_i \sum_j v_i \tau_{ij}(T_{j0}+2T_{i0})T_{j0}=18$

(E–617) $6720 \sum_i v_i T_{i0}^3=15$

$l=7$: (E–701) $72 \sum_i v_i \rho_i^7=1$

(E–702) $3024 \sum_i v_i T_{i5}=1$

(E–703) $15120 \sum_i v_i \rho_i T_{i4}=7$

(E–704) $30240 \sum_i v_i \rho_i^2 T_{i3}=21$

(E–705) $60480 \sum_i \sum_j v_i \tau_{ij} T_{j3}=1$

(E–706) $30240 \sum_i v_i \rho_i^3 T_{i2}=35$

(E–707) $181440 \sum_i \sum_j v_i(\rho_i+\rho_j)\tau_{ij}T_{j2}=12$

(E–708) $15120 \sum_i v_i \rho_i^4 T_{i1}=35$

(E–709) $362880 \sum_i \sum_j v_i \rho_i \rho_j \tau_{ij} T_{j1}=28$

(E–710) $181440 \sum_i \sum_j v_i(\rho_i^2+\rho_j^2)\tau_{ij}T_{j1}=31$

(E–711) $362880 \sum_i \sum_j \sum_k v_i \tau_{ij}\tau_{jk} T_{k1}=1$

(E–712) $181440 \sum_i v_i T_{i1} T_{i2} = 35$

(E–713) $181440 \sum_i v_i \rho_i T_{i1}^2 = 70$

(E–714) $3024 \sum_i v_i \rho_i^5 T_{i0} = 21$

(E–715) $181440 \sum_i \sum_j v_i \rho_i \rho_j (\rho_i + \rho_j) \tau_{ij} T_{j0} = 105$

(E–716) $60480 \sum_i \sum_j v_i (\rho_i^3 + \rho_j^3) \tau_{ij} T_{j0} = 45$

(E–717) $362880 \sum_i \sum_j \sum_k v_i (\rho_i + \rho_j + \rho_k) \tau_{ij} \tau_{jk} T_{k0} = 15$

(E–718) $60480 \sum_i v_i T_{i0} T_{i3} = 21$

(E–719) $181440 \sum_i v_i \rho_i T_{i0} T_{i2} = 105$

(E–720) $181440 \sum_i v_i \rho_i^2 T_{i0} T_{i1} = 210$

(E–722) $362880 \sum_i \sum_j v_i \tau_{ij} (T_{i0} T_{j1} + T_{j0} T_{j1} + T_{j0} T_{i1}) = 66$

(E–723) $30240 \sum_i v_i \rho_i^3 T_{i0}^2 = 105$

(E–724) $181440 \sum_i \sum_j v_i (2\rho_i T_{i0} + \rho_j T_{j0}) \tau_{ij} T_{j0} = 84$

(E–725) $181440 \sum_i \sum_j v_i (\rho_i T_{j0} + 2\rho_j T_{i0}) \tau_{ij} T_{j0} = 120$

(E–726) $181440 \sum_i v_i T_{i0}^2 T_{i1} = 105$

(E–727) $60480 \sum_i v_i \rho_i T_{i0}^3 = 105$

$l = 8$: (E–801) $90 \sum_i v_i \rho_i^8 = 1$

(E–802) $5040 \sum_i v_i T_{i6} = 1$

(E–803) $30240 \sum_i v_i \rho_i T_{i5} = 8$

(E–804) $75600 \sum_i v_i \rho_i^2 T_{i4} = 28$

(E–805) $151200 \sum_i \sum_j v_i \tau_{ij} T_{j4} = 1$

(E–806) $100800 \sum_i v_i \rho_i^3 T_{i3} = 56$

(E–807) $604800 \sum_i \sum_j v_i (\rho_i + \rho_j) \tau_{ij} T_{j3} = 14$

(E–808) $75600 \sum_i v_i \rho_i^4 T_{i2} = 70$

(E–809) $1814400 \sum_i \sum_j v_i \rho_i \rho_j \tau_{ij} T_{j2} = 40$

(E–810) $907200 \sum_i \sum_j v_i (\rho_i^2 + \rho_j^2) \tau_{ij} T_{j2} = 43$

(E–811) $1814400 \sum_i \sum_j \sum_k v_i \tau_{ij} \tau_{jk} T_{k2} = 1$

(E–812) $453600 \sum_i v_i T_{i2}^2 = 35$

(E–813) $30240 \sum_i v_i \rho_i^5 T_{i1} = 56$

(E–814) $1814400 \sum_i \sum_j v_i \rho_i \rho_j (\rho_i + \rho_j) \tau_{ij} T_{j1} = 192$

(E–815) $604800 \sum_i \sum_j v_i (\rho_i^3 + \rho_j^3) \tau_{ij} T_{ji} = 76$

(E–816) $3628800 \sum_i \sum_j \sum_k v_i (\rho_i + \rho_j + \rho_k) \tau_{ij} \tau_{jk} T_{k1} = 18$

(E–817) $604800 \sum_i v_i T_{i1} T_{i3} = 56$

(E–818) $1814400 \sum_i v_i \rho_i T_{i1} T_{i2} = 280$

(E–819) $907200 \sum_i v_i \rho_i^2 T_{i1}^2 = 280$

(E–820) $1814400 \sum_i \sum_j v_i \tau_{ij} T_{j1}(2T_{i1} + T_{j1}) = 66$

(E–821) $5040 \sum_i v_i \rho_i^6 T_{i0} = 28$

(E–822) $907200 \sum_i \sum_j v_i \rho_i^2 \rho_j^2 \tau_{ij} T_{j0} = 168$

(E–823) $604800 \sum_i \sum_j v_i \rho_i \rho_j (\rho_i^2 + \rho_j^2) \tau_{ij} T_{j0} = 248$

(E–824) $151200 \sum_i \sum_j v_i (\rho_i^4 + \rho_j^4) \tau_{ij} T_{j0} = 85$

(E–825) $3628800 \sum_i \sum_j \sum_k v_i (\rho_i \rho_j + \rho_j \rho_k + \rho_j \rho_k) \tau_{ij} \tau_{jk} T_{k0} = 82$

(E–826) $1814400 \sum_i \sum_j \sum_k v_i (\rho_i^2 + \rho_j^2 + \rho_k^2) \tau_{ij} \tau_{jk} T_{k0} = 49$

(E–827) $3628800 \sum_i \sum_j \sum_k \sum_l v_i \tau_{ij} \tau_{jk} \tau_{kl} T_{l0} = 1$

(E–828) $151200 \sum_i v_i T_{i0} T_{i4} = 28$

(E–829) $604800 \sum_i v_i \rho_i T_{i0} T_{i3} = 168$

(E–830) $907200 \sum_i v_i \rho_i^2 T_{i0} T_{i2} = 420$

(E–831) $1814400 \sum_i \sum_j v_i \tau_{ij} (T_{i2} T_{j0} + T_{i0} T_{j2} + T_{j0} T_{j2}) = 113$

(E–832) $604800 \sum_i v_i \rho_i^3 T_{i0} T_{i1} = 560$

(E–833) $3628800 \sum_i \sum_j v_i \tau_{ij} (\rho_j T_{i0} T_{j1} + \rho_j T_{i1} T_{j0} + \rho_i T_{j0} T_{j1}) = 360$

(E–834) $3628800 \sum_i \sum_j v_i \tau_{ij} (\rho_i T_{i0} T_{j1} + \rho_i T_{i1} T_{j0} + \rho_j T_{j0} T_{j1}) = 508$

(E–835) $1814400 \sum_i v_i T_{i0} T_{i1}^2 = 280$

(E–836) $75600 \sum_i v_i \rho_i^4 T_{i0}^2 = 210$

(E–837) $907200 \sum_i \sum_j v_i \tau_{ij} (\rho_i^2 T_{j0} + 2\rho_j^2 T_{i0}) T_{j0} = 252$

(E–838) $1814400 \sum_i \sum_j v_i \rho_i \rho_j \tau_{ij} (2T_{i0} + T_{j0}) T_{j0} = 624$

(E–839) $907200 \sum_i \sum_j v_i \tau_{ij} (\rho_j^2 T_{j0} + 2\rho_i^2 T_{i0}) T_{j0} = 465$

(E–840) $$1814400 \sum_i \sum_j \sum_k v_i \tau_{ij} (2\tau_{jk} T_{i0} T_{k0} + 2\tau_{jk} T_{j0} T_{k0} + \tau_{ik} T_{j0} T_{k0} + \tau_{jk} T_{k0}^2) = 81$$

(E–841) $907200 \sum_i v_i T_{i0}^2 T_{i2} = 210$

(E–842) $1814400 \sum_i v_i \rho_i T_{i0}^2 T_{i1} = 840$

(E–843) $302400 \sum_i v_i \rho_i^2 T_{i0}^3 = 420$

(E–844) $1814400 \sum_i \sum_j v_i \tau_{ij} T_{i0} T_{j0}^2 = 84$

(E–845) $604800 \sum_i \sum_j v_i \tau_{ij} (3T_{i0}^2 + T_{j0}^2) T_{j0} = 225$

(E–846) $151200 \sum_i v_i T_{i0}^4 = 105$

§ 1.5. Attainable Order of (1, 1)- and (1, 2)-Stage Formulas

The explicit $(1, q)$-stage formula is said to have the attainable order m if m is the largest integer for which

$$y(x+h)-y_1=O(h^{m+1})$$

among all combinations of the parameters of the formula, where $y(x)$ is the analytical solution and y_1 is given by (1.3.6). The definition of the attainable order will be extended, if necessary, to general (p, q)-stage formula.

It is obvious that a $(1, q)$-stage formula has the attainable order m if and only if the determining equations corresponding up to l have at least one solution, but they have no solution up to $l+1$, where $l=m-2$.

Theorem 5. *The attainable order of* (1, 1)*-stage formula is* 3.

Proof. The left-hand side of the equation (E–22) is equal to

$$24\sum_i v_i(\sum_j \tau_{ij}),$$

which vanishes for (1, 1)-stage formula because $\sum_j \tau_{ij}=0$. This means that the parameters v_1 and ρ_1 can satisfy merely the equations (E–0) and (E–1). □

Theorem 6. *The attainable order of* (1, 2)*-stage formula is equal to* 4.

Proof. Assume that the formula attains order 5, that is, the parameters v_1, v_2, ρ_1, ρ_2 and τ_{21} satisfy the equations (E–0) – (E–33).

$$v_1+v_2=\frac{1}{2} \tag{1.5.1}$$

$$v_1\rho_1+v_2\rho_2=\frac{1}{6} \tag{1.5.2}$$

$$v_2\tau_{21}=\frac{1}{24} \tag{1.5.3}$$

$$v_1\rho_1^2+v_2\rho_2^2=\frac{1}{12} \tag{1.5.4}$$

$$v_2\rho_2\tau_{21}=\frac{1}{40} \tag{1.5.5}$$

$$v_2\rho_1\tau_{21}=\frac{1}{120} \tag{1.5.6}$$

(1.5.7) $$\nu_1\rho_1^3+\nu_2\rho_2^3=\frac{1}{20}$$

The equations (1), (2) and (4) yield a matrix equation

$$\begin{pmatrix} 1 & 1 & 1/2 \\ \rho_1 & \rho_2 & 1/6 \\ \rho_1^2 & \rho_2^2 & 1/12 \end{pmatrix}\begin{pmatrix} \nu_1 \\ \nu_2 \\ -1 \end{pmatrix}=0,$$

which implies

(1.5.8) $$\begin{vmatrix} 1 & 1 & 1/2 \\ \rho_1 & \rho_2 & 1/6 \\ \rho_1^2 & \rho_2^2 & 1/12 \end{vmatrix}=0$$

for the existence of nontrivial solution $[\nu_1, \nu_2, -1]^t$. On the other hand, (3), (5) and (6) give the values

$$\rho_1=\frac{1}{5}, \quad \rho_2=\frac{3}{5},$$

which specify the determinant of (8) by 1/250. This contradiction implies the statement. □

Note. SHINTANI gives (1, 1)-stage formula with parameters $\nu_1=1/2$ and $\rho_1=1/3$. He also gives (1, 2)-stage formula with $\nu_1=(9+\sqrt{6})/36$, $\nu_2=(9-\sqrt{6})/36$, $\rho_1=(4-\sqrt{6})/10$, $\rho_2=(4+\sqrt{6})/10$, $\tau_{21}=(9+\sqrt{6})/50$. These parameters are not unique solution (1.5.1)–(1.5.4). The solution of them is represented with one parameter ρ by the following:

$$\begin{aligned}
&\rho_1=\rho \quad \left(\rho\neq\frac{1}{3}\right),\\
&\rho_2=(2\rho-1)/2(3\rho-1),\\
&\nu_1=1/6(6\rho^2-4\rho+1),\\
&\nu_2=(3\rho-1)^2/3(6\rho^2-4\rho+1)\\
&\tau_{21}=(6\rho^2-4\rho+1)/8(3\rho-1)^2
\end{aligned}$$

§ 1.6. Attainable Order of (1, 3)-Stage Formula

The determining equation for the explicit (1, 3)-stage formula are given as follows:

(E–0) $$\nu_1+\nu_2+\nu_3=\frac{1}{2}$$

(E–1) $$\nu_1\rho_1+\nu_2\rho_2+\nu_3\rho_3=\frac{1}{6}$$

(E–21) $$\nu_1\rho_1^2+\nu_2\rho_2^2+\nu_3\rho_3^2=\frac{1}{12}$$

(E–22) $$\nu_2\tau_{21}+\nu_3(\tau_{31}+\tau_{32})=\frac{1}{24}$$

(E–31) $$\nu_1\rho_1^3+\nu_2\rho_2^3+\nu_3\rho_3^3=\frac{1}{20}$$

(E–32) $$\nu_2\rho_2\tau_{21}+\nu_3\rho_3(\tau_{31}+\tau_{32})=\frac{1}{40}$$

(E–33) $$\nu_2\rho_1\tau_{21}+\nu_3(\rho_1\tau_{31}+\rho_2\tau_{32})=\frac{1}{120}$$

(E–41) $$\nu_1\rho_1^4+\nu_2\rho_2^4+\nu_3\rho_3^4=\frac{1}{30}$$

(E–42) $$\nu_2\rho_2^2\tau_{21}+\nu_3\rho_3^2(\tau_{31}+\tau_{32})=\frac{1}{60}$$

(E–43) $$\nu_2\rho_2\rho_1\tau_{21}+\nu_3\rho_3(\rho_1\tau_{31}+\rho_2\tau_{32})=\frac{1}{180}$$

(E–44) $$\nu_2\rho_1^2\tau_{21}+\nu_3(\rho_1^2\tau_{31}+\rho_2^2\tau_{32})=\frac{1}{360}$$

(E–45) $$\nu_2\tau_{21}^2+\nu_3(\tau_{31}+\tau_{32})^2=\frac{1}{120}$$

(E–46) $$\nu_3\tau_{21}\tau_{32}=\frac{1}{720}$$

It is remarkable that none of the factors on the left of (E–46) can vanish.

Assume that two of ρ_1, ρ_2, ρ_3 are equal, say $\rho_I=\rho_J$. Then, from (E–0), (E–1), (E–21), (E–31) and (E–41), we see that

$$\begin{bmatrix} 1 & 1 & \frac{1}{2} \\ \rho_I & \rho_K & \frac{1}{6} \\ \rho_I^2 & \rho_K^2 & \frac{1}{12} \end{bmatrix}\begin{bmatrix} \nu_I+\nu_J \\ \nu_K \\ -1 \end{bmatrix}=0,$$

$$\begin{bmatrix} 1 & 1 & \frac{1}{6} \\ \rho_I & \rho_K & \frac{1}{12} \\ \rho_I^2 & \rho_K^2 & \frac{1}{20} \end{bmatrix}\begin{bmatrix} \rho_I(\nu_I+\nu_J) \\ \rho_K\nu_K \\ -1 \end{bmatrix}=0,$$

$$\begin{bmatrix} 1 & 1 & \frac{1}{12} \\ \rho_I & \rho_K & \frac{1}{20} \\ \rho_I^2 & \rho_K^2 & \frac{1}{30} \end{bmatrix} \begin{bmatrix} \rho_I^2(v_I+v_J) \\ \rho_K^2 v_K \\ -1 \end{bmatrix} = 0 .$$

The condition that the above three equations have non-trivial solutions, implies the equations with respect to ρ_I, ρ_K as follows:

$$(\rho_K-\rho_I)\left\{\frac{1}{2}\rho_I\rho_K-\frac{1}{6}(\rho_I+\rho_K)+\frac{1}{12}\right\}=0,$$

$$(\rho_K-\rho_I)\left\{\frac{1}{6}\rho_I\rho_K-\frac{1}{12}(\rho_I+\rho_K)+\frac{1}{20}\right\}=0$$

and

$$(\rho_K-\rho_I)\left\{\frac{1}{12}\rho_I\rho_K-\frac{1}{20}(\rho_I+\rho_K)+\frac{1}{30}\right\}=0.$$

If $\rho_I \neq \rho_K$, ρ_I and ρ_K must satisfy the equations

$$\begin{aligned}\frac{1}{2}\rho_I\rho_K-\frac{1}{6}(\rho_I+\rho_K)+\frac{1}{12} &= \frac{1}{6}\rho_I\rho_K-\frac{1}{12}(\rho_I+\rho_K)+\frac{1}{20} \\ &= \frac{1}{12}\rho_I\rho_K-\frac{1}{20}(\rho_I+\rho_K)+\frac{1}{30}=0,\end{aligned}$$

which is impossible. The case of $\rho_1=\rho_2=\rho_3$ leads to a contradiction because of

$$v_1+v_2+v_3=\frac{1}{2},$$

$$\rho_1(v_1+v_2+v_3)=\frac{1}{6},$$

$$\rho_1^2(v_1+v_2+v_3)=\frac{1}{12},$$

induced by (E–0), (E–1), (E–21), respectively.

Hence no two of ρ_1, ρ_2, ρ_3 are equal. It is convenient to define

$$A_i=\sum_{j=1}^{i-1}\tau_{ij}-\frac{1}{2}\rho_i^2 \qquad (i=1, 2, 3).$$

Since we consider the explicit formula, $A_1=-\rho_1^2/2$ holds. Then, we have simultaneous linear equations

$$\begin{bmatrix} 1 & 1 & 1 \\ \rho_1 & \rho_2 & \rho_3 \\ \rho_1^2 & \rho_2^2 & \rho_3^2 \end{bmatrix} \begin{bmatrix} v_1A_1 \\ v_2A_2 \\ v_3A_3 \end{bmatrix} = 0$$

by (E–21), (E–22), (E–31), (E–32), (E–41) and (E–42). Since no two of ρ_1, ρ_2, ρ_3 are equal, all of v_1A_1, v_2A_2, v_3A_3 vanish. By virtue of the above mentioned remark, we distinguish the following four cases.

Case 1. $A_1=A_2=A_3=0$.

The equations $A_1=0$ and $A_2=0$ imply $\rho_1=0$ and $\tau_{21}=\rho_2^2/2$. Then, (E–43) and (E–44) bring the equations $v_3\rho_2\rho_3\tau_{32}=1/180$ and $v_3\rho_2^2\tau_{32}=1/360$, which give the identity $\rho_3=2\rho_2$. Thus (E–1), (E–21) and (E–31) imply the equation

$$\begin{bmatrix} \rho_2 & 2\rho_2 & \frac{1}{6} \\ \rho_2^2 & 4\rho_2^2 & \frac{1}{12} \\ \rho_2^3 & 8\rho_2^3 & \frac{1}{20} \end{bmatrix} \begin{bmatrix} v_2 \\ v_3 \\ -1 \end{bmatrix} = 0,$$

which yields a quadratic equation of ρ_2

$$20\rho_2^2-15\rho_2+3=0$$

because of $\rho_2\neq 0$. But the above quadratic equation has no real roots.

Case 2. $v_1=0$ and $A_2=A_3=0$.

In such case, we have the equations

$$\tau_{21}=\frac{1}{2}\rho_2^2$$

and

$$\tau_{31}+\tau_{32}=\frac{1}{2}\rho_3^2.$$

Substitution of $\tau_{21}=\rho_2^2/2$ and $\tau_{31}=(\rho_3^2/2)-\tau_{32}$ into (E–44) implies

$$\rho_1^2+24v_3\tau_{32}(\rho_2^2-\rho_1^2)=\frac{1}{15}.$$

Employing the equation

$$(*) \qquad v_3\rho_2^2\tau_{32}=\frac{1}{360}$$

induced by (E–46), we obtain

$$\rho_1(1-24v_3\tau_{32})=0.$$

Hence, the equation $\rho_1=0$ or $v_3\tau_{32}=1/24$ holds. The case of $\rho_1=0$ is equivalent to Case 1. The equation $v_3\tau_{32}=1/24$ yields

$$\rho_1+24\nu_3\tau_{32}(\rho_2-\rho_1)=\rho_2=\frac{1}{5}.$$

by (E–33). The equation (*), however, implies $\rho_2^2=1/15$, which leads to a contradiction.

Case 3. $\nu_2=0$ and $A_1=A_3=0$.

$A_1=0$ implies $\rho_1=0$. Then, (E–1) and (E–21) bring the equations

$$\nu_3\rho_3=\frac{1}{6}.$$

and

$$\nu_3\rho_3^2=\frac{1}{12}.$$

Hence we see $\rho_3=1/2$ and $\nu_3=1/3$. It contradicts the equation $\nu_3\rho_3^3=1/20$ induced by (E–31).

Case 4. $\nu_1=0$, $\nu_2=0$ and $A_3=0$.

The equations (E–0) and (E–1) yield $\nu_3=1/2$ and $\rho_3=1/3$. Again, it contradicts the equation $\nu_3\rho_3^3=1/20$ induced by (E–31).

Thus, we can conclude that the determining equations (E–0) – (E–46) have no solutions. The proof of the following theorem is now accomplished.

Theorem 7. *The explicit* (1, 3)-*stage formula can not attain order* 6. *Its attainable order is* 5.

Note. SHINTANI gives (1, 3)-stage formula with parameters

$$\nu_1=1/12,\ \nu_2=(5+\sqrt{5})/24, \nu_3=(5-\sqrt{5})/24,\ \rho_1=0,\ \rho_2=(5-\sqrt{5})/10,$$
$$\tau_{21}=(3-\sqrt{5})/20,\ \rho_3=(5+\sqrt{5})/10,\ \tau_{31}=0 \text{ and } \tau_{32}=(3+\sqrt{5})/20.$$

These parameters are also not unique solution of (E–0) – (E–33).

§ 1.7. Attainable Order of (1, 4)-Stage Formula

The determining equation for the explicit (1, 4)-stage formula are given by the following:

(E–0) $\quad \nu_1+\nu_2+\nu_3+\nu_4=\dfrac{1}{2}$

(E–1) $\quad \nu_1\rho_1+\nu_2\rho_2+\nu_3\rho_3+\nu_4\rho_4=\dfrac{1}{6}$

(E–21) $v_1\rho_1^2 + v_2\rho_2^2 + v_3\rho_3^2 + v_4\rho_4^2 = \frac{1}{12}$

(E–22) $v_2\tau_{21} + v_3(\tau_{31} + \tau_{32}) + v_4(\tau_{41} + \tau_{42} + \tau_{43}) = \frac{1}{24}$

(E–31) $v_1\rho_1^3 + v_2\rho_2^3 + v_3\rho_3^3 + v_4\rho_4^3 = \frac{1}{20}$

(E–32) $v_2\rho_2\tau_{21} + v_3\rho_3(\tau_{31} + \tau_{32}) + v_4\rho_4(\tau_{41} + \tau_{42} + \tau_{43}) = \frac{1}{40}$

(E–33) $v_2\rho_1\tau_{21} + v_3(\rho_1\tau_{31} + \rho_2\tau_{32}) + v_4(\rho_1\tau_{41} + \rho_2\tau_{42} + \rho_3\tau_{43}) = \frac{1}{120}$

(E–41) $v_1\rho_1^4 + v_2\rho_2^4 + v_3\rho_3^4 + v_4\rho_4^4 = \frac{1}{30}$

(E–42) $v_2\rho_2^2\tau_{21} + v_3\rho_3^2(\tau_{31} + \tau_{32}) + v_4\rho_4^2(\tau_{41} + \tau_{42} + \tau_{43}) = \frac{1}{60}$

(E–43) $v_2\rho_2\rho_1\tau_{21} + v_3\rho_3(\rho_1\tau_{31} + \rho_2\tau_{32}) + v_4\rho_4(\rho_1\tau_{41} + \rho_2\tau_{42} + \rho_3\tau_{43}) = \frac{1}{180}$

(E–44) $v_2\rho_1^2\tau_{21} + v_3(\rho_1^2\tau_{31} + \rho_2^2\tau_{32}) + v_4(\rho_1^2\tau_{41} + \rho_2^2\tau_{42} + \rho_3^2\tau_{43}) = \frac{1}{360}$

(E–45) $v_3\tau_{21}\tau_{32} + v_4(\tau_{21}\tau_{42} + \tau_{31}\tau_{43} + \tau_{32}\tau_{43}) = \frac{1}{720}$

(E–46) $v_2\tau_{21}^2 + v_3(\tau_{31} + \tau_{32})^2 + v_4(\tau_{41} + \tau_{42} + \tau_{43})^2 = \frac{1}{120}$

(E–51) $v_1\rho_1^5 + v_2\rho_2^5 + v_3\rho_3^5 + v_4\rho_4^5 = \frac{1}{42}$

(E–52) $v_2\rho_2^3\tau_{21} + v_3\rho_3^3(\tau_{31} + \tau_{32}) + v_4\rho_4^3(\tau_{41} + \tau_{42} + \tau_{43}) = \frac{1}{84}$

(E–53) $v_2\rho_2^2\rho_1\tau_{21} + v_3\rho_3^2(\rho_1\tau_{31} + \rho_2\tau_{32}) + v_4\rho_4^2(\rho_1\tau_{41} + \rho_2\tau_{42} + \rho_3\tau_{43}) = \frac{1}{252}$

(E–54) $v_2\rho_2\rho_1^2\tau_{21} + v_3\rho_3(\rho_1^2\tau_{31} + \rho_2^2\tau_{32}) + v_4\rho_4(\rho_1^2\tau_{41} + \rho_2^2\tau_{42} + \rho_3^2\tau_{43}) = \frac{1}{504}$

(E–55) $v_2\rho_1^3\tau_{21} + v_3(\rho_1^3\tau_{31} + \rho_2^3\tau_{32}) + v_4(\rho_1^3\tau_{41} + \rho_2^3\tau_{42} + \rho_3^3\tau_{43}) = \frac{1}{840}$

(E–56) $v_3(\rho_2 + \rho_3)\tau_{21}\tau_{32} + v_4(\rho_2 + \rho_4)\tau_{21}\tau_{42} + v_4(\rho_3 + \rho_4)(\tau_{31}\tau_{43} + \tau_{32}\tau_{43}) = \frac{1}{630}$

(E–57) $v_3\rho_1\tau_{21}\tau_{32} + v_4\rho_1(\tau_{21}\tau_{42} + \tau_{31}\tau_{43}) + v_4\rho_2\tau_{32}\tau_{43} = \frac{1}{5040}$

(E–58) $$\begin{aligned} &v_2\rho_1\tau_{21}^2 + v_3(\rho_1\tau_{31}^2 + \rho_1\tau_{31}\tau_{32} + \rho_2\tau_{31}\tau_{32} + \rho_2\tau_{32}^2) \\ &\quad + v_4(\rho_1\tau_{41}^2 + \rho_2\tau_{42}^2 + \rho_3\tau_{43}^2) + v_4\rho_1(\tau_{41}\tau_{42} + \tau_{41}\tau_{43}) \\ &\quad + v_4\rho_2(\tau_{41}\tau_{42} + \tau_{42}\tau_{43}) + v_4\rho_3(\tau_{31}\tau_{43} + \tau_{42}\tau_{43}) = \frac{1}{504} \end{aligned}$$

(E–59) $v_2\rho_2\tau_{21}^2 + v_3\rho_3(\tau_{31} + \tau_{32})^2 + v_4\rho_4(\tau_{41} + \tau_{42} + \tau_{43})^2 = \frac{1}{168}$

The question is whether any parameters v_i, ρ_i and τ_{ij} exist to satisfy these 22 equations simultaneously. It is helpful for investigation to introduce the following notations:

$$T_{i0}=\sum_{j=1}^{i-1}\tau_{ij},\quad T_{i1}=\sum_{j=1}^{i-1}\rho_j\tau_{ij}\qquad (i=1,2,3,4),$$

(T_{10} and T_{11} mean zero.)

$$A_i=T_{i0}-\frac{1}{2}\rho_i^2,\quad B_i=T_{i1}-\frac{1}{6}\rho_i^3\qquad (i=1,2,3,4).$$

Then, from (E–21), (E–22), (E–31), (E–32), (E–33), (E–41), (E–42), (E–43), (E–51), (E–52) and (E–53), we easily see that

$$\sum_i v_iA_i=\sum_i v_i\rho_iA_i=\sum_i v_i\rho_i^2A_i=\sum_i v_i\rho_i^3A_i=0 \tag{1.7.1}$$

and

$$\sum_i v_iB_i=\sum_i v_i\rho_iB_i=\sum_i v_i\rho_i^2B_i=0. \tag{1.7.2}$$

The equations (1) means

$$\begin{pmatrix} 1 & 1 & 1 & 1\\ \rho_1 & \rho_2 & \rho_3 & \rho_4\\ \rho_1^2 & \rho_2^2 & \rho_3^2 & \rho_4^2\\ \rho_1^3 & \rho_2^3 & \rho_3^3 & \rho_4^3 \end{pmatrix}\begin{pmatrix} v_1A_1\\ v_2A_2\\ v_3A_3\\ v_4A_4\end{pmatrix}=0.$$

We now distinguish two cases according as two of ρ_1, ρ_2, ρ_3, ρ_4 are equal or otherwise.

Case 1. Two of ρ_1, ρ_2, ρ_3, ρ_4 are equal.

Assume that two of them are equal, say $\rho_I=\rho_J$. Equations (E–0), (E–1), (E–21), (E–31), (E–41) and (E–51) give three simultaneous linear equations as follows:

$$\begin{pmatrix} 1 & 1 & 1 & \frac{1}{2}\\ \rho_I & \rho_K & \rho_L & \frac{1}{6}\\ \rho_I^2 & \rho_K^2 & \rho_L^2 & \frac{1}{12}\\ \rho_I^3 & \rho_K^3 & \rho_L^3 & \frac{1}{20} \end{pmatrix}\begin{pmatrix} v_I+v_J\\ v_K\\ v_L\\ -1\end{pmatrix}=0,$$

$$\begin{pmatrix} 1 & 1 & 1 & \frac{1}{6} \\ \rho_I & \rho_K & \rho_L & \frac{1}{12} \\ \rho_I^2 & \rho_K^2 & \rho_L^2 & \frac{1}{20} \\ \rho_I^3 & \rho_K^3 & \rho_L^3 & \frac{1}{30} \end{pmatrix} \begin{pmatrix} \rho_I(\nu_I+\nu_K) \\ \rho_K\nu_K \\ \rho_L\nu_K \\ -1 \end{pmatrix} = 0,$$

$$\begin{pmatrix} 1 & 1 & 1 & \frac{1}{12} \\ \rho_I & \rho_K & \rho_L & \frac{1}{20} \\ \rho_I^2 & \rho_K^2 & \rho_L^2 & \frac{1}{30} \\ \rho_I^3 & \rho_K^3 & \rho_L^3 & \frac{1}{42} \end{pmatrix} \begin{pmatrix} \rho_I^2(\nu_I+\nu_J) \\ \rho_K^2\nu_K \\ \rho_L^2\nu_L \\ -1 \end{pmatrix} = 0.$$

The condition that these equations have non-trivial solutions, implies the determinants of matrices to be vanishing. Hence, we see that the equations

$$\frac{1}{60}(\rho_I-\rho_K)(\rho_K-\rho_L)(\rho_L-\rho_I)\{-30\rho_I\rho_K\rho_L+10(\rho_I\rho_K+\rho_K\rho_L+\rho_L\rho_I) \\ -5(\rho_I+\rho_K+\rho_L)+3\}=0,$$

$$\frac{1}{60}(\rho_I-\rho_K)(\rho_K-\rho_L)(\rho_L-\rho_I)\{-10\rho_I\rho_K\rho_L+5(\rho_I\rho_K+\rho_K\rho_L+\rho_L\rho_I) \\ -3(\rho_I+\rho_K+\rho_L)+2\}=0$$

and

$$\frac{1}{420}(\rho_I-\rho_K)(\rho_K-\rho_L)(\rho_L-\rho_I)\{-35\rho_I\rho_K\rho_L+21(\rho_I\rho_K+\rho_K\rho_L+\rho_L\rho_I) \\ -14(\rho_I+\rho_K+\rho_L)+10\}=0$$

hold. We can distinguish three cases.

(i) At least three of ρ_i are equal.

(ii) $\rho_I=\rho_J$ and $\rho_K=\rho_L$.

(iii) ρ_I, ρ_K, ρ_L are distinct, and the above equations hold.

But, the case (i) can not hold by the similar reason mentioned at the first part of Section 1.6. In the case (ii), (E–0), (E–1), (E–21), (E–31) and (E–41) imply the equations

$$\begin{pmatrix} 1 & 1 & \frac{1}{2} \\ \rho_I & \rho_K & \frac{1}{6} \\ \rho_I^2 & \rho_K^2 & \frac{1}{12} \end{pmatrix} \begin{pmatrix} \nu_I+\nu_J \\ \nu_K+\nu_L \\ -1 \end{pmatrix} = 0,$$

$$\begin{pmatrix} 1 & 1 & \frac{1}{6} \\ \rho_I & \rho_K & \frac{1}{12} \\ \rho_I^2 & \rho_K^2 & \frac{1}{20} \end{pmatrix} \begin{pmatrix} \rho_I(\nu_I+\nu_J) \\ \rho_K(\nu_K+\nu_L) \\ -1 \end{pmatrix} = 0,$$

$$\begin{pmatrix} 1 & 1 & \frac{1}{12} \\ \rho_I & \rho_K & \frac{1}{20} \\ \rho_I^2 & \rho_K^2 & \frac{1}{30} \end{pmatrix} \begin{pmatrix} \rho_I^2(\nu_I+\nu_J) \\ \rho_K^2(\nu_K+\nu_L) \\ -1 \end{pmatrix} = 0.$$

Thus, by the same reason as for case (i), these equations lead to a contradiction.

In the case (iii), we easily see the equations

$$\rho_I+\rho_K+\rho_L=\frac{9}{7},$$

$$\rho_I\rho_K+\rho_K\rho_L+\rho_L\rho_I=\frac{3}{7}$$

and

$$\rho_I\rho_K\rho_L=\frac{1}{35},$$

which imply that ρ_I, ρ_K, ρ_L are distinct roots of the cubic equation

$$x^3-\frac{9}{7}x^2+\frac{3}{7}x-\frac{1}{35}=0. \tag{1.7.3}$$

The cubic equation is irreducible and has three distinct real roots given as follows. Let θ be an angle such that

$$\cos 3\theta=\frac{1}{5\sqrt{2}} \qquad \left(0<3\theta\leqq\frac{\pi}{2}\right). \tag{1.7.4}$$

Then, the roots are

$$\left\{\begin{aligned} R_0 &= \frac{1}{7}(3+2\sqrt{2}\cos\theta), \\ R_1 &= \frac{1}{7}(3-\sqrt{2}\cos\theta+\sqrt{6}\sin\theta), \\ R_{-1} &= \frac{1}{7}(3-\sqrt{2}\cos\theta-\sqrt{6}\sin\theta). \end{aligned}\right. \tag{1.7.5}$$

Some algebraic properties on the equation (3) are the followings:

Lemma 1.7.1. *The roots* R_0, R_1, R_{-1} *are equal to none of* 0, 1/7, 1/3.

Proof. Substitution of 0, 1/7 and 1/3 into the cubic polynomial of (3) gives $-1/35$, 16/1715 and 8/945, respectively. □

Lemma 1.7.2. *The equation* (3) *has no common roots with the cubic equation*

$$x^3-\frac{3}{8}x^2-\frac{3}{16}x+\frac{3}{64}=0. \tag{1.7.6}$$

Proof. Put

$$f_1(x)=x^3-\frac{9}{7}x^2+\frac{3}{7}x-\frac{1}{35}$$

and

$$f_2(x)=x^3-\frac{3}{8}x^2-\frac{3}{16}x+\frac{3}{64}.$$

The Sylvester's determinant $D(f_1, f_2)$ is equal to $-3437/32768000$. □

Lemma 1.7.3. *The equation* (3) *has no roots, one of which is the triple of another.*

Proof. Assume that one of roots is equal to the triple of another, then the root satisfy another cubic equation

$$27x^3-\frac{81}{7}x^2+\frac{9}{7}x-\frac{1}{35}=0.$$

That is,

$$x^3-\frac{3}{7}x^2+\frac{1}{21}x-\frac{1}{945}=0.$$

Put

$$f_1(x)=x^3-\frac{9}{7}x^2+\frac{3}{7}x-\frac{1}{35}$$

and

$$f_2(x) = x^3 - \frac{7}{3}x^2 + \frac{1}{21}x - \frac{1}{945}.$$

The Sylvester's determinant $D(f_1, f_2)$ is equal to 80384/41351522625. □

Case 1.1. $\rho_1 = \rho_2$.

From (E–45) and (E–57), the assumption gives $\rho_1 = \rho_2 = 1/7$. Due to Lemma 1.7.1, we lead to a contradiction.

Case 1.2. $\rho_1 = \rho_3$.

We may assume that ρ_1, ρ_2, ρ_4 are distinct. From (E–0), (E–1) and (E–21), we have the equation

$$\text{(1.7.9)} \qquad \begin{pmatrix} 1 & 1 & 1 \\ \rho_1 & \rho_2 & \rho_4 \\ \rho_1^2 & \rho_2^2 & \rho_4^2 \end{pmatrix} \begin{pmatrix} \nu_1 + \nu_3 \\ \nu_2 \\ \nu_4 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{6} \\ \frac{1}{12} \end{pmatrix}$$

The solution of (9) is given by

$$\begin{pmatrix} \nu_1 + \nu_3 \\ \nu_2 \\ \nu_4 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ \rho_1 & \rho_2 & \rho_4 \\ \rho_1^2 & \rho_2^2 & \rho_4^2 \end{pmatrix}^{-1} \begin{pmatrix} \frac{1}{2} \\ \frac{1}{6} \\ \frac{1}{12} \end{pmatrix}$$

$$= \begin{pmatrix} \dfrac{-6\rho_2\rho_4 + 2(\rho_2 + \rho_4) - 1}{12(\rho_1 - \rho_2)(\rho_4 - \rho_1)} \\ \dfrac{-6\rho_4\rho_1 + 2(\rho_4 + \rho_1) - 1}{12(\rho_1 - \rho_2)(\rho_2 - \rho_4)} \\ \dfrac{-6\rho_1\rho_2 + 2(\rho_1 + \rho_2) - 1}{12(\rho_2 - \rho_4)(\rho_4 - \rho_1)} \end{pmatrix}$$

Note that $\nu_1 + \nu_3$, ν_2, ν_4 can not vanish. The reason is as follows: For example, assume that $-6\rho_2\rho_4 + 2(\rho_2 + \rho_4) - 1 = 0$. Then

$$\rho_4 = \frac{2\rho_2 - 1}{6\rho_2 - 2}$$

holds. Substituting this into the cubic equation

$$\rho_4^3 - \frac{9}{7}\rho_4^2 + \frac{3}{7}\rho_4 - \frac{1}{35} = 0,$$

we see that

$$\frac{64\rho_2^3-24\rho_2^2-12\rho_2+3}{35(6\rho_2-2)^3}=0\,.$$

But, by Lemma 1.7.2, there is no common roots for the cubic equations

$$\rho_2^3-\frac{9}{7}\rho_2^2+\frac{3}{7}\rho_2-\frac{1}{35}=0$$

and

$$\rho_2^3-\frac{3}{8}\rho_2^2-\frac{3}{16}\rho_2+\frac{3}{64}=0\,.$$

Then, from the equations (1) and (2) we have

$$v_1A_1+v_3A_3=v_2A_2=v_4A_4=0$$

and

$$v_1B_1+v_3B_3=v_2B_2=v_4B_4=0.$$

Since $v_2\neq 0$, $A_2=B_2=0$ holds. This means the equations $\tau_{21}=\rho_2^2/2$ and $\rho_1\tau_{21}=\rho_2^3/6$, which imply $3\rho_1=\rho_2$. Hence, we lead to a contradiction by virtue of Lemma 1.7.3.

Case 1.3. $\rho_1=\rho_4$.
This is equivalent to Case 1.2.

Case 1.4. $\rho_2=\rho_3$.
We can assume that ρ_1, ρ_2, ρ_4 are distinct. From (E–0), (E–1), (E–21), we have the solution

$$v_1=\frac{-6\rho_2\rho_4+2(\rho_2+\rho_4)-1}{12(\rho_1-\rho_2)(\rho_4-\rho_1)}$$

$$v_2+v_3=\frac{-6\rho_4\rho_1+2(\rho_4+\rho_1)-1}{12(\rho_1-\rho_2)(\rho_2-\rho_4)}\,,$$

$$v_4=\frac{-6\rho_1\rho_2+2(\rho_1+\rho_2)-1}{12(\rho_2-\rho_4)(\rho_4-\rho_1)}\,.$$

Note that each numerator on the right can not vanish by the same reason as in Case 1.2. Then, (1) implies $v_1A_1=v_2A_2+v_3A_3=v_4A_4=0$. Since $v_1\neq 0$, we see $A_1=0$, which means $\rho_1=0$. Thus, we lead to a contradiction.

Case 1.5. $\rho_2=\rho_4$

and

Case 1.6. $\rho_3=\rho_4$.

Both of them are equivalent to Case 1.4.

Case 2. No two of ρ_1, ρ_2, ρ_3, ρ_4 are equal.

The equation (1) implies $v_1 A_1 = v_2 A_2 = v_3 A_3 = v_4 A_4 = 0$. Thus, we distinguish cases according as v_i or A_i vanishes. We have, however, the following results.

Lemma 1.7.4. *The case of* $v_J = v_K = v_L = 0$ *can not occur.*

Proof. In this case, $v_I = 1/2$ by (E–0). Then, (E–1) implies $\rho_I = 1/3$. But, they do not satisfy (E–21). □

Lemma 1.7.5. *The case for* $v_K = v_L = 0$ *leads to a contradiction.*

Proof. The equation $v_K = v_L = 0$ yields a linear system

$$v_I + v_J = \frac{1}{2},$$

$$\rho_I v_I + \rho_J v_J = \frac{1}{6}$$

by (E–0), (E–1). Since $\rho_I \neq \rho_J$, this system has the solution

$$v_I = \frac{1 - 3\rho_J}{6(\rho_I - \rho_J)}, \quad v_J = \frac{1 - 3\rho_I}{6(\rho_J - \rho_I)}.$$

Substitution of this into (E–21) and (E–31) implies

$$\frac{1}{6}(\rho_I + \rho_J) - \frac{1}{2}\rho_I \rho_J = \frac{1}{12},$$

$$\frac{1}{6}(\rho_I^2 + \rho_I \rho_J + \rho_J^2) - \frac{1}{2}\rho_I \rho_J(\rho_I + \rho_J) = \frac{1}{20}.$$

Put $X = \rho_I + \rho_J$, $Y = \rho_I \rho_J$, we have

$$2X - 6Y = 1,$$

$$10(X^2 - Y) - 30XY = 3.$$

Thus, we easily see that $X = 4/5$, $Y = 1/10$. That is, ρ_I and ρ_J are equal to the roots of the quadratic equation

$$x^2 - \frac{4}{5}x + \frac{1}{10} = 0, \tag{1.7.10}$$

which has real distinct roots. On the other hand, we see that

$$\begin{aligned} \text{the left on } (E-41) &= v_I \rho_I^4 + v_J \rho_J^4 \\ &= \frac{1}{6}(\rho_I + \rho_J)(\rho_I^2 + \rho_J^2) - \frac{1}{2}\rho_I \rho_J(\rho_I^2 + \rho_I \rho_J + \rho_J^2) \\ &= \frac{19}{600}. \end{aligned}$$

which is a contradiction. □

Due to the above Lemmas, we distinguish five cases.

Case 2.1. $\nu_1=0$ and $A_2=A_3=A_4=0$. By a similar consideration as in Case 1. we see that ρ_2, ρ_3, ρ_4 satisfy

$$\rho_2+\rho_3+\rho_4=\frac{9}{7},$$

$$\rho_2\rho_3+\rho_3\rho_4+\rho_4\rho_2=\frac{3}{7},$$

$$\rho_2\rho_3\rho_4=\frac{1}{35}.$$

Hence, they are equal to the distinct roots of the cubic equation (3). Note that, contrary to Case 1, ρ_1 is equal to none of them.

On the other hand, the equation (2) yields $\nu_2B_2=\nu_3B_3=\nu_4B_4=0$. Taking Lemma 1.7.5 into account, we are sufficient to consider the case $B_2=B_3=B_4=0$.

$A_2=B_2=0$ implies the equations $\tau_{21}=\rho_2^2/2$ and $\rho_1\tau_{21}=\rho_2^3/6$, which give $\rho_1=\rho_2/3$. $A_3=B_3=0$ implies a linear system

$$\tau_{31}+\tau_{32}=\frac{1}{2}\rho_3^2,$$

$$\rho_1\tau_{31}+\rho_2\tau_{32}=\frac{1}{6}\rho_3^3,$$

which has the solution

$$\tau_{31}=\frac{\rho_3^2(3\rho_2-\rho_3)}{4\rho_2},\quad \tau_{32}=\frac{\rho_3^2(\rho_3-\rho_2)}{4\rho_2}. \tag{1.7.11}$$

Since ρ_2, ρ_3, ρ_4 are distinct, (E–0), (E–1), (E–21) give the solution for ν_2, ν_3, ν_4 as

$$\begin{cases} \nu_2=\dfrac{-6\rho_3\rho_4+2(\rho_3+\rho_4)-1}{12(\rho_2-\rho_3)(\rho_4-\rho_2)}, \\ \nu_3=\dfrac{-6\rho_4\rho_2+2(\rho_4+\rho_2)-1}{12(\rho_2-\rho_3)(\rho_3-\rho_4)}, \\ \nu_4=\dfrac{-6\rho_2\rho_3+2(\rho_2+\rho_3)-1}{12(\rho_3-\rho_4)(\rho_4-\rho_2)}. \end{cases} \tag{1.7.12}$$

(E–44) gives the equation

$$\nu_4(\rho_1^2\tau_{41}+\rho_2^2\tau_{42}+\rho_3^2\tau_{43})=\frac{1}{360}-\nu_2\rho_1^2\tau_{21}-\nu_3(\rho_1^2\tau_{31}+\rho_2^2\tau_{32})$$
$$=\frac{1}{360}-\frac{1}{18}\nu_2\rho_2^4-\nu_3\rho_2^2\left(\frac{1}{9}\tau_{31}+\tau_{32}\right)$$
$$=\frac{1}{360}-\frac{1}{18}\nu_2\rho_2^4-\frac{1}{18}\nu_3\rho_2\rho_3^2(4\rho_3-3\rho_2)$$

by (9). Hence, we may represent the left on (E–54) as the polynomial of ρ_2 and ρ_3. By (9) and (10),

$$\nu_2\rho_2\rho_1^2\tau_{21}+\nu_3\rho_3(\rho_1^2\tau_{31}+\rho_2^2\tau_{32})+\nu_4\rho_4(\rho_1^2\tau_{41}+\rho_2^2\tau_{42}+\rho_3^2\tau_{43})-\frac{1}{504}$$
$$=\frac{1}{18}\nu_2\rho_2^5+\frac{1}{18}\nu_3\rho_2\rho_3^3(4\rho_3-3\rho_2)+\frac{\rho_4}{360}-\frac{1}{18}\nu_2\rho_2^4\rho_4$$
$$-\frac{1}{18}\nu_3\rho_2\rho_3^2\rho_4(4\rho_3-3\rho_2)-\frac{1}{504}$$
$$=\frac{1}{37800(\rho_2-\rho_3)}(525\rho_2^2\rho_3^2-360\rho_2^2\rho_3-420\rho_2\rho_3^2$$
$$-5\rho_2^2+260\rho_2\rho_3+105\rho_3^2-60\rho_3+3)\,.$$

Let us denote the numerator of the above by $\varphi(\rho_2, \rho_3)$. The question is whether $\varphi(\rho_2, \rho_3)$ vanishes for any pair (ρ_2, ρ_3). We have known the values R_0, R_1, R_{-1} which ρ_2 and ρ_3 are possible to be equal to. Calculation shows the following:

$$\varphi(R_0, R_1)=\frac{4}{343}(-420\cos^2\theta-760\sqrt{3}\sin\theta\cdot\cos\theta-630\sqrt{2}\cos\theta+60\sqrt{6}\sin\theta$$
$$+189+42\sqrt{3}),$$
$$\varphi(R_0, R_{-1})=\frac{4}{343}(-420\cos^2\theta+760\sqrt{3}\sin\theta\cdot\cos\theta-630\sqrt{2}\cos\theta-60\sqrt{6}\sin\theta$$
$$+189-42\sqrt{3}),$$
$$\varphi(R_1, R_0)=\frac{4}{343}(1350\cos^2\theta-170\sqrt{3}\cos\theta\cdot\sin\theta+405\sqrt{2}\cos\theta-285\sqrt{6}\sin\theta$$
$$-696-42\sqrt{3}),$$
$$\varphi(R_1, R_{-1})=\frac{4}{343}(-930\cos^2\theta+590\sqrt{3}\sin\theta\cdot\cos\theta+225\sqrt{2}\cos\theta-345\sqrt{6}\sin\theta$$
$$+444+42\sqrt{3}),$$
$$\varphi(R_{-1}, R_0)=\frac{4}{343}(1350\cos^2\theta+170\sqrt{3}\sin\theta\cdot\cos\theta+405\sqrt{2}\cos\theta+285\sqrt{6}\sin\theta$$
$$-696+42\sqrt{3}),$$
$$\varphi(R_{-1}, R_1)=\frac{4}{343}(-930\cos^2\theta-590\sqrt{3}\sin\theta\cdot\cos\theta+225\sqrt{2}\cos\theta+345\sqrt{6}\sin\theta$$
$$+444-42\sqrt{3}).$$

Computation by interval arithmetic shows the following:

$$\varphi(R_0, R_1) \in [-11.6391, -11.6390],$$
$$\varphi(R_0, R_{-1}) \in [-4.70784, -4.70783],$$
$$\varphi(R_1, R_0) \in [3.20479, 3.20480],$$
$$\varphi(R_1, R_{-1}) \in [0.821791, 0.821792],$$
$$\varphi(R_{-1}, R_0) \in [12.1750, 12.1751],$$
$$\varphi(R_{-1}, R_1) \in [-0.956777, -0.956776].$$

(On the interval arithmetic, see [8]. Above calculation is carried out by the program made by K. Ichida on HITAC VOS3 at the Educational Center for Information Processing, Kyoto Univ.) None of them vanishes under the condition (4) because every interval given above is away from zero. Thus, we have a contradiction.

Case 2.2. $\nu_2=0$ and $A_1=A_3=A_4=0$. $A_1=0$ implies $\rho_1=0$. Then, ρ_2, ρ_3, ρ_4 can not vanish. From (E–1), (E–21), we have

$$\nu_3=\frac{1-2\rho_4}{12\rho_3(\rho_3-\rho_4)}, \quad \nu_4=\frac{1-2\rho_3}{12\rho_4(\rho_4-\rho_3)}.$$

Substituting these into (E–31), (E–41), we see that

$$\rho_3+\rho_4-2\rho_3\rho_4=\frac{3}{5},$$

$$(\rho_3+\rho_4)^2-2\rho_3\rho_4(\rho_3+\rho_4)-\rho_3\rho_4=\frac{2}{5}.$$

Put $X=\rho_3+\rho_4$, $Y=\rho_3\rho_4$, then we have $X=1$, $Y=1/5$. The left on (E–51) is equal to

$$\frac{1}{12}(-2\rho_3^3\rho_4-2\rho_3\rho_4^3-2\rho_3^2\rho_4^2+\rho_3^3+\rho_3^2\rho_4+\rho_3\rho_4^2+\rho_4^3)$$

$$=\frac{1}{12}\{X^3-2(X^2-Y)Y-2(X+Y)Y\}=\frac{1}{100},$$

which is a contradiction.

Case 2.3. $\nu_3=0$ and $A_1=A_2=A_4=0$. Equivalent to Case 2.2.

Case 2.4. $\nu_4=0$ and $A_1=A_2=A_3=0$. Equivalent to Case 2.2.

Case 2.5. $A_1=A_2=A_3=A_4=0$. $A_1=0$ implies $\rho_1=0$, which means $B_1=0$. Then, the equations $\sum \nu_i B_i=\sum \nu_i\rho_i B_i=\sum \nu_i\rho_i^2 B_i=0$ yield $\nu_2B_2=\nu_3B_3=\nu_4B_4=0$. Since ν_2, ν_3, ν_4 are assumed to be non-zero, we have $B_2=B_3=B_4$

$=0$. $B_2=\rho_1\tau_{21}-\rho_2^3/6=0$ implies $\rho_2=0$ because $\rho_1=0$. This contradicts the assumption that no two of ρ_i are equal.

Now, we have accomplished to investigate the whole cases. In conclusion, we have

Theorem 8. *The explicit* (1, 4)*-stage formula can not attain order* 7. *Its attainable order is* 6.

Note. SHINTANI gives (1, 4)-stage formula with parameters $\nu_1=1/20$, $\nu_2=7(7+\sqrt{21})/360$, $\nu_3=8/45$, $\nu_4=7(7-\sqrt{21})/360$, $\rho_1=0$. $\rho_2=(7-\sqrt{21})/14$, $\tau_{21}=(5-\sqrt{21})/28$, $\rho_3=1/2$, $\tau_{31}=(3-\sqrt{21})/192$, $\tau_{32}=(21+\sqrt{21})/192$, $\rho_4=(7+\sqrt{21})/14$, $\tau_{41}=(21+5\sqrt{21})/294$, $\tau_{42}=(\sqrt{21}-3)/84$, $\tau_{43}=(21+\sqrt{21})/147$. These parameters are also not unique solution of (E–0) – (E–46).

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