# Resolution of Runge-Kutta-Nystrom Condition Equations through Eighth Order

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**A systematic development of general solutions of the condition equations for minimal stage Runge-Kutta-Nystrom algorithms through eighth order is made. Although it is known that, for $m$th-order accuracy, $(m-1)$-stage methods are possible through $m=6$, the general sixth-order algorithm, shown here to have two free parameters and to include Albrecht's formula as a special case, appears to be a new result. General seventh- and eighth-order algorithms, for which the number of stages is the same as the order of the method, are also developed, as well as a proof of the nonexistence of a seventh-order, six-stage method.**

## Introduction

IN 1925, Nystrom[1] investigated the numerical integration, using Runge-Kutta techniques, of a certain special class of second-order differential equations for which the right-hand sides are explicit functions only of the dependent and independent variables. He found it possible to achieve a higher degree of agreement with the Taylor series expansion of the solution for a given number of evaluations of the right-hand side of the differential equation than could be expected from the general case. Thus, with two evaluations he could achieve agreement with an error of $O(h^4)$ of $O(h^5)$ with three evaluations, and of $O(h^6)$ with four evaluations, where $h$ is the integration step size. Nystrom developed special algorithms for these three cases, which are also summarized in a textbook by Henrici.[2]

The interesting speculation as to whether or not this computational advantage persists for higher-order methods remained unanswered for 30 years. Then, in 1955, Albrecht[3] published a special, "symmetrical" (i.e., equal subdivisions of the integration interval) algorithm for a sixth-order method with five evaluations.

Most of this paper is devoted to developing general solutions of the condition equations through eighth order using the fewest number of right-hand side evaluations or "stages" as possible. The phenomenon, first observed by Nystrom, of $m-1$ stages for $m$th-order accuracy, does not seem to prevail beyond $m=6$. Indeed, an interesting proof of the nonexistence of a seventh-order, six-stage algorithm is given in a later section. By increasing the number of stages by one, however, general methods are achieved for seventh and eighth order.

To the author's knowledge, the problem of obtaining general solutions of the condition equations has not been undertaken in any systematic way. As an isolated result, Henrici includes, as a problem in his text, a one-parameter family of values for the coefficients of Nystrom's fourth-order method. (In fact, however, as will be shown, the fourth-order algorithm admits of two free parameters.)

The task of developing efficient higher-order algorithms is complicated by the fact that the number of condition equations for the parameters, many of which are nonlinear, increases with increasing order considerably faster than the number of parameters to be determined. By increasing the number of stages, the set of parameters is also enlarged. The number of equations is unchanged but the efficiency is adversely affected.

The results obtained here compare quite favorably with explicit Runge-Kutta methods applied to general first-order differential equations. It has been shown by Butcher[4] that for $m \geq 5$, an order $m$ algorithm can be achieved only if the number of stages $n$ is greater than $m$ and for $m \geq 7$, then we must have $n > m+1$. The existence of particular methods shows that his are the best possible results up to order seven. For order eight, at least 10 stages are necessary but no method has been published requiring fewer than 11. We compare in Table 1 the number of stages for Runge-Kutta methods with those of Runge-Kutta-Nystrom as obtained in this paper.

The author has elected to present his results as formulas for the Nystrom parameters expressed as functions of certain free parameters. The algorithms so obtained will have the widest possible applicability and the user may apply his own criteria for the problem at hand in selecting appropriate values for these arbitrary parameters.

## Fundamental Considerations

The Runge-Kutta-Nystrom method of numerical integration is a one-step process applied to the special class of second-order vector differential equations

$$\frac{dx}{dt}=y, \quad \frac{dy}{dt}=f(t,x)$$

where $f$ is *not* an explicit function of $y$. The particular algorithms considered in this paper are special cases of the formulas given below where $t_0$, $x_0$, $y_0$ are the initial values for the integration step, $h$ is the integration step size, $n$ is the number of stages, i.e., the number of evaluations of $f$, required.

$$x=x_0+hy_0+h^2\sum_{i=0}^{n-1}a_ik_i+O(h^{m+1})$$

**Table 1 Comparison of R-K and R-K-N methods**

| Order | Number of stages R-K | R-K-N |
|---|---|---|
| 5 | 6 | 4 |
| 6 | 7 | 5 |
| 7 | 9 | 7 |
| 8 | 11 | 8 |

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$$y=y_0+h\sum_{i=0}^{n-1}b_ik_i+O(h^{m+1})$$

$$k_0=f(t_0+hp_0,\ x_0+hp_0y_0)$$

$$\vdots \qquad \vdots$$

$$k_i=f(t_0+hp_i,\ x_0+hp_iy_0+h^2\sum_{j=0}^{i-1}c_{ij}k_j)$$

$$(i=1,\ldots,n-1)$$

where

$$c_{10}=q_1, \qquad c_{i0}=q_i-\sum_{j=1}^{i-1}c_{ij} \quad (i=2,\ldots,n-1)$$

The general problem consists of determining the parameters $p_i,q_i,c_{ij},a_i,b_i$ so that we have an $m$th-order agreement with the Taylor series expansion of $x$ and $y$ with $n$ as small as possible.

The equations of condition for these parameters are given in vector-matrix form in Table 2 for second, third, and fourth-order formulas with the number of stages one less than the order of the method. These equations are identified by greek alphabetic characters to be considered as vectors of appropriate dimension.

We make the following observations which hold in general for the higher-order equations of condition:

1) All equations for the coefficients $a_i$ are redundant with those for $b_i$ if $a_i=(1-p_i)b_i$.

2) Equations ($\alpha$) consist of $m$ linear equations for the $n$ coefficients $b_0,\ldots,b_{n-1}$ with the matrix of coefficients being a so-called Vandermode matrix. Since $n=m-1$ these equations

$$\sum_{j=0}^{m-2}p_j^ib_j=\frac{1}{i+1} \qquad (i=0,\ldots,m-1) \qquad (\alpha^i)$$

will be inconsistent unless the $m\times m$ determinant

$$D_m=\left|p_j^i,\ \frac{1}{i+1}\right| \qquad (i=0,\ldots,m-1;\ j=0,\ldots,m-2)$$

vanishes. The value of this determinant may be expressed as

$$D_m=V_{m-1}(p_0)L_m(p_0,\ldots,p_{m-2})$$

where

$$V_\ell(p_k)=|p_{j+k}^i| \qquad (i,\ j=0,\ldots,\ell-1)$$

is a Vandermonde determinant whose value is

$$V_\ell(p_k)=\prod_{i=j+1}^{\ell-1}\prod_{j=0}^{\ell-2}(p_{i+k}-p_{j+k})$$

and

$$L_\ell(p_0,\ldots,p_{\ell-2})=\sum_{j=0}^{\ell-1}\frac{1}{\ell-j}\beta_j$$

with $\beta_0,\beta_1,\ldots$ defined by

$$\prod_{j=0}^{\ell-2}(p-p_j)=\sum_{j=0}^{\ell-1}\beta_j\,p^{\ell-j-1}$$

For computational purposes, it is useful to note that the $\beta$'s may be generated recursively from

$$\beta_0=1, \quad \beta_i=-\frac{1}{i}\sum_{j=0}^{i-1}\beta_js_{i-j} \qquad (i=1,\ldots,\ell-1)$$

where

$$s_i=p_0^i+p_1^i+\ldots+p_{\ell-2}^i$$

We shall refer to these functions $L_m$ as "constraint functions." Note that they are symmetrical in their arguments

**Table 2 Equations of condition for $m=2,3,4$; $n=m-1$**

| Order, stage $(m,n)$ | Eq. nos. | $a_i$ Condition eqs. | Eq. nos. | $b_i$ Condition eqs. |
|---|---|---|---|---|
| (2,1) | ($\alpha$) | $a_0=\frac{1}{2}$ | ($\alpha$) | $\begin{bmatrix}1\\p_0\end{bmatrix}b_0=\begin{bmatrix}1\\1/2\end{bmatrix}$ |
| (3,2) | ($\alpha$) | $\begin{bmatrix}1&1\\p_0&p_1\end{bmatrix}\begin{bmatrix}a_0\\a_1\end{bmatrix}=\begin{bmatrix}1/2\\1/6\end{bmatrix}$ | ($\alpha$) | $\begin{bmatrix}1&1\\p_0&p_1\\p_0^2&p_1^2\end{bmatrix}\begin{bmatrix}b_0\\b_1\end{bmatrix}=\begin{bmatrix}1\\1/2\\1/3\end{bmatrix}$ |
| | | | ($\beta$) | $q_1b_1=\frac{1}{2}\left(\frac{1}{3}\right)$ |
| (4,3) | ($\alpha$) | $\begin{bmatrix}1&1&1\\p_0&p_1&p_2\\p_0^2&p_1^2&p_2^2\end{bmatrix}\begin{bmatrix}a_0\\a_1\\a_2\end{bmatrix}=\begin{bmatrix}1/2\\1/6\\1/12\end{bmatrix}$ | ($\alpha$) | $\begin{bmatrix}1&1&1\\p_0&p_1&p_2\\p_0^2&p_1^2&p_2^2\\p_0^3&p_1^3&p_2^3\end{bmatrix}\begin{bmatrix}b_0\\b_1\\b_2\end{bmatrix}=\begin{bmatrix}1\\1/2\\1/3\\1/4\end{bmatrix}$ |
| | ($\beta$) | $q_1a_1+q_2a_2=\frac{1}{2}\left(\frac{1}{12}\right)$ | ($\beta$) | $\begin{bmatrix}1&1\\p_1&p_2\end{bmatrix}\begin{bmatrix}q_1b_1\\q_2b_2\end{bmatrix}=\frac{1}{2}\begin{bmatrix}1/3\\1/4\end{bmatrix}$ |
| | | | ($\gamma$) | $(p_1-p_0)c_{21}b_2=\frac{1}{6}\left(\frac{1}{4}-p_0\right)$ |

and, for convenience, if any of these arguments is zero, it will be suppressed in the notation. Thus, without confusion, we shall write

$$L_4(p_2) \equiv L_4(0,0,p_2)$$

Further, it is easy to show that the constraint functions satisfy the recursive relation

$$L_\ell(p_0,\ldots,p_{\ell-2}) = L_\ell(p_0,\ldots,p_{\ell-3}) - p_{\ell-2}L_{\ell-1}(p_0,\ldots,p_{\ell-3})$$

An interesting interpretation of the constraint functions may be had using the following identity for the determinant of block partitioned matrices:

$$\begin{vmatrix} A_{kk} & B_{k\ell} \\ C_{\ell k} & D_{\ell\ell} \end{vmatrix} = |A_{kk}| \; |D_{\ell\ell} - C_{\ell k}A_{kk}^{-1}B_{k\ell}|$$

We can easily show that

$$D_m = V_{m-1}(p_0)\left(\frac{1}{m} - \sum_{j=0}^{m-2} p_j^{m-1}b_j\right) = V_{m-1}(p_0)R(\alpha^{m-1})$$

so that $L_m$ is simply the residue $R(\alpha^{m-1})$ of Eq. $(\alpha^{m-1})$. Thus, a necessary and sufficient condition for the consistency of Eqs. $(\alpha^i)$ is that

$$R(\alpha^{m-1}) = L_m(p_0,\ldots,p_{m-2}) = 0$$

and $V_{m-1}(p_0) \neq 0$. The nonvanishing of the Vandermonde determinant is equivalent to requiring that $p_i \neq p_j$ for $i \neq j$.

3) Square Vandermonde matrices have simple explicit inverses. For if we define

$$P_{m-1}^i(p) = \prod_{j=0}^{m-1}{}^i (p-p_j) = \sum_{j=0}^{m-1} \beta_j^i p^j \qquad (i=0,\ldots,m-1)$$

where the superscript $i$ on the product symbol indicates that the factor for which $j=i$ is omitted, then the inverse of the Vandermonde matrix

$$V_m(p_0) = \|p_j^i\| \qquad (i,j=0,\ldots,m-1)$$

is given by

$$V_m^{-1}(p_0) = \left\| \frac{\beta_j^i}{P_{m-1}^i(p_i)} \right\|$$

Thus, with $L_m(p_0,\ldots,p_{m-2}) = 0$, the solutions of Eqs. $(\alpha)$ are

$$b_{m-2} = \frac{D_{m-1}}{V_{m-1}(p_0)} = \frac{L_{m-1}(p_0,\ldots,p_{m-3})}{(p_{m-2}-p_0)\ldots(p_{m-2}-p_{m-3})} \qquad (0,1,\ldots,m-2)$$

with $b_0,\ldots,b_{m-3}$ obtained by a cyclic permutation of the subscripts $(0,1,\ldots,m-2)$. We shall use this notation frequently for compactness in expressing our results.

4) The constraint condition $L_m = 0$ imposed on the selection of the $p_i$'s can be eliminated by increasing the number of stages in the algorithm by one so that $m=n$. The left-hand side of each condition equation will have an obvious additional term, with a consequent increase in the number of parameters to be determined, but the number of equations will remain the same. Since we are free to assign values to these extra parameters, we may set

$$p_0 = 0, \quad p_{m-1} = 1, \quad c_{m-1,j} = a_j \quad (j=0,\ldots,m-2)$$

In this case, the last computed $k_i$ in the algorithm, $k_{m-1}$, for a given integration step will be identical with the value of $k_0$ to be computed for the next step. As a consequence, only the first integration step requires $m$ evaluations of the function $f$. All succeeding steps involve $m-1$ stages, as before.

The solutions of the equations of condition for second-, third-, and fourth-order methods are summarized in Table 3. The left-hand column gives parameter values for the conventional algorithm with $n=m-1$. The parameters listed in the right-hand column are for the algorithms with $n=m$ for the first stage only. For compactness, we have adopted the notation $p_{ij} = p_i - p_j$.

In his fundamental memoir, Nystrom gave third- and fourth-order formulas for the following values of the $p_i$'s:

$$m=3, \quad n=2: \quad p_0=0, \quad p_1=\frac{2}{3}$$

$$m=4, \quad n=3: \quad p_0=0, \quad p_1=\frac{1}{2}, \quad p_2=1$$

### Fifth-Order Method ($m=5$, $n=4$)

The relevant equations of condition for the fifth-order, four-stage algorithm are listed in Table 4. Equations $(\alpha)$ are handled as described in the previous section. Equations $(\beta)$

**Table 3 Parameters for $m$th order, $n-1$ stage algorithms ($m=2,3,4$)**

| Order, stage $(m,n)$ | Free params. | Parameters for $n=m-1$: Constraints | Parameters for $n=m-1$: Eqs. for parameters | Parameters for $n=m$ (first stage only): Constraints | Parameters for $n=m$ (first stage only): Eqs. for parameters |
|---|---|---|---|---|---|
| (2,1) | 0 | $L_2(p_0)=0$ | $b_0=1$ | $p_0=0$ | $b_0=b_1=½$ |
| | | | | $p_1=1$ | $q_1=c_{10}=a_0=(1-p_0)b_0=½$ |
| (3,2) | 1 | $L_3(p_0,p_1)=0$ | $p_{10}b_1=L_2(p_0)$ (0,1) | $p_0=0$ | $p_{20}p_{21}b_2=L_3(p_0,p_1)$ (0,1,2) |
| | | $b_1 \neq 0$ | $b_1q_1=1/6$ | $p_2=1$ | $q_i=½p_i^2$ $(i=1,2)$ |
| | | | | | $c_{2i}=a_i=(1-p_i)b_i$ $(i=0,1)$ |
| (4,3) | 2 | $L_4(p_0,p_1,p_2)=0$ | $p_{20}p_{21}b_2=L_3(p_0,p_1)$ (0,1,2) | $p_0=0$ | $p_{30}p_{31}p_{32}b_3=L_4(p_0,p_1,p_2)$ (0,1,2,3) |
| | | $b_1,b_2 \neq 0$ | $b_1q_1=\frac{1}{2p_{21}}\left(\frac{1}{3}p_2-\frac{1}{4}\right)$ (1,2) | $p_3=1$ | $q_i=½p_i^2$ $(i=1,2,3)$ |
| | | | $b_2c_{21}=\frac{1}{6p_{10}}\left(\frac{1}{4}-p_0\right)$ | $b_2 \neq 0$ | $b_2c_{21}=\frac{1}{6p_1}\left(\frac{1}{4}-b_3\right)$ |
| | | | | | $c_{3i}=a_i=(1-p_i)b_i$ $(i=0,1,2)$ |

determine $q_1, q_2, q_3$ so that Eq. ($\delta$) provides a constraint on the choice of the $p_i$'s. Similarly, Eqs. ($\gamma$), ($\epsilon$) determine $b_2c_{21}, b_3c_{31}, b_3c_{32}$ with an additional constraint implied by Eq. ($\zeta$).

To calculate the residue of Eq. ($\delta$) we first form the four-dimensional determinant $D$ of the coefficients of the $q_i$'s in Eqs. ($\beta$), ($\delta$) augmented by the right-hand sides

$$D = \begin{vmatrix} b_1 & b_2 & b_3 & 1/6 \\ p_1b_1 & p_2b_2 & p_3b_3 & 1/8 \\ p_1^2b_1 & p_2^2b_2 & p_3^2b_3 & 1/10 \\ q_1b_1 & q_2b_2 & q_3b_3 & 1/20 \end{vmatrix}$$

Solving Eqs. ($\alpha$) and ($\beta$) for $b_i$ and $q_ib_i$, we have

$$p_{10}p_{12}p_{13}b_1 = L_4(p_0.p_2,p_3) \quad (0,1,2,3)$$

$$2p_{12}p_{13}q_1b_1 = L_5(p_2,p_3) \quad (1,2,3)$$

From the constraint condition needed for the consistency of Eqs. ($\alpha$) and the recursion relation for the $L$ functions, we may establish the following to be used in the first column of $D$:

$$p_1L_4(p_0,p_2,p_3) = L_5(p_0,p_2,p_3)$$

$$p_1^2L_4(p_0,p_2,p_3) = L_6(p_0,p_2,p_3) - L_6(p_0,p_1,p_2,p_3)$$

$$p_{10}L_5(p_2,p_3) = L_6(p_0,p_2,p_3) - L_6(p_1,p_2,p_3)$$

$$p_0L_5(p_1,p_2,p_3) = p_1^2L_4(p_0,p_2,p_3) - p_{10}L_5(p_2,p_3)$$

Additional required relations may be established for the other columns of $D$.

We now substitute for the elements of the determinant $D$, subtract two times row 4 from row 3 and remove the common factors from all rows and columns. Next multiply row 3 by $L_6(p_1,p_2,p_3)$ and add to row 4. Then subtract col 2 from col 1 and col 3 from col 2 and again remove the common factors. The determinant is now three dimensional

$$D = \frac{p_0L_5(p_1,p_2,p_3)}{4V_4(p_0)p_{13}} \begin{vmatrix} L_3(p_0,p_3) & L_3(p_0,p_1) & 1/3 \\ L_4(p_0,p_3) & L_4(p_0,p_1) & 1/4 \\ L_5(p_0,p_3) & L_5(p_0,p_1) & 1/5 \end{vmatrix}$$

To finish the reduction, we subtract col 2 from col 1 and factor out $p_{13}$ from col 1. Then, to col 2 we add $p_1$ times col 1 and the determinant is now a function only of $p_0$. We have finally

$$8640\ V_4(p_0)D = p_0^3L_5(p_1,p_2,p_3)$$

To determine the residue of Eq. ($\delta$), we use the arguments of the previous section and obtain

$$R(\delta) = \frac{1}{8640\ V_4(p_0)V_3(p_1)b_1b_2b_3}p_0^3L_5(p_1,p_2,p_3)$$

In a similar manner we may obtain the residue of Eq. ($\zeta$) in the form

$$R(\zeta) = -\frac{1}{8640\ V_3(p_0)V_3(p_1)b_1b_2}p_0^2(p_3-1)^2$$

We have now established that the condition equations will be consistent if and only if the $p_i$'s are determined subject to the following constraint conditions:

$$L_5(p_0,p_1,p_2,p_3) = 0$$

$$p_0^3L_5(p_1,p_2,p_3) = 0$$

$$p_0^2(p_3-1)^2 = 0$$

The third condition requires that either $p_0 = 0$ or $p_3 = 1$. In the first case, we may select the remaining $p_i$'s subject to the constraint $L_5(p_1,p_2,p_3) = 0$. In the second case, the value of $p_0$ is arbitrary and $p_1, p_2$ are uniquely given by

$$p_1, p_2 = (4 \mp \sqrt{6})/10$$

For these values, we find $b_0 = 0$ and $b_2, b_3 \neq 0$.

In either case we may show that $q_i = \frac{1}{2}p_i^2 (i=1,2,3)$. For this purpose, we write

$$q_1 = \tfrac{1}{2}p_1^2 \frac{p_{10}L_5(p_2,p_3)}{p_1^2L_4(p_0,p_2,p_3)}$$

$$= \tfrac{1}{2}p_1^2 \frac{L_6(p_0,p_2,p_3) - L_6(p_1,p_2,p_3)}{L_6(p_0,p_2,p_3) - L_6(p_0.p_1,p_2,p_3)}$$

**Table 4 Equations of condition for $m=5$, $n=4$ [$a_i = (1-p_i)b_i$]**

| Eq. nos. | $b_i$ Condition equations |
|---|---|
| ($\alpha^i$) | $\sum_{j=0}^{3} p_j^ib_j = \frac{1}{i+1} \quad (i=0,\ldots,4)$ |
| ($\beta^i$) | $\sum_{j=1}^{3} p_j^i(q_jb_j) = \frac{1}{2(i+3)} \quad (i=0,1,2)$ |
| ($\gamma$) | $\begin{bmatrix} 1 & 1 \\ p_2 & p_3 \end{bmatrix}\begin{bmatrix} (p_1-p_0)c_{21}b_2 \\ (p_1-p_0)c_{31}b_3 + (p_2-p_0)c_{32}b_3 \end{bmatrix} = \frac{1}{6}\begin{bmatrix} (1/4)-p_0 \\ (1/5)-(3/4)p_0 \end{bmatrix}$ |
| ($\delta$) | $q_1^2b_1 + q_2^2b_2 + q_3^2b_3 = \frac{1}{4}(\frac{1}{5})$ |
| ($\epsilon$) | $[1 \quad 1]\begin{bmatrix} (p_1^2-p_0^2)c_{21}b_2 \\ (p_1^2-p_0^2)c_{31}b_3 + (p_2^2-p_0^2)c_{32}b_3 \end{bmatrix} = \frac{1}{12}(\frac{1}{5} - 2p_0^2)$ |
| ($\zeta$) | $q_1c_{21}b_2 + q_1c_{31}b_3 + q_2c_{32}b_3 = \frac{1}{120}$ |

and the conclusion follows from the second constraint condition since

$$L_6(p_0,p_1,p_2,p_3) = L_6(p_1,p_2,p_3) - p_0 L_5(p_1,p_2,p_3)$$
$$= L_6(p_1,p_2,p_3)$$

The solutions of the condition equations are summarized in Table 5. As before, the first part of the table corresponds to the conventional algorithm with $n=4$. The second part contains parameters for the algorithm with $n=5$ for the first step only. In the latter case, an additional free parameter is available.

Nystrom gave fifth-order formulas for the following values of $p_i$'s:

$$m=5,\ n=4:\ p_0=0,\ p_1=\frac{2}{5},\ p_2=\frac{2}{3}$$

$$p_0=0,\ p_1=\frac{1}{5},\ p_2=\frac{2}{3},\ p_3=1$$

## General Equations of Condition

The author derived the equations of condition for $p_0 \neq 0$ and $m \leq 5$ as given in Tables 2 and 4. For $p_0=0$ and $q_i=\frac{1}{2}p_i^2$, Fehlberg[5] derived the condition equations through $m=9$. An independent derivation through $m=7$ was made, and complete agreement with Fehlberg was found. The task is quite laborious and the number of equations increases dramatically with increasing order. For example, 13 equations (including redundant ones) evolve for $m=5$. For $m=6$, 10 more are added; for $m=7$, an additional 20, and for $m=8$, the increase is 36 or 79 in all. For a ninth-order set, the number is 151.

Successful treatment of these equations depends strongly on proper grouping of the terms. A convenient set of functions of the Nystrom parameters for this purpose is given below and the equations of condition through $m=8$ in terms of these functions are listed in Table 6.

$$H_i^k = p_i \sum_{j=i+1}^{n-1} p_j^k b_j c_{ji} \qquad i=1,\ldots,n-2 \quad k=0,\ldots$$

$$A_i^k = \frac{1}{(k-1)!} \sum_{j=1}^{i-1} c_{ij} p_j^{k-1} \qquad i=2,\ldots,n-1 \quad k=2,\ldots$$

$$A_i^{k\ell} = \frac{(\ell+1)!}{(k-1)!} \sum_{j=2}^{i-1} c_{ij} p_j^{k-\ell-2} A_j^\ell \qquad i=3,\ldots,n-1 \quad k=\ell+2,\ldots \quad \ell=2,\ldots$$

$$A_i^{k42} = \frac{5!}{(k-1)!} \sum_{j=3}^{i-1} c_{ij} p_j^{k-6} A_j^{42} \qquad i=4,\ldots,n-1 \quad k=6,\ldots$$

As already mentioned, we need only consider the equations for the $b_i$'s since we always have $a_i=(1-p_i)b_i$. The gaps in the greek alphabet labels for the equations arise from the redundancy created by the assumption that $q_i=\frac{1}{2}p_i^2$. The additional equations needed for $m=8$ (the last six in Table 6) are taken from Fehlberg and, therefore, carry a separate labeling

**Table 5 Parameters for fifth-order, four stage algorithms**

| Free params. | Constraints | Eqs. for parameters | |
|---|---|---|---|
| | | Parameters for $n=4$ | |
| 1 | $p_1,p_2=(4\mp\sqrt{6})/10$ | $p_{30}p_{31}p_{32}b_3=L_4(p_0,p_1,p_2)$ | (0,1,2,3) |
| | $p_3=1$ | $q_i=\frac{1}{2}p_i^2$ | ($i$=1,2,3) |
| | | $p_{10}b_2c_{21}=\frac{1}{6p_{23}}\left[p_0p_3-\frac{1}{4}(3p_0+p_3)+\frac{1}{5}\right]$ | |
| | | $p_{10}b_3c_{31}=\frac{1}{6p_{12}}\left[p_0p_2-\frac{1}{4}(p_0+p_2)+\frac{1}{10}\right]-p_{10}b_2c_{21}$ | |
| | | $p_{20}b_3c_{32}=\frac{1}{6p_{21}}\left[p_0p_1-\frac{1}{4}(p_0+p_1)+\frac{1}{10}\right]$ | |
| 2 | $p_0=0$; $L_5(p_1,p_2,p_3)=0$; $b_2,b_3\neq 0$ | (Same as above) | |
| | | Parameters for $n=5$ (first stage only) | |
| Free params. | Constraints | Eqs. for parameters | |
| 3 | $p_0=0$ | $p_{40}p_{41}p_{42}p_{43}b_4=L_5(p_0,p_1,p_2,p_3)$ | (0,1,2,3,4) |
| | $p_4=1$ | $q_i=\frac{1}{2}p_i^2$ | ($i$=1,2,3,4) |
| | $b_2,b_3\neq 0$ | $p_1b_2c_{21}=\frac{1}{6p_{23}}\left[p_3b_4-\frac{1}{4}(p_3+4b_4)+\frac{1}{5}\right]$ | |
| | | $p_1b_3c_{31}=\frac{1}{6p_{12}}\left[p_2b_4-\frac{1}{4}(p_2+2b_4)+\frac{1}{10}\right]-p_1b_2c_{21}$ | |
| | | $p_2b_3c_{32}=\frac{1}{6p_{21}}\left[p_1b_4-\frac{1}{4}(p_1+2b_4)+\frac{1}{10}\right]$ | |
| | | $c_{4i}=a_i=(1-p_i)b_i$ | ($i$=0,1,2,3) |

**Table 6 Equations of condition for $m=3,\ldots,8$ $[p_0=0,\ q_i=\tfrac{1}{2}p_i^2,\ a_i=(1-p_i)b_i]$**

| Eq. nos. | $b_i$ Condition equations | | Eq. nos. | $b_i$ Condition equations | |
|---|---|---|---|---|---|
| $(\alpha^i)$ | $\sum_{j=0}^{n-1} p_j^i b_j = \frac{1}{i+1}$ | $(i=0,\ldots,m-1)$ | $(e_1^i)$ | $\sum_{j=2}^{n-1} p_j^i A_j^2 A_j^3 b_j = \frac{1}{3!4!(i+8)}$ | $(i=0\ldots,m-8)$ |
| $(\gamma^i)$ | $\sum_{j=2}^{n-1} p_j^i (A_j^2 b_j) = \frac{1}{3!(i+4)} = \frac{1}{1!}\sum_{j=1}^{n-2} H_j^i$ | $\ldots,m-4)$ | $(e_2^i)$ | $\sum_{j=2}^{n-1} p_j^i (A_j^6 b_j) = \frac{1}{7!(i+8)} = \frac{1}{5!}\sum_{j=1}^{n-2} p_j^4 H_j^i$ | $\ldots,m-8)$ |
| $(\epsilon^i)$ | $\sum_{j=2}^{n-1} p_j^i (A_j^3 b_j) = \frac{1}{4!(i+5)} = \frac{1}{2!}\sum_{j=1}^{n-2} p_j H_j^i$ | $\ldots,m-5)$ | $(e_3^i)$ | $\sum_{j=3}^{n-1} p_j^i (A_j^{62} b_j) = \frac{1}{7!(i+8)} = \frac{3!}{5!}\sum_{j=2}^{n-2} p_j A_j^2 H_j^i$ | $\ldots,m-8)$ |
| $(\iota^i)$ | $\sum_{j=2}^{n-1} p_j^i (A_j^4 b_j) = \frac{1}{5!(i+6)} = \frac{1}{3!}\sum_{j=1}^{n-2} p_j^2 H_j^i$ | $\ldots,m-6)$ | $(e_4^i)$ | $\sum_{j=3}^{n-1} p_j^i (A_j^{63} b_j) = \frac{1}{7!(i+8)} = \frac{4!}{5!}\sum_{j=2}^{n-2} A_j^3 H_j^i$ | $\ldots,m-8)$ |
| $(\lambda^i)$ | $\sum_{j=3}^{n-1} p_j^i (A_j^{42} b_j) = \frac{1}{5!(i+6)} = \frac{3!}{3!}\sum_{j=2}^{n-2} \frac{1}{p_j} A_j^2 H_j^i$ | $\ldots,m-6)$ | $(e_5^i)$ | $\sum_{j=3}^{n-1} p_j^i (A_j^{64} b_j) = \frac{1}{7!(i+8)} = \frac{5!}{5!}\sum_{j=2}^{n-2} \frac{1}{p_j} A_j^4 H_j^i$ | $\ldots,m-8)$ |
| $(\pi^i)$ | $\sum_{j=2}^{n-1} p_j^i A_j^2 A_j^2 b_j = \frac{1}{3!3!(i+7)}$ | $\ldots,m-7)$ | $(e_6^i)$ | $\sum_{j=4}^{n-1} p_j^i (A_j^{642} b_j) = \frac{1}{7!(i+8)} = \frac{5!}{5!}\sum_{j=3}^{n-2} \frac{1}{p_j} A_j^{42} H_j^i$ | $\ldots,m-8)$ |
| $(\sigma^i)$ | $\sum_{j=2}^{n-1} p_j^i (A_j^5 b_j) = \frac{1}{6!(i+7)} = \frac{1}{4!}\sum_{j=1}^{n-2} p_j^3 H_j^i$ | $\ldots,m-7)$ | | | |
| $(\phi^i)$ | $\sum_{j=3}^{n-1} p_j^i (A_j^{52} b_j) = \frac{1}{6!(i+7)} = \frac{3!}{4!}\sum_{j=2}^{n-2} A_j^2 H_j^i$ | $\ldots,m-7)$ | | | |
| $(\psi^i)$ | $\sum_{j=3}^{n-1} p_j^i (A_j^{53} b_j) = \frac{1}{6!(i+7)} = \frac{4!}{4!}\sum_{j=2}^{n-2} \frac{1}{p_j} A_j^3 H_j^i$ | $\ldots,m-7)$ | | | |

**Table 7 Parameters for sixth-order, five stage algorithms**

| Free parameters | Constraints |
|---|---|
| 2 | $p_0=0, p_4=1$<br>$L_6(p_1,p_2,p_3,1)=0$<br>$b_2,b_3,b_4\neq 0$ |
| **Equations for parameters** | |
| $p_{40}p_{41}p_{42}p_{43}b_4=L_5(p_0,p_1,p_2,p_3)$ | (0,1,2,3,4) |
| $q_i=\tfrac{1}{2}p_i^2$ | $(i=1,2,3,4)$ |
| $H_1^0=\frac{1}{12p_{21}p_{31}}\left[\frac{1}{2}p_2p_3-\frac{1}{5}(p_2+p_3)+\frac{1}{10}\right]$ | (1,2,3) |
| $p_1b_2c_{21}=\frac{1}{60(1-p_2)p_{32}}\left(\frac{1}{2}p_3-\frac{1}{3}\right)$ | |
| $p_1b_3c_{31}=\frac{1}{60(1-p_3)}\left[\frac{1}{p_{21}}\left(\frac{1}{2}p_1-\frac{1}{6}\right)-\frac{1}{p_{32}}\left(\frac{1}{2}p_2-\frac{1}{3}\right)\right]$ | |
| $p_2b_3c_{32}=\frac{1}{60(1-p_3)p_{12}}\left(\frac{1}{2}p_1-\frac{1}{6}\right)$ | |
| $p_1b_4c_{41}=H_1^0-p_1b_2c_{21}-p_1b_3c_{31}$ | |
| $p_2b_4c_{42}=H_2^0-p_2b_3c_{32}$ | |
| $p_3b_4c_{43}=H_3^0$ | |

scheme. However, the grouping of the variables, in particular, the equations expressed in terms of the $H_j^i$'s, is the author's own.

We now consider separately the cases $m=6,7,8$.

## Sixth-Order Method ($m=6, n=5$)

For the five-stage, sixth-order algorithm, Eqs. ($\gamma$)-($\lambda$) consist of seven equations to determine the six parameters $c_{ij}$. The residue of Eq. ($\lambda$) may be calculated using techniques demonstrated previously by noting, from Table 6, that Eqs. $(\gamma^0)$, $(\epsilon^0)$, $(\iota)$, $(\lambda)$ provide four equations for $H_1^0, H_2^0, H_3^0$.

The augmented determinant of coefficients, formed as before, is four dimensional but is easily reduced to three dimensions by an obvious sequence of row operations. Indeed, we can readily show that this determinant is equivalent to

$$\frac{p_{21}p_{31}}{720\,b_2b_3}\begin{vmatrix} b_2 & b_3 & 5p_1-2 \\ p_2b_2 & p_3b_3 & 2p_1-1 \\ -\frac{6A_2^2b_2}{p_2p_{21}} & -\frac{6A_3^2b_3}{p_3p_{31}} & 1 \end{vmatrix}$$

Next, we obtain $A_i^2$ and $b_i$ from Eqs. ($\alpha$) and ($\gamma$), subject to the usual constraint equation $L_6(p_1,\ldots,p_4)=0$, as

$$p_2p_{21}p_{23}p_{24}b_2=L_5(p_1,p_3,p_4) \qquad (2,3)$$

$$p_2^2p_{21}p_{23}p_{24}b_2=L_6(p_1,p_3,p_4) \qquad (2,3)$$

$$6p_{23}p_{24}A_2^2b_2=L_6(p_3,p_4) \qquad (2,3)$$

These are substituted for the elements of the determinant and all common factors removed. Then the following sequence of row and column operations is performed:

1) Col 1 − col 2 → col 1 and factor $p_{23}$
2) $p_2\times$ col 1 + col 2 → col 2
3) Row 2 + row 3 → row 2 and factor $p_1$
4) Row 2 + row 1 → row 1 and factor $p_1$

The determinant is now a function only of $p_4$ and easily evaluated. The residue of Eq. ($\lambda$) is then found to be

$$R(\lambda)=\frac{1}{720^2\,V_3(p_1)\,V_3(p_2)\,p_2b_2p_3b_3}\,p_1^2(p_4-1)^2$$

Thus, the condition equations can only be consistent if either $p_1 = 0$ or $p_4 = 1$. The first option would require all of the $p_i$'s to be zero. For suppose that $p_1 = 0$. Then

$$A_2^2 = \frac{1}{6} p_{21} p_2^2 \frac{L_6(p_3,p_4)}{L_6(p_1,p_3,p_4)} = \frac{1}{6} p_2^3 \quad (2,3,4)$$

and the conclusion follows from the definition of $A_i^2$.

Therefore, a necessary and sufficient condition for the consistency of the condition equations is that

$$p_4 = 1, \quad L_6(p_1,p_2,p_3,1) = 0$$

The complete solution is summarized in Table 7. Albrecht[3] gave a sixth-order formula, which is a special case of our general formulas, for the following values of the $p_i$'s:

$$p_0 = 0, \ p_1 = 1/4, \ p_2 = 1/2, \ p_3 = 3/4, \ p_4 = 1$$

## Seventh-Order Method ($m = 7$, $n = 6$)

For a seventh-order, six-stage algorithm, Eqs. ($\alpha$) determine the coefficients $b_i$ subject to the vanishing of the residue

$$R(\alpha^6) = L_7(p_1,\ldots,p_5)$$

Then Eqs. ($\gamma$) – ($\psi$) provide 15 equations to be satisfied by the 10 parameters $c_{ij}$.

With reference to Table 6, we make the following observations:

1) Equations ($\gamma$) determine $A_j^2 (j = 2,3,4,5)$. By definition, $A_2^3 = 1/2 p_1 A_2^2$, so that Eqs. ($\epsilon$) determine $A_j^3 (j = 3,4,5)$. Equations ($\gamma^0$), ($\epsilon^0$), ($\iota^0$), ($\sigma$) determine $H_j^0 (j = 1,2,3,4)$.

2) Equations ($\pi$), ($\lambda^0$), ($\phi$), ($\psi$) then provide four additional constraints on the $p_i$'s.

3) Since, by definition, $H_4^1 = p_5 H_4^0$, Eqs. ($\lambda^1$), ($\epsilon^1$), ($\iota^1$) determine $H_j^1 (j = 1,2,3)$. Consequently, Eq. ($\lambda^1$) also provides a constraint on the $p_i$'s.

Residues for Eqs. ($\pi$), ($\lambda^0$), ($\phi$) may be determined as before. The calculations, which are considerably more complex, are outlined in the Appendix. The results are:

$$R(\pi) = -\frac{p_1^3 [L_6(p_1,\ldots,p_5) + p_1 \ldots p_5/16] L_7(p_2,\ldots,p_5)}{63(60)^3 V_5(p_1) V_4(p_2) p_2 b_2 \ldots p_5 b_5}$$

$$R(\lambda^0) = \frac{p_1^2 (p_5 - 1)^2 [L_8(p_1,\ldots,p_5) - 1/9800]}{720^2 V_4(p_1) V_4(p_2) p_2 b_2 p_3 b_3 p_4 b_4}$$

$$R(\phi) = \frac{p_1 (p_5 - 1)^2 P(p_1) L_7(p_2,\ldots,p_5)}{720^2 V_4(p_1) V_4(p_2) p_2 b_2 p_3 b_3 p_4 b_4} + p_1 R(\lambda^0)$$

where $P$ is the following third-order polynomial:

$$P(p) = p^3 - (12/7) p^2 + (6/7) p - 4/35$$

The constraint imposed by Eq. ($\psi$) is more easily handled. We observe that Eqs. ($\gamma^1$), ($\gamma^2$), ($\gamma^3$), ($\phi$), will determine $1/4 p_j A_j^2 b_j (j = 2,3,4,5)$ and they are identical with Eqs. ($\epsilon^0$), ($\epsilon^1$), ($\epsilon^2$), ($\psi$) which determine $A_j^3 b_j (j = 2,3,4,5)$. Hence, we must have

$$A_j^3 = 1/4 p_j A_j^2 \quad (j = 2,3,4,5)$$

and since by definition $A_2^2 = c_{21} p_1$ and $A_2^3 = 1/2 c_{21} p_1^2$, it follows that either $c_{21} = 0$ or $p_1 = 1/2 p_2$.

Finally, the constraint implied by Eq. ($\lambda^1$) is disposed of by calculating $H_4^i$ from Eqs. ($\gamma^i$), ($\epsilon^i$), ($\iota^i$), ($\lambda^i$) for $i = 0$, 1, as outlined in the Appendix. The result may be expressed conveniently as

$$H_4^1 - p_5 H_4^0 = \frac{120 p_{54} p_4 b_4}{7P(p_5)} \begin{vmatrix} 1 & p_4 & p_4^2 & 0 \\ L_3(p_5) & L_4(p_5) & L_5(p_5) & 84 - 105 p_5 \\ L_4(p_5) & L_5(p_5) & L_6(p_5) & 35 - 42 p_5 \\ L_5(p_5) & L_6(p_5) & L_7(p_5) & 18 - 21 p_5 \end{vmatrix}$$

We shall now examine the possibility of determining appropriate values of the $p_i$'s which satisfy the constraint equations.

*Case 1:* If $p_5 = 1$, then $R(\lambda^0) = R(\phi) = 0$. However, $H_4^1 - p_5 H_4^0$ can then only be zero if $p_4$ is also equal to one.

*Case 2:* If $p_1 = 0$ and $R(\alpha^6) = 0$, then $R(\pi) = R(\lambda^0) = R(\phi) = 0$. However, from Eqs. ($\alpha$), since $p_1 b_1 = 0$ it follows that

$$L_6(p_2,\ldots p_5) = 0$$

Also, from Eqs. ($\gamma$) and the definition $A_2^2 = p_1 c_{21}$, we also have

$$L_7(p_3,p_4,p_5) = 0$$

The three condition equations are equivalent to

$$L_5(p_3,p_4,p_5) = 0, \quad L_6(p_3,p_4,p_5) = 0, \quad L_7(p_3,p_4,p_5) = 0$$

from which we find $P(p_j) = 0$ $(j = 3,4,5)$. Unfortunately, $p_4$ and $p_5$ will not satisfy the requirement $H_4^1 - p_5 H_4^0 = 0$.

*Case 3:* If

$$L_7(p_1,\ldots,p_5) = L_7(p_2,\ldots,p_5) - p_1 L_6(p_2,\ldots,p_5) = 0$$

$$L_7(p_2,\ldots,p_5) = 0$$

then $R(\alpha^6) = R(\pi) = 0$ and $R(\phi) = p_1 R(\lambda^0)$. It follows that

$$b_1 = L_6(p_2,\ldots,p_5) = 0$$

and also

$$A_2^2 = \frac{1}{6} p_2^3 \frac{p_{21} L_7(p_3,p_4,p_5)}{p_2^2 L_6(p_1,p_3,p_4,p_5)} = \frac{1}{6} p_2^3 \quad (2,3,4,5)$$

$$A_j^3 = 1/4 p_j A_j^2 = \frac{1}{24} p_j^4 \qquad (j = 2,3,4,5)$$

Furthermore, by subtracting Eqs. ($\iota^i$) and ($\lambda^i$), we find that $p_1^2 H_1^i = 0$. Since $p_1$ cannot be zero, then $H_1^i = 0$ $(i = 0, 1)$.

The three equations

$$L_6(p_2,\ldots,p_5) = 0, \quad L_7(p_2,\ldots,p_5) = 0, \quad H_1^0 = 0$$

can be expressed as

$$L_3(p_5)\beta_3 + L_4(p_5)\beta_2 + L_5(p_5)\beta_1 + L_6(p_5) = 0$$

$$L_4(p_5)\beta_3 + L_5(p_5)\beta_2 + L_6(p_5)\beta_1 + L_7(p_5) = 0$$

$$(1/4)\beta_3 + (1/10)\beta_2 + (1/20)\beta_1 + 1/35 = 0$$

where

$$\beta_1 = -(p_2 + p_3 + p_4), \quad \beta_2 = p_2 p_3 + p_2 p_4 + p_3 p_4,$$

$$\beta_3 = -p_2 p_3 p_4$$

Solving for the $\beta_i$'s, we have

$$(p_5-1)^2\beta_1=-\frac{12}{7}(p_5-1)^2,\quad (p_5-1)^2\beta_2=\frac{6}{7}(p_5-1)^2,$$

$$(p_5-1)^2\beta_3=-\frac{4}{35}(p_5-1)^2$$

Since $p_5$ cannot be one, it follows that $P(p_j)=0(j=2,3,4)$.

The polynomial equation $P(p)=0$ has three real and unequal roots but, unfortunately, $b_5$ is then zero. With $b_5=0$, the number of stages in the algorithm would be five and it is easy to see that the resulting condition equations cannot be satisfied.

*Case 4:* If

$$P(p_1)=0,\quad L_8(p_1,\ldots,p_5)=1/9800,\quad L_7(p_1,\ldots,p_5)=0$$

then $R(\alpha^6)=R(\lambda^0)=R(\phi)=0$. Assume for the moment that also $b_2=0$, or equivalently

$$L_6(p_1,p_3,p_4,p_5)=0$$

Then the three constraint function equations may be written as

$$L_3(p_1)\beta_3+L_4(p_1)\beta_2+L_5(p_1)\beta_1+L_6(p_1)=0$$

$$L_4(p_1)\beta_3+L_5(p_1)\beta_2+L_6(p_1)\beta_1+L_7(p_1)=0$$

$$L_5(p_1)\beta_3+L_6(p_1)\beta_2+L_7(p_1)\beta_1+L_8(p_1)=1/9800$$

where

$$\beta_1=-(p_3+p_4+p_5),\quad \beta_2=p_3p_4+p_3p_5+p_4p_5,$$

$$\beta_3=-p_3p_4p_5$$

Solving for the $\beta_i$'s we have

$$P(p_1)\beta_1=-(12/7)P(p_1),\quad P(p_1)\beta_2=(6/7)P(p_1),$$

$$P(p_1)\beta_3=-(4/35)P(p_1)$$

and since $P(p_1)=0$, the rank of the three equations is two. Hence, under the assumptions stated for this case, $b_2$ is automatically zero.

The three constraint function equations are symmetrical in $p_1,p_3,p_4,p_5$, so that if any $p_j$ were such that $P(p_j)\neq 0$, then we could solve for the corresponding $\beta$'s and find that $P(p_i)=0$ for $i\neq j$. We must conclude that $P(p_j)=0$ for $j=1,3,4,5$, which is possible only if two of the $p_j$'s are equal.

Having exhausted the possibilities, we reluctantly conclude that a seventh-order, six-stage algorithm does not exist.

## Seventh-Order Method ($m=7$, $n=7$)

If the number of stages is increased to seven, the number of $c_{ij}$'s increases to 15 but the number of equations remains 15. The set of parameters in Eqs. ($\alpha$) has also been expanded to include $p_6$ and $b_6$ so that no constraint condition is required.

To simplify the solution of these equations we will introduce as assumptions $b_1=0$ and $A_i^2=p_i^3/6$ $(i=2,\ldots,6)$. The first imposes a constraint on the $p_i$'s, i.e.,

$$L_7(p_2,\ldots,p_6)=0$$

The second requires $H_1^i=0$ $(i=0,1)$, as can be seen by subtracting Eqs. ($\iota^i$) and ($\lambda^i$). The importance of these assumptions is that Eqs. ($\gamma$) and ($\pi$) are then identical to certain of the Eqs. ($\alpha$). Furthermore, Eqs. ($\lambda$) and ($\iota$) are the same, as are also Eqs. ($\phi$) and ($\sigma$).

In addition, we find it convenient to assume that $A_i^3=p_i^4/24$ $(i=2,\ldots,6)$ so that Eqs. ($\epsilon$) will be identical to the last three of Eqs. ($\alpha$) and Eq. ($\psi$) will be identical to Eq. ($\phi$). However, in so doing, it follows from the definitions of $A_2^2$ and $A_2^3$ that $p_1=\frac{1}{2}p_2$ and $c_{21}=\frac{1}{3}p_2^2$.

The condition equations are now 13 in number and consist of

$$A_i^k=\frac{1}{(k-1)!}\sum_{j=1}^{i-1}c_{ij}p_j^{k-1}=\frac{1}{(k+1)!}p_i^{k+1}\quad (i=3,\ldots,n-1)\ (k=2,3)$$

$$H_1^k=p_1\sum_{j=2}^{n-1}p_j^kb_jc_{j1}=0\qquad (k=0,\ldots,n-6)$$

$$\sum_{j=3}^{n-1}p_j^ib_jA_j^{k2}=\frac{1}{(k+1)!(i+k+2)}\qquad (i=0,\ldots,n-k-2)\ (k=4,\ldots,n-2)$$

where

$$A_i^{k2}=\frac{1}{(k-1)!}\sum_{j=2}^{i-1}c_{ij}p_j^{k-1}\qquad (i=3,\ldots,n-1)\ (k=4,\ldots,n-2)$$

and the number of parameters $c_{ij}$ to be determined is 14, since $c_{21}$ has already been established. With $c_{41}$ regarded as a free parameter, these equations may be regrouped, as shown in

**Table 8 Parameters for seventh-order, seven stage and eighth-order, eight stage algorithms**

| Free parameters | Constraints |
|---|---|
| 5 <br> $c_{41}$ is arbitrary | $p_0=0, p_1=\frac{1}{2}p_2$ <br> $p_7=1$ for $m=n=8$ <br> $L_n(p_2,\ldots,p_{n-1})=0$ <br> $b_5,\ldots,b_{n-1}\neq 0$ |

Equations for parameters

$$(p_{n-1}-p_0)\ldots(p_{n-1}-p_{n-2})b_{n-1}=L_n(p_0,\ldots,p_{n-2})$$

$$q_i=\tfrac{1}{2}p_i^2\qquad (0,1,\ldots,n-1)$$

$$c_{21}=\tfrac{1}{3}p_2^2\qquad (i=1,\ldots,n-1)$$

$$\sum_{j=1}^{2}p_j^{k-2}(p_jc_{3j})=\frac{(k-1)!}{(k+1)!}p_3^{k+1}\qquad (k=2,3)$$

$$\sum_{j=2}^{3}p_j^{k-2}(p_jc_{4j})=\frac{(k-1)!}{(k+1)!}p_4^{k+1}-p_1^{k-1}c_{41}\qquad (k=2,3)$$

$$\sum_{j=5}^{n-1}p_j^k\,(b_jc_{j1})=-\sum_{j=2}^{4}p_j^kb_jc_{j1}\qquad (k=0,\ldots,n-6)$$

Repeat the following for $k=4,\ldots,n-2$:

$$A_i^{k2}=\frac{1}{(k-1)!}\sum_{j=2}^{i-1}c_{ij}p_j^{k-1}\qquad (i=3,\ldots,k)$$

$$\sum_{j=k+1}^{n-1}p_j^i(b_jA_j^{k2})=\frac{1}{(k+1)!(i+k+2)}-\sum_{j=3}^{k}p_j^ib_jA_j^{k2}\qquad (i=0,\ldots,n-k-2)$$

$$\sum_{j=2}^{k}p_j^i(p_jc_{k+1,j})=\begin{cases}\dfrac{(i+1)!}{(i+3)!}p_{k+1}^{i+3}-p_1^{i+1}c_{k+1,1} & (i=0,1)\\[2ex] (i+1)!\,A_{k+1}^{i+2,2} & (i=2,\ldots,k-2)\end{cases}$$

Table 8, in the form of linear equations, having Vandermonde coefficient matrices, to be solved for the $c_{ij}$'s.

A note of caution in obtaining the $c_{ij}$'s from Table 8 is appropriate. High-order Vandermonde matrices can be ill-conditioned so that the explicit analytic inverse should be used rather than a standard computer matrix inversion routine.

## Eighth-Order Method ($m=8$, $n=8$)

For an eighth-order algorithm with eight stages, Eqs. ($\gamma$) through ($e_6$) provide 29 equations to determine the 21 parameters $c_{ij}$. As before, we will assume

$$b_1=0, \quad A_i^2=p_i^3/6, \quad A_i^3=p_i^4/24 \quad (i=2,\ldots,7)$$

Thus, we impose the constraint $L_8(p_2,\ldots,p_7)=0$ and have also

$$p_1=\tfrac{1}{2}p_2, \quad c_{21}=\tfrac{1}{3}p_2^2$$

Again by subtracting Eqs. ($\iota^i$) and ($\lambda^i$), we find $H_1^i=0$ ($i=0,1,2$). Equations ($\gamma$), ($\epsilon$), ($\pi$) and ($e_1$) are identical to certain of the Eqs. ($\alpha$). Furthermore, the following sets of equations are identical: Eqs. ($\lambda$), ($\iota$), Eqs. ($\sigma$), ($\phi$), ($\psi$) and Eqs. ($e_2$), ($e_3$), ($e_4$). There are, therefore, 21 condition equations remaining to determine the 20 parameters $c_{ij}$.

Equations ($\gamma^0$), ($\epsilon^0$), ($\iota^0$), ($\sigma^0$), ($e_2$) determine $H_j^0$ ($j=2,\ldots,6$), so that Eqs. ($e_5$) and ($e_6$) provide additional constraints on the $p_i$'s. Note also, with the assumption $A_i^2=p_i^3/6$ and the use of Eq. ($e_6$), that Eq. ($e_5$) may be written as

$$\sum_{j=2}^{6} \frac{1}{p_j} c_{j1} H_j^0 = 0 \qquad (e_5)$$

The author has not succeeded in calculating useful expressions for the residues of Eqs. ($e_5$) and ($e_6$). However, it has been determined by numerical experiment that $R(e_5)=R(e_6)=0$ if $p_7=1$.

Subject to the constraints $p_7=1$ and $L_8(1, p_2,\ldots,p_6)=0$, the reduced set of 19 condition equations is the same as listed in the previous section for the seventh-order case and the number of parameters $c_{ij}$ is 20. Again we may regard $c_{41}$ as arbitrary, making the total number of free parameters five. The solution may be obtained from the equations given in Table 8.

## Appendix

We provide here, in brief outline form, the various steps required to obtain the equation residues which were given without proof in the section treating the seventh-order, six-stage method.

#### Residue of Eq. ($\pi$)

Form the five-dimensional determinant of the coefficients of the $A_i^2$'s in Eqs. ($\gamma$), ($\pi$) augmented by the right-hand sides. Solve Eqs. ($\alpha$) and ($\gamma$) for $b_i$ and $A_i^2 b_i$

$$p_2 p_{12} p_{32} p_{42} p_{52} b_2 = L_6(p_1,p_3,p_4,p_5) \qquad (1,2,3,4,5)$$

$$6 p_2 p_{12} p_{32} p_{42} p_{52} A_2^2 b_2 = p_2 p_{21} L_7(p_3,p_4,p_5) \qquad (2,3,4,5)$$

Establish the following to be used in the first column, with similar relations for the other columns:

$$p_2 L_6(p_1,p_3,p_4,p_5) = L_7(p_1,p_3,p_4,p_5)$$

$$p_2^2 L_6(p_1,p_3,p_4,p_5) = L_8(p_1,p_3,p_4,p_5) - L_8(p_1,\ldots,p_5)$$

$$p_2^3 L_6(p_1,p_3,p_4,p_5) = p_2 L_8(p_1,p_3,p_4,p_5) - p_2 L_8(p_1,\ldots,p_5)$$

$$p_2 p_{21} L_7(p_3,p_4,p_5) = p_2 L_8(p_1,p_3,p_4,p_5) - p_2 L_8(p_2,\ldots,p_5)$$

Note that

$$p_2 L_8(p_1,p_3,p_4,p_5) = L_9(p_1,p_3,p_4,p_5) - L_9(p_1,\ldots,p_5)$$

$$p_1 p_2 L_7(p_2,p_3,p_4,p_5) = p_2^3 L_6(p_1,p_3,p_4,p_5) - p_2 p_{21} L_7(p_3,p_4,p_5)$$

Substitute for the elements of the determinant and remove the common factors from all rows and columns. Then

1) Row 4 − row 3 → row 4 and factor $-p_1 L_7(p_2,\ldots,p_5)$.
2) $L_8(p_1,\ldots,p_5)\times$ row 4 + row 3 → row 3.
3) Col 1 − col 2 → col 1 and factor $p_{23}$.
4) Col 2 − col 3 → col 2 and factor $p_{34}$.
5) Col 3 − col 4 → col 3 and factor $p_{45}$.
6) Col 1 − col 2 → col 1 and factor $p_{24}$.
7) Col 2 − col 3 → col 2 and factor $p_{35}$.
8) $-p_5\times$ col 3 + col 4 → col 4.

The determinant is now four dimensional.

9) Col 1 − col 2 → col 1 and factor $p_{25}$.
10) $p_4 p_5\times$ col 2 + col 3 → col 3.
11) $p_2\times$ col 1 + col 2 → col 2.
12) $-p_3 p_4 p_5\times$ col 1 + col 3 → col 3.
13) Col 2 − col 4 → col 2 and factor $-p_1$.
14) Col 1 − col 2 → col 1 and factor $-p_1$.
15) $p_2 p_3 p_4 p_5\times$ col 1 + col 3 → col 3.

The element in the first row, third column can be simplified using the identity

$$L_6(p_1,\ldots,p_5) + p_1\ldots p_5 = L_6(p_1,\ldots,p_4) - p_5 L_5(p_1,p_2,p_3) + p_4 p_5 L_4(p_1,p_2) - p_3 p_4 p_5 L_3(p_1) + p_2 p_3 p_4 p_5 L_2(0)$$

The determinant is now

$$\begin{vmatrix} 1/2 & 1/3 & L_6(p_1,\ldots,p_5)+p_1\ldots p_5 & 1/4 \\ 1/3 & 1/4 & (1/2)p_1..p_5 & 1/5 \\ 1/4 & 1/5 & (1/3)p_1\ldots p_5 & 1/6 \\ 1/5 & 1/6 & (1/4)p_1\ldots p_5 & 1/7 \end{vmatrix}$$

multiplied by all of the factors which have been removed in the reduction process. The final result follows easily.

#### Residue of Eq. ($\lambda^0$)

Form the five-dimensional determinant of the coefficients of the $H_i^0$'s in Eqs. ($\gamma^0$), ($\epsilon^0$), ($\iota^0$), ($\sigma$), ($\lambda^0$) augmented by the right-hand sides. By an obvious sequence of row operations, reduce this to the following four-dimensional determinant:

$$\frac{p_{21}p_{31}p_{41}}{144 b_2 b_3 b_4} \begin{vmatrix} b_2 & b_3 & b_4 & \frac{2}{5}-p_1 \\ p_2 b_2 & p_3 b_3 & p_4 b_4 & \frac{1}{5}-\frac{2}{5}p_1 \\ p_2^2 b_2 & p_3^2 b_3 & p_4^2 b_4 & \frac{4}{35}-\frac{1}{5}p_1 \\ \frac{6A_2^2 b_2}{p_2 p_{21}} & \frac{6A_3^2 b_3}{p_3 p_{31}} & \frac{6A_4^2 b_4}{p_4 p_{41}} & \frac{1}{5} \end{vmatrix}$$

Substitute for the determinant elements and remove all common factors. Then

1) Col 1 − col 2 → col 1 and factor $p_{23}$.
2) Col 2 − col 3 → col 2 and factor $p_{34}$.
3) Col 1 − col 2 → col 1 and factor $p_{24}$.
4) $p_3\times$ col 2 + col 3 → col 3.

5) $p_2 \times$ col 1 + col 2 → col 2.
6) $p_2 \times$ col 2 + col 3 → col 3.
7) Row 2 − row 4 → row 2 and factor $-p_1$.
8) Row 1 − row 2 → row 1 and factor $-p_1$.
9) $p_1 \times$ row 4 + row 3 → row 3.
10) Interchange row 3 and row 4.

The determinant is now

$$\begin{vmatrix} L_3(p_5) & L_4(p_5) & L_5(p_5) & 1 \\ L_4(p_5) & L_5(p_5) & L_6(p_5) & 2/5 \\ L_5(p_5) & L_6(p_5) & L_7(p_5) & 1/5 \\ L_6(p_5) & L_7(p_5) & L_8(p_5) - L_8(p_1,\ldots,p_5) & 4/35 \end{vmatrix}$$

where again the factors removed in the reduction process are not displayed. The rest is straightforward.

**Residue of Eq. ($\phi$)**

Begin the reduction in the same manner as in the previous case with Eq. ($\phi$) replacing Eq. ($\lambda^0$), so that the last row of the preliminary four-dimensional determinant is replaced by

$$\frac{6A_2^2 b_2}{p_{21}} \quad \frac{6A_3^2 b_3}{p_{31}} \quad \frac{6A_4^2 b_4}{p_{41}} \quad \frac{4}{35}$$

The first six steps in the reduction are the same. Then
7) Row 3 − row 4 → row 3 and factor $-p_1$.
8) Row 2 − row 3 → row 2 and factor $-p_1$.
9) Row 1 − row 2 → row 1 and factor $-p_1$.

Thus the determinant, omitting the display of the common factors as before, is

$$\begin{vmatrix} L_3(p_5) & L_4(p_5) & L_5(p_5) - p_1 L_7(p_2,\ldots,p_5)/p_1^3 & 1 \\ L_4(p_5) & L_5(p_5) & L_6(p_5) - p_1 L_7(p_2,\ldots,p_5)/p_1^2 & 2/5 \\ L_5(p_5) & L_6(p_5) & L_7(p_5) - p_1 L_7(p_2,\ldots,p_5)/p_1 & 1/5 \\ L_6(p_5) & L_7(p_5) & L_8(p_5) - p_1 L_7(p_2,\ldots,p_5) - L_8(p_1,\ldots,p_5) & 4/35 \end{vmatrix}$$

The final expression is readily obtained without further details.

*$H_4^1 - p_5 H_4^0$*

Apply Cramer's rule to Eqs. ($\gamma^i$), ($\epsilon^i$) ($\iota^i$), ($\lambda^i$) with $i=0$, 1. Reduce the four-dimensional denominator determinant, which is the same for both $H_4^0$ and $H_4^1$, to the following three-dimensional one by an obvious sequence of row operations:

$$\begin{vmatrix} p_{21} & p_{31} & p_{41} \\ p_2 p_{21} & p_3 p_{31} & p_4 p_{41} \\ A_2^2/p_2 & A_3^2/p_3 & A_4^2/p_4 \end{vmatrix}$$

Substitute for the determinant elements and remove all common factors. Then
1) Row 2 − row 3 → row 2 and factor $-p_1$.
2) Row 1 − row 2 → row 1 and factor $-p_1$.
3) Col 1 − col 2 → col 1 and factor $p_{23}$.
4) Col 2 − col 3 → col 2 and factor $p_{34}$.
5) $p_3 \times$ col 2 + col 3 → col 3.
6) Col 1 − col 2 → col 1 and factor $p_{24}$.
7) $p_2 \times$ col 1 + col 2 → col 2.
8) $p_2 \times$ col 2 + col 3 → col 3.

The denominator determinant is now

$$-\frac{p_1^2}{6V_4(p_2)p_2b_2p_3b_3p_4b_4} \begin{vmatrix} L_3(p_5) & L_4(p_5) & L_5(p_5) \\ L_4(p_5) & L_5(p_5) & L_6(p_5) \\ L_5(p_5) & L_6(p_5) & L_7(p_5) \end{vmatrix}$$

which is equal to $p_1^2 P(p_5)/259200 V_4(p_2)p_2b_2p_3b_3p_4b_4$.

The reduction of the numerator determinants follows an identical pattern, so the details are omitted. We have

$$H_4^1 - p_5 H_4^0 = \frac{43200 p_4 b_4 p_{54}}{P(p_5)} \begin{vmatrix} L_4(p_4,p_5) & L_5(p_4,p_5) & \frac{1}{30} - \frac{1}{24}p_5 \\ L_5(p_4,p_5) & L_6(p_4,p_5) & \frac{1}{72} - \frac{1}{60}p_5 \\ L_6(p_4,p_5) & L_7(p_4,p_5) & \frac{1}{140} - \frac{1}{120}p_5 \end{vmatrix}$$

The alternate form, as given in the text, is obtained using $L_i(p_4,p_5) = L_i(p_5) - p_4 L_{i-1}(p_5)$ and a straightforward manipulation of the determinant elements.

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