Hermite–Birkhoff Differential Equation Solvers

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Abstract

We construct a new six-stage general linear Hermite–Birkhoff (HB) method of order 9 with 4 off-step points and 2 backstep points. Particular choices of the off-step points produce corresponding particular variable-step and constant-step methods. Similar methods of order 10 and 11 are also considered. These methods lie between multistep and Runge–Kutta methods. It is seen that the regions of absolute stability of HB methods, obtained by a scanning method, are larger than those of multistep methods of comparative order. A local error estimator is used to control the stepsize. These methods were tested with the non-stiff DETEST two-body problems of class D and compared with the Dormand–Prince Runge–Kutta pair DP(8,7)13M of order 8. Generally, the HB methods have lower global errors and use fewer function evaluations.

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Résumé

On construit des méthodes d’Hermite–Birkhoff (HB) linéaires générales à 6 étages d’ordre 9 avec 4 points hors-noeud et 2 noeuds rétrogrades. Des choix appropriés des pas hors-noeuds produisent des méthodes particulières correspondantes à pas variable et à pas constant. On considère aussi des méthodes d’ordre 10 et 11. Ces méthodes HB se situent entre les méthodes multipas et celles de Runge–Kutta. On voit que la région de stabilité absolue des méthodes HB, obtenue par balayage, est plus grande que celle des méthodes multipas d’ordre correspondant. Un estimateur de l’erreur locale contrôle le pas. On a testé ces méthodes sur les problèmes de 2 corps de classe D de DETEST non-raides et on les compare à la paire DP(8,7)13M de méthodes de Runge–Kutta imbriquées de Dormand–Prince d’ordre 8. En général, les méthodes HB admettent une erreur globale inférieure et utilisent moins d’évaluations de fonctions que DP.
1 Introduction

The search for improved numerical methods to solve initial value problems for ordinary differential equations continues to fascinate applied mathematicians, scientists, and engineers. One is looking for more accurate, more stable, and faster methods. There is a deep mathematical theory behind these issues \cite{1} and its implementation has resulted in ingenious programming achievements.

The general linear methods considered in this paper fall somewhere between conventional multistep methods, on the one hand, and Runge–Kutta methods, on the other hand. Like multistep methods, they use information prior to the last step and, like Runge–Kutta methods, they use derivative evaluations at points partway through a step. The link between the two types of methods is that values at off-step points are obtained by means of predictors which use values at previous points.

Since the new methods make use of Hermite–Birkhoff (HB) interpolation polynomials, they will be called HB methods.

We let \( \text{HB}(p, q; p_1)\{s, k\} \) denote an HB method for systems of first-order differential equations of the form \( y' = f(x, y) \). The parameters appearing in these methods are defined in Table \ref{tab:parameters}.

An initial value problem for a non-stiff system of ordinary differential equations of first order:

\[
y' = f(x, y), \quad y(x_0) = y_0, \tag{1}
\]

can be solved numerically by an explicit linear \( k \)-step methods of the form

\[
y_{n+1} = \alpha_0 y_n + \alpha_1 y_{n-1} + \cdots + \alpha_k y_{n-k+1} + h(\beta_0 f_n + \beta_1 f_{n-1} + \cdots + \beta_k f_{n-k+1}), \tag{2}
\]

where \( \alpha_i \) and \( \beta_i \) are constants, \( x_{n+1} = x_n + h_{n+1} \), \( y_n \) is a numerical approximation to \( y(x_n) \) and \( f_n = f(x_n, y_n) \). Some method is used to supply the \( k - 1 \) starting values \( y_2, y_3, \ldots, y_{k-1} \). If formula \( (2) \) is exact for any polynomial \( y(x) \) of degree \( p \), we say that \( (2) \) is a method of order \( p \).

It has been noted in \cite{3, 4, 10, 5} and \cite{8} that general linear methods incorporate function evaluations at off-step points in order to reduce the number of steps of \( (2) \) without lowering the order. The purpose of the present paper is to derive and test HB methods and show that they have higher order and larger region of stability and use fewer steps than multistep methods.

The \( s \)-stage HB methods considered here are generalizations of \( s \)-stage Runge–Kutta methods. They will have \( s - 2 \) off-step points since the first and last stages will be at \( x_n \) and \( x_{n+1} \) which are not off-step points. In particular, they will have four or five off-step points. Increased speed is generally achieved by higher-order methods. Higher order is achieved by using standard or modified Hermite–Birkhoff polynomials (HBP) of increasing degree as predictors, \( P_1, P_2, \ldots \), to satisfy the associated order conditions and approximate \( y(x) \) at off-step points, \( x_{n+c_2}, x_{n+c_3}, \ldots \). For a given integration formula, the predictors are chosen experimentally to increase the accuracy of the HB method and minimize the global error of the solution. It was found experimentally that increasing

\[2\] Table 1: The parameters entering HB\((p, q; p_1)\{s, k\} \).

| \( p \) | order of the method |
| \( q \) | order of the step control predictor, SCP |
| \( p_j \) | order of the \( j \)th predictor, \( j = 1, 2, \ldots \) |
| \( s \) | number of stages |
| \( k \) | number of backstep points |
Table 2: Orders $p$ of the method, $q$ of the step control predictor (SCP), $p_1$, $p_2$, ... of predictors P1, P2, ... for three HB($p, q; p_1$)\{s, k\} with s stages and k backstep points.

<table>
<thead>
<tr>
<th>HB($p, q; p_1$){s, k}</th>
<th>$p$</th>
<th>$q$</th>
<th>$p_1$</th>
<th>$p_2$</th>
<th>$p_3$</th>
<th>$p_4$</th>
<th>$p_5$</th>
<th>$p_6$</th>
<th>s</th>
<th>k</th>
</tr>
</thead>
<tbody>
<tr>
<td>HB(9, 7; 5){6, 2}</td>
<td>9</td>
<td>7</td>
<td>5</td>
<td>6</td>
<td>6</td>
<td>6</td>
<td>5</td>
<td></td>
<td>6</td>
<td>2</td>
</tr>
<tr>
<td>HB(10, 7; 5){7, 2}</td>
<td>10</td>
<td>7</td>
<td>5</td>
<td>6</td>
<td>7</td>
<td>6</td>
<td>7</td>
<td>5</td>
<td>7</td>
<td>2</td>
</tr>
<tr>
<td>HB(11, 8; 7){6, 3}</td>
<td>11</td>
<td>8</td>
<td>7</td>
<td>8</td>
<td>8</td>
<td>8</td>
<td>7</td>
<td></td>
<td>6</td>
<td>3</td>
</tr>
</tbody>
</table>

the number of back-step points is more efficient in increasing the accuracy of HB methods than increasing the number of off-step points.

A modified Hermite–Birkhoff Step Control Predictor (SCP) produces an extrapolated value, $\tilde{y}_{n+1}$, at the next node, $x_{n+1}$, to control the stepsize by means of the difference $|y_{n+1} - \tilde{y}_{n+1}|$.

Table 2 lists the orders of the integration formula, the predictors, P1, P2, ..., and step control predictor for three HB methods.

It will be seen that there is a marked difference in the implementation of order 9 and 11 methods and the order 10 method.

The methods were tested on the nonstiff DETEST two-body problems of class D [9] and were found to compare favorably with the 13-stage FSAL Runge-Kutta pair DP(8,7)13M of Dormand–Prince [11] and [6]. A k-stage Runge-Kutta method is said to be FSAL (First Same As Last) if the first stage at the next step is the same as the last stage of the previous step. Thus, the method reduces to a $(k-1)$-stage method if the step is accepted.

In section 2 and 3 we define a general HB method of order 9 and derive the order conditions for this method. We mention that a general HB method of order 11 can be derived similarly. In section 4 we present a particular variable-step method of order 9, which we illustrate with constant stepsize method in section 5. Section 6 briefly describes the structure of general HB methods of order 10 and a particular variable-step method which is illustrated with a constant-step method. In section 7, the regions of stability of these methods are obtained by a scanning method. Section 8 deals with the variable stepsize control. In sections 9 and 10, the HB methods are compared between themselves and with the Dormand–Prince Runge-Kutta pair DP(8,7)13M on the basis of their maximum global error and the number of function evaluations used in solving the five non-stiff DETEST elliptic problems of class D. Section 11 is a conclusion.

2 Definition of general HB($9, 7; 5$)\{6, 2\}

An HB method is said to be a general HB method if it contains free parameters besides the variable positions of the back-step points. When the positions of the off-step points are specified, a general HB method is said to be a particular variable-step method. When the stepsize, $h$, is constant, we have a constant-step HB method.

A general HB($9, 7; 5$)\{6, 2\} method with $s = 6$ stages and $k = 2$ backstep points is defined by the following formulae. (Note that $c_6 = 1$.)

(P1) An HBP of degree 5 is used as P1 to obtain $\tilde{y}_{n+c_2}$ to order 5,

\[
\tilde{y}_{n+c_2} = \alpha_{20}y_{n} + \alpha_{21}y_{n-1} + \alpha_{22}y_{n-2} + h_{n+1}(a_{21}f_{n} + \beta_{21}f_{n-1} + \beta_{22}f_{n-2}).
\]  

(P2) An HBP of degree 6 is used as P2 to obtain $\tilde{y}_{n+c_3}$,

\[
\tilde{y}_{n+c_3} = \alpha_{30}y_{n} + \alpha_{31}y_{n-1} + \alpha_{32}y_{n-2} + h_{n+1}(a_{32}\tilde{f}_{n+c_2} + a_{31}f_{n} + \beta_{31}f_{n-1} + \beta_{32}f_{n-2}).
\]
(P3) An HBP of degree 7 is used as P3 to obtain \( \hat{y}_{n+c_4} \) to order 7,
\[
\hat{y}_{n+c_4} = \alpha_{40} y_n + \alpha_{41} y_{n-1} + \alpha_{42} y_{n-2} + h_{n+1} (a_{43} \hat{f}_{n+c_3} + a_{42} \hat{f}_{n+c_2} + a_{41} f_n + \beta_{41} f_{n-1} + \beta_{42} f_{n-2}).
\]
(5)

(P4) An HBP of degree 8 is used as P4 to obtain \( \hat{y}_{n+c_5} \),
\[
\hat{y}_{n+c_5} = \alpha_{50} y_n + \alpha_{51} y_{n-1} + \alpha_{52} y_{n-2} + h_{n+1} (a_{54} \hat{f}_{n+c_4} + a_{53} \hat{f}_{n+c_3} + a_{52} \hat{f}_{n+c_2} + a_{51} f_n + \beta_{51} f_{n-1} + \beta_{52} f_{n-2}).
\]
(6)

(P5) An HBP of degree 9 is used as last predictor, P5, to obtain \( \hat{y}_{n+c_6} \),
\[
\hat{y}_{n+c_6} = \alpha_{60} y_n + \alpha_{61} y_{n-1} + \alpha_{62} y_{n-2} + h_{n+1} (a_{65} \hat{f}_{n+c_5} + a_{64} \hat{f}_{n+c_4} + a_{63} \hat{f}_{n+c_3} + a_{62} \hat{f}_{n+c_2} + a_{61} f_n + \beta_{61} f_{n-1} + \beta_{62} f_{n-2}).
\]
(7)

(HBIF9) A seven-point HBP of degree 9 is used as integration formula, HBIF9, to obtain \( y_{n+1} \) to order 9 (note that \( b_2 = 0 \)):
\[
y_{n+1} = A_0 y_n + A_1 y_{n-1} + A_2 y_{n-2} + h_{n+1} [(b_0 \hat{f}_{n+c_6} + b_5 \hat{f}_{n+c_5} + b_4 \hat{f}_{n+c_4} + b_3 \hat{f}_{n+c_3} + b_2 \hat{f}_{n+c_2} + b_1 f_n + B_1 f_{n-1} + B_2 f_{n-2})].
\]
(8)

(SCP) A six-point HBP of degree 7 is used as SCP to control the stepsize, \( h_{n+1} \), and obtain \( \tilde{y}_{n+1} \) to order 7 (note that \( a_{72} = 0 \)),
\[
\tilde{y}_{n+1} = \alpha_{70} y_n + \alpha_{71} y_{n-1} + h_{n+1} (a_{76} \hat{f}_{n+c_6} + a_{75} \hat{f}_{n+c_5} + a_{74} \hat{f}_{n+c_4} + a_{73} \hat{f}_{n+c_3} + a_{72} f_n + \beta_{72} f_{n-1}).
\]
(9)

In these formulae,
\[
c_k = \sum_{j=1}^{k-1} a_{kj} + B(k,1), \quad k = 2, 3, \ldots, 6,
\]
(10)

where, in general,
\[
B(k, j) = \sum_{i=1}^{2} \left[ \alpha_{ki} \frac{\eta_{i+1}^j}{j!} + \beta_{ki} \frac{\eta_{i+1}^{j-1}}{(j-1)!} \right], \quad j = 1, \cdots, 9, \quad k = 2, 3, \ldots, 6.
\]
(11)

and
\[
\eta_2 = -\frac{h_n}{h_{n+1}}, \quad \eta_3 = -\frac{h_n + h_{n-1}}{h_{n+1}}.
\]
(12)

We choose to have a negative sign in the right-hand sides in the definition of \( \eta_2 \) and \( \eta_3 \) to avoid negative signs everywhere below.

The coefficients
\[
\{a_{21}, a_{31}, a_{32}, \ldots, a_{7,6}\}, \quad \{\alpha_{20}, \alpha_{21}, \ldots, \alpha_{70}, \alpha_{71}\}, \quad \{\beta_{21}, \beta_{22}, \ldots, \beta_{61}, \beta_{62}, \beta_{71}\},
\]
\[
\{b_1, b_2, \ldots, b_6, \ldots\}, \quad \{A_0, A_1, A_2\}, \quad \{B_1, B_2\}
\]
(13)

are solutions of seven linear systems of equations of condition for order 9, namely, (21), (22), (27), (30), (33), (36) and (40) below.
As in similar search for ODE solvers, we impose the following simplifying assumptions on the coefficients of the method:

\[ \sum_{i=j+1}^{8} b_i a_{ij} = b_j (1 - c_j), \quad j = 2, \ldots, 5, \quad (14) \]

\[ \sum_{j=1}^{i-1} a_{ij} c_j^k + k! B(i, k + 1) = \frac{1}{k + 1} c_i^{k+1}, \quad \begin{cases} i = 3, \ldots, 6, \\ k = 0, 1, 2, \ldots, 5, \end{cases} \quad (15) \]

\[ b_2 = 0. \quad (16) \]

Thus, we need to solve the remaining three sets of equations,

\[ \sum_{i=2}^{6} b_i c_i^k + k! B_Q(k + 1) = \frac{1}{k + 1}, \quad k = 0, 1, \ldots, 8, \quad (17) \]

\[ \sum_{i=1}^{6} b_i c_i \left\{ \sum_{j=1}^{i-1} a_{ij} \left[ \sum_{k=1}^{j-1} a_{ijk} \frac{c_k}{k!} + B(j, 6) \right] + B(i, 7) \right\} + 8 B_Q(9) = \frac{8}{9!}, \quad (18) \]

\[ \sum_{i=1}^{6} b_i c_i \left[ \sum_{j=1}^{i-1} a_{ij} \frac{c_j^6}{6!} + B(i, 7) \right] + 8 B_Q(9) = \frac{8}{9!}, \quad (19) \]

where the backstep parts, \( B_Q(j) \), are defined by

\[ B_Q(j) = A_1 \frac{\eta_j^j}{j!} + A_2 \frac{\eta_j^j}{j!} + B_1 \frac{\eta_j^{j-1}}{(j-1)!} + B_2 \frac{\eta_j^{j-1}}{(j-1)!}, \quad j = 1, \ldots, 9, \quad (20) \]

and \( B(k, j) \) are defined in (11).

The coefficients of HBIF9 satisfy the following ten order conditions:

\[
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \eta_2 & \eta_3 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & \eta_2^2/2! & \eta_3^2/2! & c_6 & c_5 & c_4 & c_3 & 0 & \eta_2 & \eta_3 \\
0 & \eta_2^3/3! & \eta_3^3/3! & c_6^2/2! & c_5^2/2! & c_4^2/2! & c_3^2/2! & 0 & \eta_2^2/2! & \eta_3^2/2! \\
0 & \eta_2^4/4! & \eta_3^4/4! & c_6^3/3! & c_5^3/3! & c_4^3/3! & c_3^3/3! & 0 & \eta_2^3/3! & \eta_3^3/3! \\
0 & \eta_2^5/5! & \eta_3^5/5! & c_6^4/4! & c_5^4/4! & c_4^4/4! & c_3^4/4! & 0 & \eta_2^4/4! & \eta_3^4/4! \\
0 & \eta_2^6/6! & \eta_3^6/6! & c_6^5/5! & c_5^5/5! & c_4^5/5! & c_3^5/5! & 0 & \eta_2^5/5! & \eta_3^5/5! \\
0 & \eta_2^7/7! & \eta_3^7/7! & c_6^6/6! & c_5^6/6! & c_4^6/6! & c_3^6/6! & 0 & \eta_2^6/6! & \eta_3^6/6! \\
0 & \eta_2^8/8! & \eta_3^8/8! & c_6^7/7! & c_5^7/7! & c_4^7/7! & c_3^7/7! & 0 & \eta_2^7/7! & \eta_3^7/7! \\
0 & \eta_2^9/9! & \eta_3^9/9! & c_6^8/8! & c_5^8/8! & c_4^8/8! & c_3^8/8! & 0 & \eta_2^8/8! & \eta_3^8/8! \\
\end{bmatrix}
\begin{bmatrix}
A_0 \\
A_1 \\
A_2 \\
A_3 \\
A_4 \\
A_5 \\
A_6 \\
A_7 \\
A_8 \\
A_9 \\
\end{bmatrix} =
\begin{bmatrix}
1 \\
0 \\
1/2! \\
1/3! \\
1/4! \\
1/5! \\
1/6! \\
1/7! \\
1/8! \\
1/9! \\
\end{bmatrix}.
\]
The leading error term of HBIF9 is
\[ A_1 \frac{\eta^2_{10}}{10!} + A_2 \frac{\eta^3_{10}}{10!} + \sum_{j=3}^{6} b_j c_j^2 \frac{\eta^j}{j!} + B_1 \frac{\eta^2_9}{9!} + B_2 \frac{\eta^3_9}{9!} - \frac{1}{10!} \] \[ h^{10}_{n+1} y^{(10)} \].

The coefficients of Predictor P1 satisfy the six order conditions:
\[
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \eta_2 & \eta_3 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & \eta_2^2/2! & \eta_3^2/2! & 0 & \eta_2 & \eta_3 & \alpha_22 & \alpha_21 & \alpha_2 & c_2 \\
0 & \eta_2^3/3! & \eta_3^3/3! & 0 & \eta_2^2/2! & \eta_3^2/2! & \alpha_22 & \alpha_21 & \alpha_2 & \eta_2^2/2! & \eta_3^2/2! \\
0 & \eta_2^4/4! & \eta_3^4/4! & 0 & \eta_2^3/3! & \eta_3^3/3! & \alpha_22 & \alpha_21 & \alpha_2 & \eta_2^2/2! & \eta_3^2/2! \\
0 & \eta_2^5/5! & \eta_3^5/5! & 0 & \eta_2^4/4! & \eta_3^4/4! & \alpha_22 & \alpha_21 & \alpha_2 & \eta_2^2/2! & \eta_3^2/2! \\
\end{bmatrix} =
\begin{bmatrix}
\alpha_{20} \\
\alpha_{21} \\
\alpha_{22} \\
\alpha_{23} \\
\alpha_{24} \\
\alpha_{25} \\
\end{bmatrix} =
\begin{bmatrix}
1 \\
c_2 \\
c_2^2/2! \\
c_2^3/3! \\
c_2^4/4! \\
c_2^5/5! \\
\end{bmatrix}.
\] (22)

The coefficients of \( h^j_{n+1}, j = 1, 2, \ldots, 10 \), in the truncated Taylor series expansion of the right-hand side of (3) for \( y(x) \) and \( y' = f(x, y) \) about \( x_n \) are
\[ L_2(j) = \alpha_21 \eta_2 + \alpha_22 \eta_3 + a_21 + \beta_21 + \beta_22, \] (23)
\[ L_2(j) = \alpha_21 \frac{\eta_2^j}{j!} + \alpha_22 \frac{\eta_3^j}{j!} + \beta_21 \frac{\eta_2^{j-1}}{(j-1)!} + \beta_22 \frac{\eta_3^{j-1}}{(j-1)!}, \] (24)
where \( \alpha_21, \alpha_22, \beta_21, \beta_22 \) are solutions of system (22). In other words, \( L_2(j) \) is the term associated with \( h^j_{n+1} \) in the truncated series
\[ y_n + c_2 h_{n+1} y'_n + \sum_{j=2}^{9} L_2(j) h^j_{n+1} y^{(j)}_n. \] (25)

We note that P1 is of order 5 because
\[ L_2(j) = \frac{c_2^j}{j!}, \quad j = 2, \ldots, 5. \] (26)

The leading error term of P1 is
\[
\left[ L_2(6) - \frac{c_2^6}{6!} \right] h^6 y^{(6)}.
\]

The coefficients of P2 satisfy the following seven order conditions:
\[
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \eta_2 & \eta_3 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & \eta_2^2/2! & \eta_3^2/2! & 0 & \eta_2 & \eta_3 & \eta_2 c_3 & \alpha_31 & \alpha_30 & \alpha_3 \\
0 & \eta_2^3/3! & \eta_3^3/3! & 0 & \eta_2^2/2! & \eta_3^2/2! & \eta_2 c_3 & \alpha_31 & \alpha_30 & \alpha_3 \\
0 & \eta_2^4/4! & \eta_3^4/4! & 0 & \eta_2^3/3! & \eta_3^3/3! & \eta_2 c_3 & \alpha_31 & \alpha_30 & \alpha_3 \\
0 & \eta_2^5/5! & \eta_3^5/5! & 0 & \eta_2^4/4! & \eta_3^4/4! & \eta_2 c_3 & \alpha_31 & \alpha_30 & \alpha_3 \\
0 & \eta_2^6/6! & \eta_3^6/6! & 0 & \eta_2^5/5! & \eta_3^5/5! & \eta_2 c_3 & \alpha_31 & \alpha_30 & \alpha_3 \\
\end{bmatrix} =
\begin{bmatrix}
\alpha_{30} \\
\alpha_{31} \\
\alpha_{32} \\
\alpha_{33} \\
\alpha_{34} \\
\alpha_{35} \\
\end{bmatrix} =
\begin{bmatrix}
1 \\
c_3 \\
c_3^2/2! \\
c_3^3/3! \\
c_3^4/4! \\
c_3^5/5! \\
\end{bmatrix}.
\] (27)

The coefficients of \( h^j_{n+1}, j = 1, 2, \ldots, 10 \), in the truncated Taylor series expansion of the right-hand side of (4) for \( y(x) \) and \( y' = f(x, y) \) about \( x_n \) are
\[ L_3(j) = \alpha_31 \frac{\eta_2^j}{j!} + \alpha_32 \frac{\eta_3^j}{j!} + a_31 + a_32 + \beta_31 + \beta_32, \] (28)
\[ L_3(j) = \alpha_31 \frac{\eta_2^j}{j!} + \alpha_32 \frac{\eta_3^j}{j!} + a_31 L_2(j-1) + \beta_31 \frac{\eta_2^{j-1}}{(j-1)!} + \beta_32 \frac{\eta_3^{j-1}}{(j-1)!}, \] (29)
\[ j = 2, \ldots, 10. \]
The coefficients of $P_3$ satisfy the following eight order conditions:

$$
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & \eta_2 & \eta_3 & 1 & 1 & 1 & 1 & 1 \\
0 & \eta_2^2/2! & \eta_3^2/2! & c_3 & c_3 & c_3 & 0 & \eta_2 & \eta_3 \\
0 & \eta_2^3/3! & \eta_3^3/3! & c_3^2/2! & c_3^2/2! & 0 & \eta_2^2/2! & \eta_3^2/2! \\
0 & \eta_2^4/4! & \eta_3^4/4! & c_3^3/3! & c_3^3/3! & 0 & \eta_2^3/3! & \eta_3^3/3! \\
0 & \eta_2^5/5! & \eta_3^5/5! & c_3^4/4! & c_3^4/4! & 0 & \eta_2^4/4! & \eta_3^4/4! \\
0 & \eta_2^6/6! & \eta_3^6/6! & c_3^5/5! & c_3^5/5! & 0 & \eta_2^5/5! & \eta_3^5/5! \\
0 & \eta_2^7/7! & \eta_3^7/7! & c_3^6/6! & c_3^6/6! & 0 & \eta_2^6/6! & \eta_3^6/6! \\
\end{bmatrix}
\begin{bmatrix}
\alpha_{40} \\
\alpha_{41} \\
\alpha_{42} \\
\alpha_{43} \\
\alpha_{44} \\
\alpha_{45} \\
\alpha_{46} \\
\alpha_{47} \\
\end{bmatrix}
= 
\begin{bmatrix}
1 \\
c_4 \\
c_4^2/2! \\
c_4^3/3! \\
c_4^4/4! \\
c_4^5/5! \\
c_4^6/6! \\
c_4^7/7! \\
\end{bmatrix}.
\tag{30}
$$

The coefficients of $h_{n+1}^j$, $j = 1, 2, \ldots, 10$, in the truncated Taylor series expansion of the right-hand side of (5) for $y(x)$ and $y' = f(x, y)$ about $x_n$ are

$$
L_4(1) = \alpha_{41} \eta_2 + \alpha_{42} \eta_3 + a_{43} + a_{44} + \alpha_{41} + \beta_{41} + \beta_{42},
\tag{31}
$$

$$
L_4(j) = \alpha_{41} \frac{\eta_2^j}{j!} + \alpha_{42} \frac{\eta_3^j}{j!} + a_{43} L_3(j-1) + a_{44} L_2(j-1)
\quad + \beta_{41} \frac{\eta_2^{j-1}}{(j-1)!} + \beta_{42} \frac{\eta_3^{j-1}}{(j-1)!},
\quad j = 2, \ldots, 10.
\tag{32}
$$

The coefficients of $P_4$ satisfy the following nine order conditions:

$$
\begin{bmatrix}
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \eta_2 & \eta_3 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & \eta_2^2/2! & \eta_3^2/2! & c_4 & c_3 & c_2 & 0 & \eta_2 & \eta_3 \\
0 & \eta_2^3/3! & \eta_3^3/3! & c_4^2/2! & c_3^2/2! & c_2^2/2! & 0 & \eta_2^2/2! & \eta_3^2/2! \\
0 & \eta_2^4/4! & \eta_3^4/4! & c_4^3/3! & c_3^3/3! & c_2^3/3! & 0 & \eta_2^3/3! & \eta_3^3/3! \\
0 & \eta_2^5/5! & \eta_3^5/5! & c_4^4/4! & c_3^4/4! & c_2^4/4! & 0 & \eta_2^4/4! & \eta_3^4/4! \\
0 & \eta_2^6/6! & \eta_3^6/6! & c_4^5/5! & c_3^5/5! & c_2^5/5! & 0 & \eta_2^5/5! & \eta_3^5/5! \\
0 & \eta_2^7/7! & \eta_3^7/7! & c_4^6/6! & c_3^6/6! & c_2^6/6! & 0 & \eta_2^6/6! & \eta_3^6/6! \\
0 & \eta_2^8/8! & \eta_3^8/8! & c_4^7/7! & c_3^7/7! & c_2^7/7! & 0 & \eta_2^7/7! & \eta_3^7/7! \\
0 & \eta_2^9/9! & \eta_3^9/9! & c_4^8/8! & c_3^8/8! & c_2^8/8! & 0 & \eta_2^8/8! & \eta_3^8/8! \\
0 & \eta_2^{10}/10! & \eta_3^{10}/10! & c_4^9/9! & c_3^9/9! & c_2^9/9! & 0 & \eta_2^9/9! & \eta_3^9/9! \\
\end{bmatrix}
\begin{bmatrix}
\alpha_{50} \\
\alpha_{51} \\
\alpha_{52} \\
\alpha_{53} \\
\alpha_{54} \\
\alpha_{55} \\
\alpha_{56} \\
\alpha_{57} \\
\end{bmatrix} = 
\begin{bmatrix}
1 \\
c_5 \\
c_5^2/2! \\
c_5^3/3! \\
c_5^4/4! \\
c_5^5/5! \\
c_5^6/6! \\
c_5^7/7! \\
\end{bmatrix},
\tag{33}
$$

where the 8th row, $a(8, :)$, is

$$
a(8, :) = (1 - c_5) b_5 \begin{bmatrix}
0 & \eta_2^7/7! & \eta_3^7/7! & c_4^6/6! & c_3^6/6! & c_2^6/6! & 0 & \eta_2^6/6! & \eta_3^6/6! \\
\end{bmatrix}.
$$

The right-hand sides, $r_7$ and $r_8$, of the 8th and 9th equations in (33) are

$$
r_7 = \frac{1}{9!} - \left\{ (1-c_2) b_2 B(2, 7) + (1-c_3) b_3 \left[ a_{32} \frac{c_2^6}{6!} + B(3, 7) \right] \\
+ (1-c_4) b_4 \left[ a_{43} \frac{c_3^6}{6!} + a_{44} \frac{c_2^6}{6!} + B(4, 7) \right] + B_Q(8) - 8 B_Q(9) \right\}
$$

$$
r_8 = -\left[ b_2 (c_3 - 1) a_{32} + b_4 (c_4 - 1) a_{42} \right] \ldots
$$

The coefficients of $h_{n+1}^j$, $j = 1, 2, \ldots, 10$, in the truncated Taylor series expansion of the right-
The coefficients of $h^j_{x+1}$, $j = 1, 2, \ldots, 10$, in the truncated Taylor series expansion of the right-hand side of  (7) for $y(x)$ and $y' = f(x, y)$ about $x_n$ are

$$L_5(1) = \alpha_{51} \eta_2 + \alpha_{52} \eta_3 + \sum_{j=1}^{4} a_{5j} + \beta_{51} + \beta_{52},$$

$$L_5(j) = \alpha_{51} \frac{\eta_j^j}{j!} + \alpha_{52} \frac{\eta_3^j}{j!} + \sum_{k=2}^{4} a_{5k} L_k(j - 1) + \beta_{51} \frac{\eta_2^{j-1}}{(j - 1)!} + \beta_{52} \frac{\eta_3^{j-1}}{(j - 1)!}, \quad j = 2, \ldots, 10. \tag{35}$$

The coefficients of the last predictor, P5, satisfy the following ten conditions:

$$\begin{bmatrix}
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \eta_2 & \eta_3 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & \eta_2^2 / 2! & \eta_2^3 / 2! & c_5 & c_4 & c_3 & c_2 & 0 & \eta_2 & \eta_3 \\
0 & \eta_2^3 / 3! & \eta_2^3 / 3! & c_5^2 / 2! & c_4^2 / 2! & c_3^2 / 2! & c_2^2 / 2! & 0 & \eta_2^2 / 2! & \eta_3^2 / 2! \\
0 & \eta_2^4 / 4! & \eta_2^4 / 4! & c_5^3 / 3! & c_4^3 / 3! & c_3^3 / 3! & c_2^3 / 3! & 0 & \eta_2^3 / 3! & \eta_3^3 / 3! \\
0 & \eta_2^5 / 5! & \eta_2^5 / 5! & c_5^4 / 4! & c_4^4 / 4! & c_3^4 / 4! & c_2^4 / 4! & 0 & \eta_2^4 / 4! & \eta_3^4 / 4! \\
0 & 0 & 0 & 0 & b_6 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & b_6 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & b_6 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & b_6 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & b_6 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_6 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & b_6 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
\alpha_{60} \\
\alpha_{61} \\
\alpha_{62} \\
\alpha_{63} \\
\alpha_{64} \\
\alpha_{65} \\
\alpha_{66} \\
\alpha_{67} \\
\beta_{61} \\
\beta_{62} \\
\end{bmatrix}
= \begin{bmatrix}
1 \\
c_6 \\
c_6^2 / 2! \\
c_6^3 / 3! \\
c_6^4 / 4! \\
c_6^5 / 5! \\
r_7 \\
r_8 \\
r_9 \\
r_{10} \\
\end{bmatrix}, \tag{36}$$

where

$$r_7 = b_5(1 - c_5), \quad r_8 = b_4(1 - c_4) - (b_5 a_{54}), \quad r_9 = b_3(1 - c_3) - (b_4 a_{43} + b_5 a_{53}), \quad r_{10} = -(b_3 a_{32} + b_4 a_{42} + b_5 a_{52}).$$

The coefficients of $h^j_{y+1}$, $j = 1, 2, \ldots, 10$, in the truncated Taylor series expansion of the right-hand side of  (7) for $y(x)$ and $y' = f(x, y)$ about $x_n$ are

$$L_6(1) = \alpha_{61} \eta_2 + \alpha_{62} \eta_3 + \sum_{j=1}^{5} a_{6j} + \beta_{61} + \beta_{62},$$

$$L_6(j) = \alpha_{61} \frac{\eta_2^j}{j!} + \alpha_{62} \frac{\eta_3^j}{j!} + \sum_{k=2}^{5} a_{6k} L_k(j - 1) + \beta_{61} \frac{\eta_2^{j-1}}{(j - 1)!} + \beta_{62} \frac{\eta_3^{j-1}}{(j - 1)!}, \quad j = 2, \ldots, 10. \tag{39}$$

The coefficients of SCP satisfy the following eight order conditions:

$$\begin{bmatrix}
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \eta_2 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & \eta_2^2 / 2! & c_6 & c_5 & c_4 & c_3 & 0 & \eta_2 \\
0 & \eta_2^3 / 3! & c_6^2 / 2! & c_5^2 / 2! & c_4^2 / 2! & c_3^2 / 2! & 0 & \eta_2^2 / 2! \\
0 & \eta_2^4 / 4! & c_6^3 / 3! & c_5^3 / 3! & c_4^3 / 3! & c_3^3 / 3! & 0 & \eta_2^3 / 3! \\
0 & \eta_2^5 / 5! & c_6^4 / 4! & c_5^4 / 4! & c_4^4 / 4! & c_3^4 / 4! & 0 & \eta_2^4 / 4! \\
0 & \eta_2^6 / 6! & c_6^5 / 5! & c_5^5 / 5! & c_4^5 / 5! & c_3^5 / 5! & 0 & \eta_2^5 / 5! \\
0 & \eta_2^7 / 7! & c_6^6 / 6! & c_5^6 / 6! & c_4^6 / 6! & c_3^6 / 6! & 0 & \eta_2^6 / 6! \\
\end{bmatrix}
\begin{bmatrix}
\alpha_{70} \\
\alpha_{71} \\
\alpha_{72} \\
\alpha_{73} \\
\alpha_{74} \\
\alpha_{75} \\
\alpha_{76} \\
\beta_{71} \\
\beta_{72} \\
\beta_{73} \\
\beta_{74} \\
\end{bmatrix}
= \begin{bmatrix}
1 \\
1/2! \\
1/3! \\
1/4! \\
1/5! \\
1/6! \\
1/7! \\
\end{bmatrix}. \tag{40}$$
which determine by choice, reduce the global error and extend the region of absolute stability of a method. Particular values of some of the parameters, say, the location of the off-step points, in order to the parameters entering in the method. To circumvent this difficulty, one can run many cases with \( \eta \) and \( \eta_c \) to (note that, \( c_2, c_3, c_4, c_5 \), are derived similarly. It would be a formidable task to optimize an HB method by solving all the equations for all the parameters entering in the method. To circumvent this difficulty, one can run many cases with particular values of some of the parameters, say, the location of the off-step points, in order to reduce the global error and extend the region of absolute stability of a method.

### 4 Particular variable-step HB\((9, 7; 5)\{6, 2\}\)

The 6-stage general HB\((9, 7; 5)\{6, 2\}\) method contains four free coefficients, \( c_2, c_3, c_4, c_5 \) (note that, by choice, \( c_1 = 0 \) and \( c_6 = 1 \)). It also depends on \( h_{n+1} \) and the previous nodes \( x_n, x_{n-1} \) and \( x_{n-2} \), which determine \( \eta_2 \) and \( \eta_3 \) in (12).

A particular variable-step HB\((9, 7; 5)\{6, 2\}\) is obtained with the choice of the six coefficients

\[
c_1 = 0, \quad c_2 = \frac{1}{5}, \quad c_3 = 0.3, \quad c_4 = 0.8, \quad c_5 = \frac{8}{9}, \quad c_6 = 1,
\]

of DP\((5,4)7M\). This method still depends on the choice of \( \eta_2 \) and \( \eta_3 \). Thus at each step, all the linear systems for the order conditions have to be solved for the coefficients of the method for given \( c_i \).

Among many experimental choices of the \( c_i \), the choice (41) produces a very good method as testified by the results of sections [9] and [10].

### Remark 1

Eleventh-order general HB\((11, 8; 7)\{6, 3\}\) with six stages and four degrees of freedom, \( c_2, c_3, c_4, c_5 \), are derived similarly.

It would be a formidable task to optimize an HB method by solving all the equations for all the parameters entering in the method. To circumvent this difficulty, one can run many cases with particular values of some of the parameters, say, the location of the off-step points, in order to reduce the global error and extend the region of absolute stability of a method.

### 5 Constant-step HB\((9, 7; 5)\{6, 2\}\)

As an illustration, we list a constant-step HB\((9, 7; 5)\{6, 2\}\). This method uses the coefficients (41), and \( \eta_2 = -1 \) and \( \eta_3 = -2 \) given in (12). The variable stepsize \( h_{n+1} \) appearing in (3) to (9) is replaced here by the constant stepsize \( h \).
• Predictors

\[ \hat{y}_{n+c_2} = \frac{2178}{3125} y_n + \frac{121}{625} y_{n-1} + \frac{342}{3125} y_{n-2} + h \left( \frac{1089}{3125} f_n + \frac{726}{3125} f_{n-1} + \frac{99}{3125} f_{n-2} \right) , \]

\[ \hat{y}_{n+c_3} = \frac{805971}{797086} y_n - \frac{14283}{166000} y_{n-1} - \frac{2699}{1061497} y_{n-2} + h \left( \frac{268203}{1168640} \hat{f}_{n+c_2} + \frac{100616}{1556867} \hat{f}_n - \frac{21623}{3025770} f_{n-1} - \frac{407}{606974} f_{n-2} \right) , \]

\[ \hat{y}_{n+c_4} = \frac{2212488}{614311} y_n - \frac{1083725}{556444} y_{n-1} - \frac{343393}{525077} y_{n-2} + h \left( \frac{2306105}{660914} \hat{f}_{n+c_3} - \frac{3565709}{1355847} \hat{f}_{n+c_2} - \frac{3098733}{2198969} f_n - \frac{1609256}{929887} f_{n-1} - \frac{51039}{291344} f_{n-2} \right) , \]

\[ \hat{y}_{n+c_5} = \frac{31219381}{2647362} y_n - \frac{70238926}{8753129} y_{n-1} - \frac{2988661}{1079680} y_{n-2} + h \left( \frac{366958}{1058017} \hat{f}_{n+c_4} + \frac{18705772}{1752259} \hat{f}_{n+c_3} - \frac{16408084}{1915593} \hat{f}_{n+c_2} - \frac{2190913}{339853} f_n - \frac{7515704}{1037417} f_{n-1} - \frac{1862651}{2505150} f_{n-2} \right) , \]

\[ \hat{y}_{n+c_6} = \frac{5430577}{489076} y_n - \frac{11633252}{1558477} y_{n-1} - \frac{1331324}{504433} y_{n-2} + h \left( \frac{240731}{979101} \hat{f}_{n+c_5} + \frac{392052}{1307593} \hat{f}_{n+c_4} + \frac{6526988}{810229} \hat{f}_{n+c_3} - \frac{10626781}{1794820} \hat{f}_{n+c_2} - \frac{8289751}{1298137} f_n - \frac{2920544}{427285} f_{n-1} - \frac{312432}{439501} f_{n-2} \right) . \]

• Integrator

\[ y_{n+1} = \frac{333233}{329916} y_n - \frac{11425}{1205826} y_{n-1} - \frac{255}{440231} y_{n-2} + h \left( \frac{89185}{819532} \hat{f}_{n+c_6} - \frac{136035}{564908} \hat{f}_{n+c_5} + \frac{247375}{425959} \hat{f}_{n+c_4} + \frac{310995}{655018} \hat{f}_{n+c_3} - \frac{191543}{2744934} f_n - \frac{6589}{1714584} f_{n-1} - \frac{67}{544750} f_{n-2} \right) . \]

• Step Control Predictor

\[ \tilde{y}_{n+1} = \frac{82976}{82893} y_n - \frac{83}{82893} y_{n-1} + h \left( \frac{133214}{1038941} \hat{f}_{n+c_6} - \frac{220531}{707727} \hat{f}_{n+c_5} + \frac{5782154}{9015245} \hat{f}_{n+c_4} + \frac{377256}{832813} \hat{f}_{n+c_3} + \frac{54392}{616119} f_n - \frac{217}{82058} f_{n-1} \right) . \]

6 HB(10, 7; 5) {7, 2}

The general HB(10, 7; 5) {7, 2} with s = 7 stages and predictor P1 of order p1 = 5 must satisfy 36 order conditions. In addition to the simplifying assumptions (14) to (16) and the order conditions,
there are three additional simplifying assumptions to be satisfied:

\[ \sum_{i=3}^{6} b_i (1 - c_i) a_{i2} = 0, \quad \sum_{i=3}^{5} b_i (1 - c_i) (c_6 - c_i) a_{i2} = 0, \] (42)

\[ \sum_{i=4}^{6} \sum_{j=3}^{i-1} b_i (1 - c_i) a_{ij} a_{j2} = 0. \] (43)

The solution of the equations of condition for HB(10, 7; 5)\{7, 2\} is generalized from that of Butcher [2] who derived a sixth-order Runge–Kutta formula with seven stages.

In HB(10, 7; 5)\{7, 2\}, at each step,

- The coefficient \( c_2 \) is chosen so that P2 becomes a Hermite–Birkhoff–Radau quadrature with 1 off-step point (in other words, P2 is of order 7 if P1 is of order 6).
- The coefficients of the predictors are calculated so that all the order conditions and simplifying assumptions are satisfied except the following condition for predictor P5:

\[ \alpha_61 \eta_2^2 + \alpha_62 \eta_3^2 + a_{65} c_5 + a_{64} c_4 + a_{63} c_3 + a_{62} c_2 + \beta_61 \eta_2 + \beta_62 \eta_3 = \frac{c_2^2}{2!}. \] (44)

The coefficient \( c_4 \) is then chosen by the bisection method such that (44) is satisfied.

Thus, we obtain a general HB(10, 7; 5)\{7, 2\} of order 10 with 7 stages and three undetermined coefficients, \( c_3, c_5, c_6 \) (note that, by choice, \( c_1 = 0 \) and \( c_7 = 1 \)).

With the choice

\[ c_1 = 0, \quad c_3 = \frac{2}{9}, \quad c_5 = \frac{3}{5}, \quad c_6 = \frac{4}{5}, \quad c_7 = 1, \] (45)

we have a particular variable-step HB(10, 7; 5)\{7, 2\} with \( \eta_2, \eta_3, c_2, c_4 \) as variables. To avoid solving linear systems and calculating \( c_2, c_4 \) whenever the stepsize changes, in the applications, it may be enough to quantize the stepsize to a small number of predefined stepsizes at the expense of a small increase in the number of function evaluations. One may solve 64 sets of equations of conditions once for all for the 64 combinations of \( h_{n+1} \) listed in Table 3 as in the HB(9, 7; 5)\{6, 2\} case.

The structure of this method is illustrated by the following constant-step HB(10, 7; 5)\{7, 2\} with the following coefficients

\[ c_1 = 0, \quad c_2 = \frac{66202}{421143}, \quad c_3 = \frac{2}{9}, \quad c_4 = \frac{1207021}{4906615}, \quad c_5 = \frac{3}{5}, \quad c_6 = \frac{4}{5}, \quad c_7 = 1, \] (46)

and the parameters \( \eta_2 = -1, \eta_3 = -2 \) as defined in (12). The constant stepsize is \( h \).

- **Predictors**

\[
\hat{y}_{n+2} = \frac{1495619}{1816834} y_n + \frac{83923}{729825} y_{n-1} + \frac{180917}{2927046} y_{n-2} \\
+ h \left( \frac{67983}{277604} f_n + \frac{117952}{886413} f_{n-1} + \frac{23004}{1289071} f_{n-2} \right),
\]

\[
\hat{y}_{n+3} = \frac{603999}{605549} y_n + \frac{2175}{907513} y_{n-1} + \frac{159}{975455} y_{n-2} + h \left( \frac{101515}{659884} \hat{f}_{n+c2} \\
+ \frac{264984}{3778531} f_n + \frac{672}{714013} f_{n-1} + \frac{29}{778749} f_{n-2} \right),
\]
\[
\begin{align*}
\hat{y}_{n+c_4} &= \frac{1499401}{1503602} y_n + \frac{2033}{777788} y_{n-1} + \frac{149}{827159} y_{n-2} + h \left( \frac{9757}{315427} \hat{f}_{n+c_3} \right. \\
&\quad + \frac{237752}{1636935} \hat{f}_{n+c_2} + \frac{4557}{63535} f_n + \frac{1553}{1504089} f_{n-1} + \frac{55}{1335029} f_{n-2} \right), \\
\hat{y}_{n+c_5} &= \frac{634854}{1341353} y_n + \frac{250169}{521567} y_{n-1} + \frac{36583}{777412} y_{n-2} + h \left( \frac{42377990}{3966537} \hat{f}_{n+c_4} - \frac{5623019}{513497} \hat{f}_{n+c_3} \\
&\quad - \frac{382649}{583588} \hat{f}_{n+c_2} + \frac{1135127}{609816} f_n + \frac{205204}{918065} f_{n-1} + \frac{9121}{823983} f_{n-2} \right), \\
\hat{y}_{n+c_6} &= \frac{4164809}{2439493} y_n - \frac{502199}{772242} y_{n-1} - \frac{240380}{4222327} y_{n-2} + h \left( \frac{629753}{917806} \hat{f}_{n+c_5} - \frac{37411960}{2028531} \hat{f}_{n+c_4} + \frac{15327901}{752193} \hat{f}_{n+c_3} \\
&\quad + \frac{283739}{1094399} \hat{f}_{n+c_2} - \frac{2870365}{1128999} f_n - \frac{193914}{671651} f_{n-1} - \frac{19632}{1485809} f_{n-2} \right), \\
\hat{y}_{n+c_7} &= -\frac{3347544}{2412229} y_n + \frac{3232588}{1458077} y_{n-1} + \frac{310633}{1819574} y_{n-2} + h \left( \frac{882438}{920477} \hat{f}_{n+c_6} \\
&\quad - \frac{8620783}{3639588} \hat{f}_{n+c_5} + \frac{65044157}{737027} f_{n+c_4} - \frac{99048035}{1050988} \hat{f}_{n+c_3} \\
&\quad - \frac{472229}{1412704} \hat{f}_{n+c_2} + \frac{14057623}{1361879} f_n + \frac{1238898}{1329155} f_{n-1} + \frac{46694}{1195287} f_{n-2} \right).
\end{align*}
\]

- **Integrator**

\[
\begin{align*}
y_{n+1} &= \frac{474137}{477957} y_n + \frac{13018}{1662697} y_{n-1} + \frac{149}{914657} y_{n-2} + h \left( \frac{55228}{915547} \hat{f}_{n+c_7} \\
&\quad + \frac{359985}{1244986} \hat{f}_{n+c_6} + \frac{366771}{2642521} \hat{f}_{n+c_5} + \frac{2386955}{1221228} \hat{f}_{n+c_4} \\
&\quad - \frac{2304703}{1431490} \hat{f}_{n+c_3} + \frac{330869}{1910638} f_n + \frac{1401}{655927} f_{n-1} + \frac{31}{1000599} f_{n-2} \right).
\end{align*}
\]

- **Step Control Predictor**

\[
\begin{align*}
\tilde{y}_{n+1} &= \frac{2373973}{2371300} y_n - \frac{2673}{2371300} y_{n-1} + \frac{300662}{4403675} \hat{f}_{n+c_7} + \frac{430122}{1783447} \hat{f}_{n+c_6} + \frac{120317}{493615} \hat{f}_{n+c_5} \\
&\quad + \frac{513389}{1360282} \hat{f}_{n+c_4} + \frac{84319}{1230572} f_n - \frac{493}{1914726} f_{n-1}.
\end{align*}
\]

## 7 Region of absolute stability of the methods

The region of absolute stability, $R$, of an HB method is obtained by a scanning method. A complex number $\lambda h$, with small $h > 0$, in the left-half complex plane is in $R$ if the numerical solution, $y_n$, of the linear test equation

\[ y' = \lambda y, \quad y_0 = 1, \]
converges to 0 as $n \to \infty$. The regions of absolute stability of HB methods of orders 9, 10 and 11 are shown in Figs. 1, 2 and 3. The corresponding intervals of absolute stability, $(\alpha, 0)$, of HB methods, the fifth-order method, DP(5,4)7M, and the eighth-order method, DP(8,7)13M, are given in Table 4. The norm of the principal local truncation coefficients (PLTC) of these constant-step HB methods and DP(8,7)13M (see [6]) are given in Table 5.

8 Controlling stepsize

We use the following simple procedure to calculate the coefficients of the predictors and the integration formula whenever the stepsize changes. First, an estimate $y_{n+1} - \tilde{y}_{n+1}$ and $h_n$ can be used to calculate the stepsize $h_{n+1}$ by means of formula [9]:

$$h_{new} = \min \left\{ h_{max}, \beta h_{old} \left( \frac{\text{tolerance}}{|y_{n+1} - \tilde{y}_{n+1}|} \right)^{1/\kappa} \right\},$$  \hspace{1cm} (47)
Figure 3: Region of absolute stability, $R$, of HB(11, 7; 7)\{6, 3\}.

Table 4: Abscissae of absolute stability $\alpha$.

<table>
<thead>
<tr>
<th>Method</th>
<th>$\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HB(9, 7; 5){6, 2}</td>
<td>$-3.2$</td>
</tr>
<tr>
<td>HB(10, 7; 5){7, 2}</td>
<td>$-2.5$</td>
</tr>
<tr>
<td>HB(11, 7; 7){6, 3}</td>
<td>$-3.4$</td>
</tr>
<tr>
<td>DP(8,7)13M</td>
<td>$-5.1$</td>
</tr>
</tbody>
</table>

Table 5: Norm of the principal local truncation coefficients.

<table>
<thead>
<tr>
<th>Method</th>
<th>Norm of PLTC</th>
</tr>
</thead>
<tbody>
<tr>
<td>HB(9, 7; 5){6, 2}</td>
<td>$3.12e-5$</td>
</tr>
<tr>
<td>HB(10, 7; 5){7, 2}</td>
<td>$8.11e-6$</td>
</tr>
<tr>
<td>HB(11, 7; 7){6, 3}</td>
<td>$5.44e-6$</td>
</tr>
<tr>
<td>DP(8,7)13M</td>
<td>$4.51e-6$</td>
</tr>
</tbody>
</table>
except that $h_{new}$ is not allowed to differ from $h_{old}$ by more than a factor of 4. The values of the constants $\beta = 0.9$ and $\kappa$ are:

<table>
<thead>
<tr>
<th></th>
<th>HB(9, 7; 5){6, 2}</th>
<th>HB(10, 7; 5){7, 2}</th>
<th>HB(11, 8; 7){6, 3}</th>
<th>DP(8, 7)13M</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\kappa$</td>
<td>8</td>
<td>8</td>
<td>9</td>
<td>8</td>
</tr>
</tbody>
</table>

In fact, $\kappa = q + 1$.

Next, we calculate the coefficients of the integration formula HBIF9 and of the predictors P1, P2, P3, P4 and P5 for HB(9, 7; 5){6, 2}. These depend only on the values of $\eta_2$ and $\eta_3$ defined in (12) and on the off-step points determined by the choice of the $c_i$. Solving system (21), we obtain the coefficients of HBIF9. To obtain the coefficients of P1, P2, P3, P4, P5 and SCP we solve systems (22), (27), (30), (33), (36) and (40), respectively.

## 9 Comparison of numerical results

Two objective criteria are used to compared the numerical methods considered in this paper.

### 9.1 Comparison based on the maximum global error

As a first comparison, the Maximum Global Error (MGE) has been plotted for the methods treated here. In Fig. 4 the horizontal axis is the number of function evaluations (NFE) for a given tolerance and the vertical axis is

$$\log_{10}\left(\sum |\text{MGE}|\right),$$

(48)

where the sum is over the problems considered.

It is seen from the figure that HB(9, 7; 5){6, 2}, HB(10, 7; 5){7, 2} and HB(11, 8; 7){6, 3} have lower global maximum errors than the comparative method DP(8, 7)13M for wide ranges of tolerance.
Table 6: Global NFE PEG of three HB methods over DP(8,7)13M for the DETEST problems of class D.

<table>
<thead>
<tr>
<th>HB method</th>
<th>Global NFE PEG</th>
</tr>
</thead>
<tbody>
<tr>
<td>HB(9, 7; 5){6, 2}</td>
<td>16%</td>
</tr>
<tr>
<td>HB(10, 7; 5){7, 2}</td>
<td>59%</td>
</tr>
<tr>
<td>HB(11, 8; 7){6, 3}</td>
<td>50%</td>
</tr>
</tbody>
</table>

9.2 Comparison based on the number of function evaluations percentage efficiency gain

As a second comparison, Table 6 lists the global Number of Function Evaluations Percentage Efficiency Gain (NFE PEG) which is defined by a formula similar to the one used by Sharp [12],

$$\text{Global NFE PEG} = 100 \left( \frac{\sum_{i,j} \text{NFE}_{2,i,j}}{\sum_{i,j} \text{NFE}_{1,i,j}} - 1 \right),$$

where NFE_{1,i,j} and NFE_{2,i,j} are the number of function evaluations of methods 1 and 2, respectively, associated with problem $i$ and Maximum Global Error $10^{-j}$, with stepsize control (47).

10 Testing methods on DETEST problems of class D

The above HB methods were tested on the five non-stiff DETEST two-body problems of class D [7] given by the initial value equations

$$y_1' = y_3,$$
$$y_2' = y_4,$$
$$y_3' = -y_1/(y_1^2 + y_2^2)^{3/2},$$
$$y_4' = -y_2/(y_1^2 + y_2^2)^{3/2},$$

where the eccentricity, $\epsilon$, of the five problems is $\epsilon = 0.1, 0.3, 0.5, 0.7, 0.9$, respectively.

We consider numerical solutions of these problems by means of HB(9, 7; 5)\{6, 2\}, HB(10, 7; 5)\{7, 2\} and HB(11, 8; 7)\{6, 3\}, of order 9, 10 and 11, respectively, and DP(8,7)13M of order 8.

The integration was carried to the point $x = 20$ and the starting values were obtained by ODE45 or ODE113 of the MATLAB ODE suite. Table 6 lists the global NFE PEG of the three HB methods as compared with DP(8,7)13M. The coefficients $c_i$ of HB(9, 7; 5)\{6, 2\} and HB(11, 8; 7)\{6, 3\} are those of DP(5,4)7M listed in (41).

11 Conclusion

The new methods, HB(9, 7; 5)\{6, 2\}, HB(10, 7; 5)\{7, 2\} and HB(11, 8; 7)\{6, 3\}, compare favorably with DP(8,7)13M as tested on the five DETEST two-body problems of class D on the basis of the global error and the percentage efficiency gain of the number of function evaluation.
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