On contractivity-preserving 2- and 3-step predictor-corrector series for ODEs

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Abstract

New optimal, contractivity-preserving (CP), \( d \)-derivative, 2- and 3-step, predictor-corrector, Hermite–Birkhoff–Obrechkoff series methods, denoted by HBO\((d,k,p)\), \( k = 2,3 \), with nonnegative coefficients are constructed for solving nonstiff first-order initial value problems \( y' = f(t,y) \), \( y(t_0) = y_0 \). The upper bounds \( p_u \) of order \( p \) of HBO\((d,k,p)\), \( k = 2,3 \) methods are approximately 1.4 and 1.6 times the number of derivatives \( d \), respectively. Their stability regions have generally a good shape and grow with decreasing \( p - d \). Two selected CP HBO methods: 9-derivative 2-step HBO of order 13, denoted by HBO\((9,2,13)\), which has maximum order 13 based on the CP conditions, and 8-derivative 3-step HBO of order 14, denoted by HBO\((8,3,14)\), compare well with Adams–Cowell of order 13 in PECE mode, denoted by AC\((13)\), in solving standard N-body problems over an interval of 1000 periods on the basis of the relative error of energy as a function of the CPU time. They also compare well with AC\((13)\) in solving standard N-body problems on the basis of the growth of relative error of energy and 10000 periods of integration. The coefficients of selected HBO methods are listed in the appendix.

Keywords: Contractivity-preserving, Hermite–Birkhoff–Obrechkoff series method, predictor-corrector multiderivative methods, Taylor series methods, Series methods for ODEs, N-body simulation.

1. Introduction

In this paper, only \( d = 2,3, \ldots, 9 \), Taylor coefficients, with \( d < p \), are required by a new contractivity-preserving (CP), explicit, \( d \)-derivative, 2- and 3-step, predictor-corrector, Hermite–Birkhoff–Obrechkoff method of order \( p \) up to 13 and 16, respectively, for solving nonstiff ODEs,

\[
y' = f(t,y), \quad y(t_0) = y_0, \quad \text{where } ' = \frac{d}{dt} \quad \text{and} \quad y \in \mathbb{R}^n. \tag{1}
\]
The new methods are denoted by \( \text{HBO}(d, k, p) \), \( k = 2, 3 \), which use \( y', y'', \ldots y^{(d)} \), as in Obrechkoff methods [21].

The Taylor series methods have been an excellent choice in astronomical calculations [3], numerical integration of ordinary differential equations (ODEs) and differential algebraic equations (DAEs) [1], sensitivity analysis of ODEs/DAEs [2], in solving general problems [5] and validating solutions of ODEs by means of interval analysis [18, 11].

The main cost in solving ODEs by the Taylor method of order \( p \) (T(p)) lies in the repeated evaluation of the \( p \) Taylor coefficients of the functions involved.

Following Steffensen and Rabe [25, 22], recursive computation of Taylor coefficients is used to compute sums, differences, products and powers of power series, etc. (see [3, 17], and [10, pp. 46–49]).

Deprit and Zahar [6] showed that such recursive computation is very effective in achieving high accuracy, even with little computing time and large step sizes.

The current investigation and the results are offered as potentially useful additions to the contemporary repertory of numerical integrators. This paper explores an alternative way to improve the stability and the order of predictor-corrector methods. In our construction of \( \text{HBO}(d, k, p) \), we replace the forward Euler (FE) method,

\[
y_{n+1} = y_n + \Delta t f(t_n, y_n),
\]

used by Gottlieb et al. and Huang [7, 12] in establishing strong stability preserving (SSP) Runge–Kutta (RK) methods as convex combinations of FE methods, by rewriting \( \text{HBO}(d, k, p) \) as a convex combination of the special \( d \)-derivative extension of FE, which we denote by \( S(d) \):

\[
y_{n+1} = y_n + \Delta t f(t_n, y_n) + \sum_{m=2}^{d} \eta_m (\Delta t)^m f^{(m-1)}(t_n, y_n),
\]

where the coefficients \( \eta_m \) satisfy the inequality \( \eta_m \leq \frac{1}{m!} \). If equality holds, then \( S(d) \) reduces to the Taylor method of order \( d, T(d) \). The error in \( S(d) \) is of order \( \ell \geq 2 \) if there exists a smallest \( \ell \in \{2, 3, \ldots, d\} \) such that \( \eta_{\ell} < \frac{1}{\ell!} \). If \( S(d) \) is contractive in a given norm, then \( \text{HBO}(d, k, p) \) will be contractive as a convex combination of \( S(d) \) with modified step sizes.

The region of absolute stability of \( \text{HBO}(d, k, p) \) is derived under the assumption that two solutions, \( y \) and \( \tilde{y} \), to problem (1) are contractive:

\[
\|y(t + \Delta t) - \tilde{y}(t + \Delta t)\| \leq \|y(t) - \tilde{y}(t)\|, \quad \forall \Delta t \geq 0.
\]

We assume that there exists a maximum stepsize \( \Delta t_{S(d)} \) such that \( f \) satisfies a discrete analog of (4) when \( S(d) \) is employed with \( \Delta t \leq \Delta t_{S(d)} \):

\[
\|y_{n+1} - \tilde{y}_{n+1}\| \equiv \|y_n + \Delta t f(t_n, y_n) + \sum_{m=2}^{d} \eta_m (\Delta t)^m f^{(m-1)}(t_n, y_n) - \left( \tilde{y}_n + \Delta t f(t_n, \tilde{y}_n) + \sum_{m=2}^{d} \eta_m (\Delta t)^m f^{(m-1)}(t_n, \tilde{y}_n) \right)\| \leq \|y_n - \tilde{y}_n\|.
\]

Here \( y_n \) and \( \tilde{y}_n \) are two numerical solutions generated by \( S(d) \) with different neighbouring starting (or previous) values \( y_0 = y(t_0) \) and \( \tilde{y}_0 = \tilde{y}(t_0) \).

By interpreting \( \tilde{y}_0 \) as a perturbation of \( y_0 \) due to numerical error, we see that contractivity implies that these errors do not grow as they are propagated.
We are interested in a higher-order HBO($d, k, p$) that maintains the contractivity-preserving property

$$\|y_{n+1} - \tilde{y}_{n+1}\| \leq \max_{0 \leq \ell \leq (k-1)} \|y_{n-\ell} - \tilde{y}_{n-\ell}\|,$$

(6)

for $0 \leq \Delta t \leq \Delta t_{\text{max}} = c\Delta t_{S(d)}$ whenever inequality (5) holds. Here $c$, called the CP coefficient, depends only on the numerical integration method but not on $f$. This definition of the CP coefficient of HBO($d, k, p$) follows closely the definition of the SSP coefficient of RK (see [7]).

In [15], similar CP RK methods have been constructed and tested on DETEST problems [14]. The aim of HBO($d, k, p$) is to maintain the CP property (6) while achieving higher-order accuracy, perhaps with a modified time-step restriction, measured here with the CP coefficient $c(HBO(d, k, p))$:

$$\Delta t \leq c(HBO(d, k, p))\Delta t_{S(d)}.$$

(7)

This coefficient describes the ratio of the maximal HBO($d, k, p$) time step to the time step $\Delta t_{S(d)}$, for which condition (5) holds.

The upper bounds $p_u$ of order $p$ of HBO($d, k, p$), $k = 2, 3$ methods are approximately 1.4 and 1.6 times the number of derivatives $d$, respectively. It can be shown that HBO($d, k, p$)) are absolutely stable for $d = 1$ to infinity. Their stability regions have generally a good shape and grow with decreasing $p - d$. This result suggests that, for large $d$, HBO($d, k, p$) methods have order $p$ large enough to take into account many problems where a very high precision of the solution is required, similar to Taylor methods.

Similar to Huang et al. [13], we, first, compare the numerical performance of HBO($9,2,13$), HBO($8,3,14$) and Adams–Cowell of order 13 in PECE mode, denoted by AC(13), on Kepler circular orbit with eccentricity $e = 0.3$, $e = 0.5$ and $e = 0.7$ over an interval of 1000 periods on the basis of $\log_{10}(\text{EE})$ as a function of CPU time. It is seen that HBO($9,2,13$) and HBO($8,3,14$) win. Next, these two HBO methods compare well with AC(13) in solving eccentric Kepler orbit with eccentricity $e = 0.3$, $e = 0.5$ and $e = 0.7$ over an interval of 10000 periods on the basis of the growth of relative error of energy and long intervals of integration.

Section 2 introduces $d$-derivative HBO($d, k, p$) methods and the necessary order conditions are listed in Section 3. Section 4 derives HBO($d, k, p$) in Shu–Osher form. In Section 5, the existence, the stability properties of HBO($d, k, p$) methods are considered. Section 6 describes the region of absolute stability and the principal error term of two selected HBO methods: HBO($9,2,13$), HBO($8,3,14$). In Section 7, numerical results are used to compare HBO($9,2,13$), HBO($8,3,14$) with AC(13). New selected HBO($9,2,13$), HBO($8,3,14$) methods are listed in Appendix A.

2. Predictor-corrector CP Hermite–Birkhoff–Obrechkoff methods

All HBO methods considered in this paper are CP, so the denomination “CP” will generally be omitted in what follows.

The $k$-step, predictor-corrector HBO($d, k, p$) are constructed, as a subclass of multiderivative, multistep, multistage methods, by the following two formulae which perform integration from $t_n$ to $t_{n+1}$. Let $\Delta t$ denote the step size. The abscissa vector $[c_1, c_2]^T$ defines the two off-step points $t_n + c_i\Delta t$, $j = 1, 2$. In all cases $c_1 = 0$ and, by convention, $c_1^T = 1$. Let $F_1 = f_{n}$.

A Hermite–Birkhoff (HB) polynomial is used as stage formula P$_2$ to obtain the stage value $Y_2$ to order $p - 1$,

$$Y_2 = y_{B,U,2Y_n} + \Delta t a_{21} F_1 + \sum_{m=2}^{d} (\Delta t)^m y_{0,2,m}^{(m)} + \sum_{\ell=1}^{k-1} \sum_{m=0}^{d} (\Delta t)^m \gamma_{\ell,2,m}^{(m)} y_{n-\ell}^{(m)},$$

(8)

A HB polynomial is used as the integration formula to obtain $y_{n+1} = Y_3$ to order $p$, 

$$y_{n+1} = Y_3 = \sum_{m=0}^{d} (\Delta t)^m y_{n+1}^{(m)} f_n.$$
Next, we have to solve the following equations for the backsteps of the method. First, we need to satisfy the set of consistency conditions:

\[ y_{n+1} = Y_3 = v_{BU,3}y_n + \Delta t (b_1 F_1 + b_2 F_2) + \sum_{m=2}^{d} (\Delta t)^m \gamma_{0,3,m} y_n^{(m)} + \sum_{\ell=1}^{k-1} \sum_{m=0}^{d} (\Delta t)^m \gamma_{\ell,3,m} y_{n-\ell}^{(m)} \]  \hspace{1cm} (9)

where \( F_2 := f(t_n + c_2 \Delta t, Y_2) \) denotes the stage derivative. Here the subscript BU refers to the Butcher form, while the subscript SO will be used later for the Shu–Osher form.

Formulae (8)–(9) are the Butcher form of HBO(d, k, p). One sees that the derivatives \( y_n^{(m)} \), \( m = 2, 3, \ldots, d \), are computed only once per step at \( t = t_n \). The defining formulae of the 2- and 3-step HBO(d, k, p) involve the usual RK parameters \( c_i, a_{ij} \) and \( b_j \) and the Taylor expansion parameters \( \gamma_{\ell,ij,m} \), \( \ell = 0, 1, \ldots, k - 1 \). Thus we can represent HBO(d, k, p) by its coefficient scheme \( (A, b, y_0, y_1, \ldots, y_{k-1}) \), where \( A = (a_{ij}) \) is a 2 × 2 matrix, \( b = (b_1, b_2)^T \) is a 2-vector \( y_0 = (y_{0,j}) \) is 3 × (d − 1) matrix and \( y_{\ell} = (y_{\ell,j}) \), \( \ell = 1, 2, \ldots, k - 1 \), are \( k - 1 \times (d + 1) \) matrices. One can display the coefficient scheme \( (A, b, y_0, y_1, \ldots, y_{k-1}) \) and the \( c_i \) in the Butcher tableau

\[
\begin{array}{c|cccc}
1 & c_1 & c_2 & a_{2,1} & b_2 \\
\hline
& b_1 &
\end{array}
\]

the 3 × (d − 1) matrix \( y_0 \)

\[
y_0 = \begin{bmatrix}
0 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 \\
\gamma_{0,2,2} & \gamma_{0,2,3} & \cdots & \gamma_{0,2,d} \\
\gamma_{0,3,2} & \gamma_{0,3,3} & \cdots & \gamma_{0,3,d}
\end{bmatrix}, \hspace{1cm} (10)
\]

and the 3 × (d + 1) matrices \( y_{\ell} \), \( \ell = 1, 2, \ldots, k - 1 \),

\[
y_{\ell} = \begin{bmatrix}
0 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 \\
\gamma_{\ell,2,0} & \gamma_{\ell,2,1} & \cdots & \gamma_{\ell,2,d} \\
\gamma_{\ell,3,0} & \gamma_{\ell,3,1} & \cdots & \gamma_{\ell,3,d}
\end{bmatrix}. \hspace{1cm} (11)
\]

3. Order conditions for predictor-corrector HBO(d, k, p)

To derive the order conditions of HBO(d, k, p), we shall use the following expressions coming from the backsteps of the method. First, we need to satisfy the set of consistency conditions:

\[
v_{BU,j} + \sum_{\ell=1}^{k-1} y_{\ell,j,0} = 1, \hspace{1cm} j = 2, 3. \hspace{1cm} (12)
\]

Next, we have to solve the following equations for \( a_{21}, c_2, b_1, b_2 \):

\[
a_{21} c_1^k + k! B_2(k + 1) = \frac{1}{k + 1} c_2^{k+1}, \hspace{1cm} k = 0, 1, \ldots, (p - 2), \hspace{1cm} (13)
\]

\[
b_1 c_1^k + b_2 c_2^k + k! B(k + 1) = \frac{1}{k + 1}, \hspace{1cm} k = 0, 1, \ldots, (p - 1), \hspace{1cm} (14)
\]

where the backstep parts, \( B_2(j) \) and \( B(j) \), are defined by
This form generalizes the modified Shu–Osher form for RK methods (see [8]). We can rearrange the stage

\[ B_2(j) = \gamma_{0,2,j} + \sum_{\ell=1}^{k-1} \sum_{m=0}^{j} \gamma_{\ell,2,m} \frac{(-1)^{j-m}}{(j-m)!}, \quad j = 1, 2, \ldots, d, \]

\[ B_2(j) = \sum_{\ell=1}^{k-1} \sum_{m=0}^{d} \gamma_{\ell,2,m} \frac{(-1)^{j-m}}{(j-m)!}, \quad j = d + 1, d + 2, \ldots, p - 1, \]

\[ B(j) = \gamma_{0,3,j} + \sum_{\ell=1}^{k-1} \sum_{m=0}^{j} \gamma_{\ell,3,m} \frac{(-1)^{j-m}}{(j-m)!}, \quad j = 1, 2, \ldots, d, \]

\[ B(j) = \sum_{\ell=1}^{k-1} \sum_{m=0}^{d} \gamma_{\ell,3,m} \frac{(-1)^{j-m}}{(j-m)!}, \quad j = d + 1, d + 2, \ldots, p. \]

4. From modified Shu–Osher form to canonical Shu–Osher form of \(k\)-step HBO\((d, k, p)\)

Gottlieb, Ketcheson and Shu presented canonical Shu–Osher forms in compact vector notation for RK methods (see [8, Section 3.1–3.4] for details). Our construction of the canonical Shu–Osher form of HBO\((d, k, p)\) proceeds in three steps in Subsections 4.1–4.3.

4.1. Modified Shu–Osher form of \(k\)-step HBO\((d, k, p)\)

Similar to the generalization to HB methods [20] of the Shu-Osher form of RK methods [24], equations (8)–(9) can be written in the form

\[ Y_i = \left[ \sum_{j=1}^{i-1} \alpha_{ij} Y_j + \Delta t \beta_{ij} F_j \right] + \sum_{m=2}^{d} (\Delta t)^m \delta_{0,i,m} y_n^{(m)} \]

\[ + \sum_{\ell=1}^{k-1} \sum_{m=0}^{d} (\Delta t)^m \delta_{\ell,i,m} y_{n-\ell}^{(m)}, \quad i = 2, 3, \]

\[ y_{n+1} = Y_3, \]

with consistency conditions:

\[ \sum_{j=1}^{i-1} \alpha_{ij} + \sum_{\ell=1}^{k-1} \delta_{\ell,i,0} = 1, \quad i = 2, 3. \]

Form (19) is called the Shu–Osher form of HBO\((d, k, p)\). By setting \(v_i = \alpha_{i1}\) and \(w_i = \beta_{i1}, i = 2, 3\), in (19), we have the modified Shu–Osher form of HBO\((d, k, p)\):

\[ Y_i = \left[ v_i y_n + \Delta t w_i f_n + \sum_{m=2}^{d} (\Delta t)^m \delta_{0,i,m} y_n^{(m)} \right] \]

\[ + \left[ \sum_{\ell=1}^{k-1} \sum_{m=0}^{d} (\Delta t)^m \delta_{\ell,i,m} y_{n-\ell}^{(m)} \right] + \sum_{j=2}^{i-1} \alpha_{ij} Y_j + \Delta t \beta_{ij} F_j \], \quad i = 2, 3,

\[ y_{n+1} = Y_3. \]

This form generalizes the modified Shu–Osher form for RK methods (see [8]). We can rearrange the stage
Thus we obtain the di-

Y_i = v_i \left[ y_n + \Delta t \frac{w_i}{v_i} f_n + \sum_{m=2}^{d} (\Delta t)^m \frac{b_{0,i,m}}{v_i} y_n^{(m)} \right] + \sum_{\ell=1}^{k-1} \delta_{\ell,i,0} \left[ y_{n-\ell} + \sum_{m=1}^{d} (\Delta t)^m \frac{b_{\ell,i,m}}{v_i} y_{n-\ell}^{(m)} \right] + \sum_{j=2}^{i-1} \alpha_{ij} \left( Y_j + \Delta t \frac{\beta_{ij}}{\alpha_{ij}} F_j \right), \quad i = 2, 3, (22)

with consistency conditions:

\[ v_i + \sum_{\ell=1}^{k-1} \delta_{\ell,i,0} + \sum_{j=2}^{i-1} \alpha_{ij} = 1, \quad i = 2, 3. \quad (23) \]

Thus we obtain the difference \( Y_i - \bar{Y}_i, i = 2, 3, \) from (22) as follows:

\[
Y_i - \bar{Y}_i = v_i \left[ (y_n + \Delta t \frac{w_i}{v_i} f_n + \sum_{m=2}^{d} (\Delta t)^m \frac{b_{0,i,m}}{v_i} y_n^{(m)}) - (\bar{y}_n + \Delta t \frac{w_i}{v_i} \bar{f}_n + \sum_{m=2}^{d} (\Delta t)^m \frac{b_{0,i,m}}{v_i} \bar{y}_n^{(m)}) \right] - \sum_{\ell=1}^{k-1} \delta_{\ell,i,0} \left[ (y_{n-\ell} + \sum_{m=1}^{d} (\Delta t)^m \frac{b_{\ell,i,m}}{v_i} y_{n-\ell}^{(m)}) - (\bar{y}_{n-\ell} + \sum_{m=1}^{d} (\Delta t)^m \frac{b_{\ell,i,m}}{v_i} \bar{y}_{n-\ell}^{(m)}) \right] + \sum_{j=2}^{i-1} \alpha_{ij} \left[ (Y_j + \Delta t \frac{\beta_{ij}}{\alpha_{ij}} F_j) - (\bar{Y}_j + \Delta t \frac{\beta_{ij}}{\alpha_{ij}} \bar{F}_j) \right], \quad i = 2, 3. (24)

Provided all the coefficients of (22) are nonnegative, the following straightforward extension of a result presented in [9, 12] holds.

**Theorem 1.** If \( f \) satisfies condition (4) of the \( S(d) \) method, then the \( k \)-step, predictor-corrector \( HBO(p) \) method (22) satisfies the CP property

\[ \|y_{n+1} - \bar{y}_{n+1}\| \leq \max_{0 \leq \ell \leq k-1} \|y_{n-\ell} - \bar{y}_{n-\ell}\| \]

provided

\[ \Delta t \leq c_{\text{feasible}} \Delta t_{S(d)}, \]

where

- the feasible CP coefficient, \( c_{\text{feasible}} \), is the minimum of the following numbers:
  \[
  \left\{ \frac{a_{32}}{\beta_{32}}, r_{i0} = \frac{v_i}{w_i}, \quad \text{and} \quad r_{i\ell} = \left( \frac{\delta_{\ell,i,0}}{\delta_{\ell,i,1}} \right)^m \right\}, \quad \left\{ \begin{array}{c} i = 2, 3, \\ \ell = 1, 2, \ldots, k - 1, \end{array} \right. \quad (25)
  \]

- the following conditions are imposed on \( \delta_{\ell,i,m} \):
  \[
  \frac{\delta_{0,i,m}}{v_i} \leq \left[ \frac{1}{r_{i0}} \right]^m \frac{1}{m!}, \quad \frac{\delta_{\ell,i,m}}{\delta_{\ell,i,0}} \leq \left[ \frac{1}{r_{i\ell}} \right]^m \frac{1}{m!}, \quad \left\{ \begin{array}{c} i = 2, 3, \\ m = 2, 3, \ldots, d, \\ \ell = 1, 2, \ldots, k - 1, \end{array} \right. \quad (26)
  \]

under the assumption that all coefficients of (22) are nonnegative, with the convention that the ratios \( a/0 = +\infty \), and the ratios \( 0/0 \) are ignored.
Proof. The difference \( Y_i - \tilde{Y}_i \) of HBO(\( d, k, p \)) can be rewritten as a convex combination of the three terms on the right-hand side of (24). Thus, by the convexity of the norm \( \| \cdot \| \), we have

\[
\| Y_i - \tilde{Y}_i \| \leq v_i \left\| \left( y_n + \Delta t \frac{w_l}{v_i} f_n + \sum_{m=2}^{d} (\Delta t)^m \frac{\delta_{0,i,m}}{v_i} y_n^{(m)} \right) \right. \\
- \left( \tilde{y}_n + \Delta t \frac{w_l}{v_i} \tilde{f}_n + \sum_{m=2}^{d} (\Delta t)^m \frac{\delta_{0,i,m}}{v_i} \tilde{y}_n^{(m)} \right) \bigg\| \\
+ \sum_{\ell=1}^{k-1} \delta_{\ell,i,0} \left\| \left( y_{n-\ell} + \sum_{m=1}^{d} (\Delta t)^m \frac{\delta_{\ell,i,m}}{\delta_{\ell,i,0}} y_{n-\ell}^{(m)} \right) \right. \\
- \left( \tilde{y}_{n-\ell} + \sum_{m=1}^{d} (\Delta t)^m \frac{\delta_{\ell,i,m}}{\delta_{\ell,i,0}} \tilde{y}_{n-\ell}^{(m)} \right) \bigg\| \\
+ \sum_{j=2}^{i-1} \alpha_{ij} \left\| \left( Y_j + \Delta t \frac{\beta_{ij}}{\alpha_{ij}} F_j \right) - \left( \tilde{Y}_j + \Delta t \frac{\beta_{ij}}{\alpha_{ij}} \tilde{F}_j \right) \right\|, \quad i = 2, 3. \tag{27}
\]

The first two terms on the right-hand side of (27) have the following upper bounds:

\[
v_i \left\| \left( y_n + \Delta t \frac{w_l}{v_i} f_n + \sum_{m=2}^{d} (\Delta t)^m \frac{\delta_{0,i,m}}{v_i} y_n^{(m)} \right) \right. \\
- \left( \tilde{y}_n + \Delta t \frac{w_l}{v_i} \tilde{f}_n + \sum_{m=2}^{d} (\Delta t)^m \frac{\delta_{0,i,m}}{v_i} \tilde{y}_n^{(m)} \right) \bigg\| \\
+ \sum_{\ell=1}^{k-1} \delta_{\ell,i,0} \left\| \left( y_{n-\ell} + \sum_{m=1}^{d} (\Delta t)^m \frac{\delta_{\ell,i,m}}{\delta_{\ell,i,0}} y_{n-\ell}^{(m)} \right) \right. \\
- \left( \tilde{y}_{n-\ell} + \sum_{m=1}^{d} (\Delta t)^m \frac{\delta_{\ell,i,m}}{\delta_{\ell,i,0}} \tilde{y}_{n-\ell}^{(m)} \right) \bigg\| \\
\leq v_i \left\| y_n - \tilde{y}_n \right\| + \sum_{\ell=1}^{k-1} \delta_{\ell,i,0} \left\| y_{n-\ell} - \tilde{y}_{n-\ell} \right\| \quad \text{by (4)}
\]

\[
\leq (v_i + \sum_{\ell=1}^{k-1} \delta_{\ell,i,0}) \max_{0 \leq \ell \leq k-1} \left\| y_{n-\ell} - \tilde{y}_{n-\ell} \right\|, \quad i = 2, 3,
\]

since

\[
\frac{1}{\tau_{\ell,t}} \Delta t \leq \frac{\Delta t}{c_{\text{feasible}}} \leq \Delta t s_{(d)} \ell = 0, 1, \ldots, k - 1.
\]

The third term on the right-hand side of (27) has the following upper bound:

\[
\sum_{j=2}^{i-1} \alpha_{ij} \left\| \left( Y_j + \Delta t \frac{\beta_{ij}}{\alpha_{ij}} F_j \right) - \left( \tilde{Y}_j + \Delta t \frac{\beta_{ij}}{\alpha_{ij}} \tilde{F}_j \right) \right\| \\
\leq \sum_{j=2}^{i-1} \alpha_{ij} \left\| \left( Y_j + \Delta t \frac{\beta_{ij}}{c_{\text{feasible}}} F_j \right) - \left( \tilde{Y}_j + \Delta t \frac{\beta_{ij}}{c_{\text{feasible}}} \tilde{F}_j \right) \right\| \\
\leq \sum_{j=2}^{i-1} \alpha_{ij} \max_{0 \leq \ell \leq k-1} \left\| y_{n-\ell} - \tilde{y}_{n-\ell} \right\|, \quad i = 2, 3, \quad \text{by (4)},
\]
since $\frac{\beta_{ij} \Delta t}{\alpha_{ij}} \leq \frac{\Delta t}{c_{\text{feasible}}} \leq \Delta t$.  

Because $v_i$, $\sum_{\ell=1}^{k-1} \delta_{\ell,i,0}$ and $\alpha_{ij}$ are nonnegative and $v_i + \sum_{\ell=1}^{k-1} \delta_{\ell,i,0} + \sum_{j=1}^{i} \alpha_{ij} = 1$, we have the inequality

$$
\|Y_i - \bar{Y}_i\| \leq \left( v_i + \sum_{\ell=1}^{k-1} \delta_{\ell,i,0} \right) \max_{0 \leq s \leq 1} \|y_n - \bar{y}_n - \tilde{y}_n - \ell\| + \sum_{j=2}^{i} \alpha_{ij} \max_{0 \leq s \leq 1} \|y_n - \bar{y}_n - \ell\|
$$

$$
\leq \max_{0 \leq s \leq 1} \|y_{n-j} - \bar{y}_{n-j}\|, \quad i = 2, 3.
$$

We thus obtain $\|Y_i - \bar{Y}_i\| \leq \max_{0 \leq s \leq 1} \|y_{n-j} - \bar{y}_{n-j}\|$ for $i = 2, 3$. In particular, this yields $\|y_{n+1} - \bar{y}_{n+1}\| \leq \max_{0 \leq s \leq 1} \|y_{n-j} - \bar{y}_{n-j}\|$. \hfill \qed

It is to be noted here that each representation of (22) with coefficients $v_i$, $w_i$, $\alpha_{ij}$, $\beta_{ij}$, and $\delta_{\ell,i,m}$ will produce a feasible CP coefficient, $c_{\text{feasible}}$, defined in Theorem 1 and a feasible HBO($d,k,p$) in modified Shu–Osher form (22). What we really want is not merely a feasible method HBO($d,k,p$) in Shu–Osher form but a best HBO($d,k,p$). This question will be considered in Subsection 4.4.

Transforming formulae (8)–(9) into the modified Shu–Osher form (21) of HBO($d,k,p$) and vice versa will be considered in Subsection 4.2.

4.2. Vector notation of HBO($d,k,p$)

Vector and matrix notation will help represent HBO($d,k,p$) in canonical Shu–Osher form. We define 3-vectors

$$v = [0, v_2, v_3]^T, \quad w = [0, w_2, w_3]^T,$$

strictly lower triangular matrices $\alpha, \beta \in \mathbb{R}^{3 \times 3}$, rectangular matrices $\delta_0 \in \mathbb{R}^{3 \times (d-1)}$ and $\delta_1, \delta_2, \ldots, \delta_{k-1} \in \mathbb{R}^{3 \times (d+1)}$ with zero first row. The components $v_i$, $w_i$, $\alpha_{ij}$, $\beta_{ij}$, $\delta_{\ell,i,m}$ come from the modified Shu–Osher form (21) of HBO($d,k,p$). Moreover,

$$Y = [0, Y_2, Y_3]^T, \quad F = [0, F_2, F_3]^T,$$

$$\varphi_n = [(\Delta t)^2 y_n^{(2)}, (\Delta t)^3 y_n^{(3)}, \ldots, (\Delta t)^d y_n^{(d)}]^T,$$

$$\varphi_{n-\ell} = [(\Delta t)^0 y_{n-\ell}^{(0)}, (\Delta t)^1 y_{n-\ell}^{(1)}, (\Delta t)^2 y_{n-\ell}^{(2)}, \ldots, (\Delta t)^d y_{n-\ell}^{(d)}]^T,$$

$$\ell = 1, 2, \ldots, k-1,$$

with the following $N$-vectors: $Y_j F_j$ for $j = 1, 2, 3$, $y_{n-\ell} f_{n-\ell}$ for $\ell = 0, 1, \ldots, k-1$, $Y_1 = y_n$, $F_1 = f_n$, $Y_3 = y_{n+1}$ and $F_3 = f_{n+1}$.

4.2.1. Modified Shu–Osher form in vector notation

Using the above notation, we rewrite the modified Shu–Osher form (21) of HBO($d,k,p$) in vector notation:

$$Y = v y_n^T + \Delta t w f_n^T + \delta_0 \varphi_n + \sum_{\ell=1}^{k-1} \delta_{\ell} \varphi_{n-\ell}$$

$$+ \alpha Y + \Delta t \beta F,$$

$$y_{n+1} = Y_3.$$

with consistency conditions (20),

$$v + \sum_{\ell=1}^{k-1} \delta_{\ell,0} + \alpha e_3 = e_3,$$
where
\[ \delta_{\ell,0} = [0, \delta_{\ell,2,0}, \delta_{\ell,3,0}]^T, \ell = 1, 2, \ldots, k - 1, \text{ and } e_3 = [0, 1, 1]^T \in \mathbb{R}^3. \] (31)

It is to be noted that, by setting the first row of matrices \( Y, F \) equal zero, \( \alpha_{i1} \) and \( \beta_{i1}, i = 2, 3 \) are not used in formulae (29) and are replaced by \( v_i \) and \( w_i, i = 2, 3 \), respectively.

### 4.2.2. Butcher form in vector notation

If \( \alpha = 0 \), then the modified Shu–Osher form (29) becomes

\[ Y = v_n y_n^T + \Delta t w_0 f_n^T + \delta_0 \varphi_n + \sum_{\ell=1}^{k-1} \delta_{\ell} \varphi_{n-\ell} + \Delta t \beta F, \]

\[ y_{n+1} = Y_3. \] (32)

which is the Butcher form. The elements \( v, w, \delta_0, \delta_\ell, \beta \) of (32) are then denoted as \( v_0, w_0, \gamma_0, \gamma_\ell, \beta_0 \) respectively, and hence the Butcher form (32) can be rewritten as

\[ Y = v_0 y_n^T + \Delta t w_0 f_n^T + \gamma_0 \varphi_n + \sum_{\ell=1}^{k-1} \gamma_{\ell} \varphi_{n-\ell} + \Delta t \beta_0 F, \]

\[ y_{n+1} = Y_3, \] (33)

with the consistency condition,

\[ v_0 + \sum_{\ell=1}^{k-1} Y_{\ell,0} = e_3, \] (34)

where \( Y_{\ell,0} = [0, \gamma_{\ell,2,0}, \gamma_{\ell,3,0}]^T, \ell = 1, 2, \ldots, k - 1, \) and \( e_3 \) is defined in (31).

To find the relation between the Shu–Osher coefficients and the Butcher coefficients, we can solve (29) for \( Y \) since \( I - \alpha \) is invertible because the matrix \( \alpha \) is strictly lower triangular,

\[ Y = (I - \alpha)^{-1} v y_n^T + \Delta t (I - \alpha)^{-1} w f_n^T + (I - \alpha)^{-1} \delta_0 \varphi_n + \sum_{\ell=1}^{k-1} (I - \alpha)^{-1} \gamma_{\ell} \varphi_{n-\ell} + \Delta t (I - \alpha)^{-1} \beta F. \] (35)

Comparing (35) with (33), we have the following relations between the generalized Shu–Osher coefficients and the Butcher coefficients,

\[ v_0 = (I - \alpha)^{-1} v, \quad w_0 = (I - \alpha)^{-1} w, \quad \gamma_0 = (I - \alpha)^{-1} \delta_0, \]

\[ \gamma_\ell = (I - \alpha)^{-1} \delta_\ell, \quad \beta_0 = (I - \alpha)^{-1} \beta. \] (36) (37)

These relations allow a simple transformation of the vectors and matrices \( v, w, \delta_0, \delta_\ell, \) \( \ell = 1, 2, \ldots, k - 1, \) \( \beta \) of a Shu–Osher form into \( v_0, w_0, \gamma_0, \gamma_\ell, \) \( \ell = 1, 2, \ldots, k - 1, \) \( \beta_0 \) of a Butcher form and vice versa.

In fact, the form (33) is the Butcher form (8) and (9) with

\[ v_0 = [0, v_{BU2}, v_{BU3}]^T, \quad w_0 = [0, a_{21}, b_1]^T, \]

\[ \beta_0 = \begin{bmatrix} 0 & 0 & 0 \\ a_{21} & 0 & 0 \\ b_1 & b_2 & 0 \end{bmatrix}, \]

\( \gamma_0 \) defined in (10), \( \gamma_\ell, \) \( \ell = 1, 2, \ldots, k - 1 \) in (11), and \( \varphi_n, \varphi_{n-\ell}, F, \) in (28), respectively.
4.3. Canonical Shu–Osher form of HBO($d, k, p$) in vector notation

To find the CP coefficient of HBO($d, k, p$), it is useful to consider a particular modified Shu–Osher form (29) where the elements of the matrices $a$ and $b$ satisfy the ratios

$$r = \frac{\alpha_{32}}{\beta_{32}}, \text{ such that } \beta_{32} \neq 0,$$

(40)

or, in vector notation,

$$\alpha_r = r\beta_r.$$

(41)

Substituting this relation into (37), we can solve for $\beta_r$ in terms of $\beta_0$ and $r$. First, we have

$$(I - r\beta_r)^{-1} \beta_r = \beta_0 \iff \beta_r = \beta_0 - r\beta_0 \iff \beta_r(I + r\beta_0) = \beta_0.$$

Then, since $I + r\beta_0$ is invertible, the coefficients of the Shu–Osher form (29) are given in terms of the coefficients of the Butcher form (33) by the expressions

$$v_r = (I + r\beta_0)^{-1} v_0 = (I - \alpha_r) v_0,$$

(42)

$$w_r = (I + r\beta_0)^{-1} w_0 = (I - \alpha_r) w_0,$$

(43)

$$\delta_{0,r} = (I + r\beta_0)^{-1} \gamma_0 = (I - \alpha_r) \gamma_0,$$

(44)

$$\delta_{\ell,r} = (I + r\beta_0)^{-1} \gamma_{\ell} = (I - \alpha_r) \gamma_{\ell},$$

(45)

$$\alpha_r = r\beta_r = r\beta_0(I + r\beta_0)^{-1} = \beta_0(I - \alpha_r),$$

(46)

$$\beta_r = \beta_0(I + r\beta_0)^{-1} = \beta_0(I - \alpha_r),$$

(47)

where the identity $(I - \alpha_r) = (I + r\beta_0)^{-1}$ follows from

$$(I - \alpha_r)(I + r\beta_0) = (I - r\beta_r)(I + r\beta_0) = I + r\beta_0 - r\beta_r - r^2\beta_0 = I$$

since $r\beta_r = r\beta_0 - r^2\beta_0$.

It is to be noted that using (37) and (47), $\beta_r$ can then be written as

$$\beta_r = \beta_0(I + r\beta_0)^{-1} = \beta_0(I - \alpha_r) = (I - \alpha_r) \beta_0 = (I + r\beta_0)^{-1} \beta_0.$$

(48)

As in [8], we shall refer to the form given by the coefficients (42)–(47), as the canonical Shu–Osher form of HBO($d, k, p$):

$$Y = v_r y_n^T + \Delta t w_r f_n^T + \delta_{0,r} q_n + \sum_{\ell=1}^{k-1} \delta_{\ell,r} q_{n-\ell} + \alpha_r Y + \Delta t \beta_r F,$$

(49)

which can be written solely in terms of the vectors and matrices $v_0, w_0, \gamma_0, \gamma_{\ell}, \beta_0$ of the Butcher form (33),

$$Y = (I + r\beta_0)^{-1} v_0 y_n^T + \Delta t (I + r\beta_0)^{-1} w_0 f_n^T + (I + r\beta_0)^{-1} \gamma_0 q_n + \sum_{\ell=1}^{k-1} (I + r\beta_0)^{-1} \gamma_{\ell} q_{n-\ell} + r\beta_0 (I + r\beta_0)^{-1} Y + \Delta t \beta_0 (I + r\beta_0)^{-1} F.$$

(50)
The canonical Shu–Osher form (49) and the Shu–Osher form (50), will allow us to formulate simply the optimization problem considered in Subsection 4.4.

Using (48) and (50), we obtain

\[ Y = (I + r\beta_0)^{-1} \left[ v_0y_n^T + \Delta tw_0f^T_n + \gamma_0p_n + \sum_{\ell=1}^{k-1} \gamma_{\ell}p_{n-\ell} + \beta_0(rY + \Delta F) \right]. \tag{51} \]

Here consistency requires that

\[ (I + r\beta_0)^{-1} v_0 + \sum_{\ell=1}^{k-1} (I + r\beta_0)^{-1} \gamma_{\ell,0} + r(I + r\beta_0)^{-1} \beta_0 e_3 = e_3, \tag{52} \]

where \( \gamma_{\ell,0} = [0, \gamma_{\ell,2,0}, \gamma_{\ell,3,0}]^T \) and \( e_3 \) is defined in (31). Condition (52) is equivalent to the consistency condition (30).

Note that the vectorial Butcher form (33), with \( v_0, w_0, \gamma_0, \gamma_{\ell}, \beta_0 \), corresponds to the canonical Shu–Osher form (49) or (51) with \( r = 0 \).

Relations (42)–(47) will enable us to obtain simply the vectors and matrices of a canonical Shu–Osher form (49) from those of a Butcher form (33) and vice versa.

To simplify notation, in the following theorem, the ratio \( r = \frac{\alpha_{32}}{\beta_{32}} \) becomes a feasible CP coefficient of HBO\( (d,k,p) \). Hence,

1. \( r \) must satisfy the conditions:

\[ r \leq r_{i0} = \frac{v_i}{w_i}, \quad r \leq r_{i\ell} = \left\{ \frac{\delta_{i,0}}{\delta_{i,1}} \right\}, \quad \left\{ \begin{array}{ll} \ell = 2, 3, \quad i = 2, 3, \\ \ell = 1, 2, \ldots, k-1, \end{array} \right. \tag{53} \]

2. conditions (26) are imposed on \( \delta_{i,0, m}, \ell = 0, 1, \ldots, k-1 \). To enhance the performance of the optimization software, conditions (26) can be rewritten as

\[ \delta_{i,0, m} m! v_i - 1 \leq 0, \quad \delta_{i, m} r_{i, m} m! - \delta_{i,0, m} \leq 0. \tag{54} \]

Therefore, the following slight modification of Theorem 1 holds.

**Theorem 2.** If \( f \) satisfies condition (4) of the S\( (d) \) method, then the \( k \)-step, predictor-corrector HBO\( (p) \) method (22) satisfies the CP property

\[ \|y_{n+1} - \tilde{y}_{n+1}\| \leq \max_{0 \leq \ell \leq k-1} \|y_{n-\ell} - \tilde{y}_{n-\ell}\| \]

provided

\[ \Delta t \leq c(v_r, w_r, \delta_{0,r}, \delta_{f,r}, \alpha_r, \beta_r) \Delta t_{S(d)}, \]

where

- \( c(v_r, w_r, \delta_{0,r}, \delta_{f,r}, \alpha_r, \beta_r) \) is equal to

\[ r = \left[ \begin{array}{c} \alpha_{32} \\ \beta_{32} \end{array} \right], \tag{55} \]

and satisfies conditions (53),

- conditions (54) are imposed on \( \delta_{i,0, m}, \ell = 0, 1, \ldots, k-1, i = 2, 3, m = 2, 3, \ldots, d, \)

under the assumption that all coefficients of (22) are nonnegative, with the convention that ratios \( a/0 = +\infty, \) and ratios \( 0/0 \) are ignored.
4.4. Optimizing \( c \) of HBO\((d, k, p)\)

With the newly defined \( r \), to optimize HBO\((d, k, p)\) and obtain \( c(\text{HBO}(d, k, p)) \), by Theorem 2, we maximize

\[ r = c(v_r, w_r, \delta_{0,r}, \delta_{r,\ell}, \alpha_r, \beta_r). \]

In the optimization formulation with any feasible initial data, the ratio \( r \) becomes the variable \( r \) which satisfies the following nonlinear equation in the variables \( \alpha_{32}, r, \beta_{32} \),

\[ \alpha_{32} - r\beta_{32} = 0, \]

together with conditions (53) and (54).

We can now formulate the optimization problem, using the Shu–Osher form (50) which is written solely in terms of the vectors and matrices of the Butcher form. Hence, the problem of optimizing HBO\((d, k, p)\) can be formulated as,

\[ c(\text{HBO}(d, k, p)) = \max_{v_r, w_r, \delta_{0,r}, \delta_{r,\ell}, \alpha_r, \beta_r} r, \] (56)

subject to the componentwise inequalities

\[
\begin{align*}
    v_r &= (I + r\beta_0)^{-1} v_0 \geq 0, \quad \text{(57)} \\
    w_r &= (I + r\beta_0)^{-1} w_0 \geq 0, \quad \text{(58)} \\
    \delta_{0,r} &= (I + r\beta_0)^{-1} \gamma_0 \geq 0, \quad \text{(59)} \\
    \beta_r &= \beta_0(I + r\beta_0)^{-1} \geq 0, \quad \text{(60)} \\
    \delta_{r,\ell} &= (I + r\beta_0)^{-1} \gamma_{\ell} \geq 0, \quad \ell = 1, 2, \ldots, k - 1, \quad \text{(61)}
\end{align*}
\]

together with conditions (53), (54) and order conditions (12) to (14) for order \( p \).

Since the consistency condition (52) is satisfied, condition (57) is equivalent to the following condition, in vector notation,

\[ \sum_{\ell=1}^{k-1} (I + r\beta_0)^{-1} \gamma_{\ell,0} + r\beta_0(I + r\beta_0)^{-1} e_3 \leq e_3. \]

It is to be noted here that each representation of the canonical Shu–Osher form (49) of HBO\((d, k, p)\) with coefficients \((v_r, w_r, \delta_{0,r}, \delta_{r,\ell}, \alpha_r, \beta_r)\), which satisfies conditions (57)–(61) together with conditions (53)–(54) and order conditions (12)–(14) for order \( p \), will produce a feasible CP coefficient \( c(v_r, w_r, \delta_{0,r}, \delta_{r,\ell}, \alpha_r, \beta_r) \) and a feasible HBO\((d, k, p)\) in Shu–Osher form (22).

4.5. Conditions to obtain CP predictor-corrector HBO\((d, k, p)\) series

We consider the following formula obtained from formula (22) using the relations \( r = \frac{\alpha_{ij}}{\beta_{ij}}, \quad r_{0} = \frac{v_i}{w_j} \) and \( r_{i,\ell} = \frac{\delta_{i,\ell,0}}{\delta_{i,\ell,1}} \) from (40) and (53),

\[
Y_i = v_i \left[ y_n + \Delta t \frac{1}{r_{0}} f_n + \sum_{m=2}^{d} (\Delta t)^n \frac{\delta_{0,i,m}}{v_i} y_n^{(m)} \right] + \sum_{\ell=1}^{k-1} \delta_{i,\ell,0} \left[ y_{n-\ell} + \Delta t \frac{1}{r_{i,\ell}} f_{n-\ell} \right] \\
+ \sum_{m=2}^{d} (\Delta t)^n \frac{\delta_{i,0,m}}{\delta_{i,0,0}} y_n^{(m)} + \sum_{j=2}^{i-1} \alpha_{ij} \left( Y_j + \Delta t \frac{1}{r_{i}} f_j \right), \quad i = 2, 3, \] (62)
The first two terms and the third term on the right hand side of (62) form the Taylor part and Runge–Kutta part respectively of HBO methods.

From formula (62), we can form the maximum stepsize $\Delta t_{RK}$ and $\Delta t_T$ of Runge–Kutta part and Taylor part, respectively,

\[
\Delta t_{RK} = r \Delta t_{FE},
\]

\[
\Delta t_T = \min_{i=2,3, \ell=0,1,\ldots,k-1} \{ r_{i\ell} \Delta t_{s(d)} \}.
\]

When HBO($d,k,p$) methods are applied to the test problem $y' = -y$, $\Delta t_{RK}$ and $\Delta t_T$ of (63) and (64) follow approximately the conditions:

\[
\Delta t_{RK} = r \cdot 2,
\]

\[
\Delta t_T \leq \min_{i=2,3, \ell=1,2,\ldots,k-1} \{ r_{i0}, r_{i\ell} \} |x_{\min,T}(d)|,
\]

where $x_{\min,T}(d)$, the lower end of the interval of stability of T($d$), Taylor method of order $d$, for all $d$, follows the formula

\[
|x_{\min,T}(d)| = 0.3725d + 1.3614,
\]

given by [3].

To guarantee the property that the stability intervals of HBO($d,k,p$) methods grow as order $p$ increases, like Taylor methods, $\Delta t_{RK}$ must exceed substantially $\Delta t_T$ (and, hence, $|x_{\min,T}(d)|$) as follows:

\[
\Delta t_{RK} = \Theta |x_{\min,T}(d)|,
\]

where the security factor $\Theta$ can be between 2 to 3, and, consequently, from (65) and (68), $r$ must satisfy,

\[
r = \frac{\Theta |x_{\min,T}(d)|}{2} = \frac{\Theta (0.3725d + 1.3614)}{2}.
\]

4.6. Optimizing $c$ of predictor-corrector HBO($d,k,p$) series

With the newly defined $r$ in (69), the problem of optimizing HBO($d,k,p$) can be formulated as,

\[
c(HBO(d,k,p)) = \max r_T,
\]

subject to component-wise inequalities (57)–(61) together with following conditions

\[
r_T \leq r_{i0} = \frac{v_i}{w_i}, \quad r_T \leq r_{i\ell} = \frac{\delta_{i,j,0}}{\delta_{i,j,m}}, \quad \begin{cases} i = 2,3, \\ \ell = 1,2,\ldots,k-1, \end{cases}
\]

condition (54) and order conditions (12)–(14) for order $p$.

Since HBO($d,k,p$) contains many free parameters, the MATLAB Optimization Toolbox was used to search for the methods with largest $c(HBO(d,k,p))$ under the tolerance $10^{-12}$ on the objective function $c(HBO(d,k,p))$, provided all the constraints are satisfied to tolerance $8 \times 10^{-14}$.

5. Existence and stability properties of HBO($d,k,p$) series methods

5.1. Existence of HBO($d,k,p$) series methods as a function of $d$ derivatives

HBO($d,k,p$) coefficients were obtained using security factor $\Theta = 2$ and formula $|x_{\min,T}(d)| = 0.4d + 1.4$ which is larger than $|x_{\min,T}(d)|$ in (67) for $d > 0$. 

For a given \( d \), Table 1 lists the upper bound \( p_u \) of \( p \) of HBO\((d, k, p)\), \( k = 2, 3 \), which exist and \( x_{\min}(p_u) \) of order \( p_u \). Here, it is seen that \( x_{\min}(p_u) \) compare positively with \( x_{\min} = -2 \) of the most stable member of the predictor-corrector Adams–Bashforth–Moulton method family.

\[
\begin{array}{c|cc|cc}
 d & p_u & x_{\min}(p_u) & p_u & x_{\min}(p_u) \\
\hline
 2 & 3 & -3.64 & 4 & -3.28 \\
 3 & 5 & -3.36 & 7 & -2.24 \\
 4 & 6 & -4.24 & 8 & -2.00 \\
 5 & 7 & -2.96 & 9 & -3.76 \\
 6 & 8 & -4.56 & 11 & -1.92 \\
 7 & 11 & -2.00 & 13 & -2.24 \\
 8 & 12 & -2.58 & 14 & -2.04 \\
 9 & 13 & -3.01 & 16 & -2.38 \\
\hline
\text{Average} & -3.29 & \text{Average} & -2.48
\end{array}
\]

Table 1: For a given \( d \), the table lists the upper bound \( p_u \) of \( p \) of HBO\((d, k, p)\), \( k = 2, 3 \), which exist and \( x_{\min}(p_u) \) of order \( p_u \).

For a given \( k = 2, 3 \), Table 2 lists the equations of line \( p_u = \eta d + \zeta \) of best fit for a set of ordered pairs \((d, k, p_u)\), appearing in Table 1.

\[
\begin{array}{c|c|c}
 k = 2 & k = 3 \\
\hline
 p_u = 1.4404 d + 0.2023 & p_u = 1.6190 d + 1.3452 \\
\end{array}
\]

Table 2: For a given \( k = 2, 3 \), the table lists the equations of line \( p_u = \eta d + \zeta \) of best fit for a set of ordered pairs \((d, k, p_u)\), appearing in Table 1.

![Figure 1](image)

Figure 1: Upper bounds \( p_u \) of order \( p \) of HBO\((d, 3, p)\) methods as an increasing function of \( d \), number of their derivatives.

As an example, Fig. 1 depicts the upper bounds \( p_u \) of CP HBO\((d, 3, p)\) methods as an increasing function of \( d \), number of derivatives and shows that the upper bound \( p_u \) of order \( p \) seems to be linear with the number of derivatives \( d \) and a linear least square fit is given in Table 2 where the slope \( \eta = 1.6190 \) is expected, since an increase of order \( p \) by one requires two additional order conditions while an increase of \( d \) by one yields 6 additional variables. Here, for any positive \( d \), lower bounds \( x_{\min} \) of the unscaled intervals of stability \((x_{\min}, 0)\) of HBO\((d, k, p_u)\)) satisfy generally the relation \( |x_{\min}| \geq 2 \times c(\text{HBO}(d, k, p_u)) \) from condition (7) and, hence, CP HBO\((d, k, p)\)) are absolutely stable for \( d = 1 \) to infinity. This analysis suggests that, for large \( d \), HBO\((d, k, p)\) methods have order \( p \) large enough to take into account many problems which require a very high precision of the solution, similar to Taylor methods which have the slope \( \eta = 1 \).

Since \( p_u \) follows the equations shown in Table 2, when we slow down the growth of order \( p \) as \( d \) increases
as follows: \( p = \lfloor \eta d \rfloor \) where
\[
1 \leq \eta \leq \eta_{\max}, \tag{72}
\]
HBO\((d,k,p)\) method has desirable stability properties considered in Subsection 5.3. Here, \( \eta_{\max} > 1 \) should not be much larger than 1. From Table 4, \( \eta_{\max} \) seems to be about 1.4 or less.

5.2. Regions of absolute stability of HBO\((d,k,p)\)
To obtain the regions of absolute stability, \( R \), of HBO\((d,k,p)\), we apply the stage formula \( P_2 \) and the integration formula with constant step \( h = \Delta t \) to the linear test equation
\[
y' = \lambda y, \quad y_0 = 1.
\]
Thus we obtain
\[
Y_2 = v_{BU,2} y_n + \lambda \Delta t a_{21} y_n + \sum_{m=2}^{d} (\lambda \Delta t)^{m} y_{0,2,m} y_n + \sum_{\ell=1}^{k-1} \sum_{m=0}^{d} (\lambda \Delta t)^{m} y_{\ell,2,m} y_{n-\ell}, \tag{73}
\]
and
\[
y_{n+1} = v_{BU,3} y_n + \lambda \Delta t [b_1 y_n + b_2 Y_2] + \sum_{m=2}^{d} (\lambda \Delta t)^{m} y_{0,3,m} y_n + \sum_{\ell=1}^{k-1} \sum_{m=0}^{d} (\lambda \Delta t)^{m} y_{\ell,3,m} y_{n-\ell}. \tag{74}
\]
It is seen that \( Y_2 \) in (73) is expressed only in terms of \( y_{n-\ell}, \ell = 0, 1, \ldots, k - 1 \). Then, \( y_{n+1} \) in (74) is expressed only in terms of \( y_{n-\ell}, \ell = 0, 1, \ldots, k - 1 \); thus we obtain the following second-order difference equation and associated linear characteristic equation:
\[
\sum_{j=0}^{k} C_j y_{n+j} = 0, \quad \sum_{j=0}^{k} C_j \gamma^j = 0. \tag{75}
\]
A complex number \( \hat{h} = \lambda h \) is in \( R \) if the \( k \) roots of the characteristic equation satisfy the root condition \( |r_s| \leq 1, \) \( s = 1, 2, \ldots, k, \) provided the multiple roots satisfy \( |r_s| < 1 \). The scanning method used to find \( R \) is similar to the one used for Runge–Kutta methods (see [16, pp. 70 and 204]). As an example, the grey regions in Fig. 3 depict \( R \) in the half-plane \( \text{Im}(\hat{h}) > 0 \) for two selected HBO methods: HBO\((9,2,13)\) and HBO\((8,3,14)\). Here the lower ends of the intervals of stability, denoted by \( x_{\min} \), of HBO\((9,2,13)\) and HBO\((8,3,14)\) are \( x_{\min} = -3.00 \) and \( x_{\min} = -2.08 \) respectively.

5.3. Stability properties of HBO methods for a given step number \( k \)
In this section, we analyze some stability properties and list the principal error term of CP HBO\((d,k,p)\) methods with \( p = \lfloor \eta d \rfloor \) and \( \eta \) satisfying (72). Similar to the case of Taylor series methods, the use of high number \( d \) gives HBO series methods of high order.

We are now interested in the size of the stability regions of CP HBO\((d,k,p)\) methods. The percentage stability gain (PSG) of method 2 over method 1 is defined by the formula (cf. Sharp [23]),
\[
(\text{PSG}) = 100 \sum_{d} \left[ \frac{|x_{\min}(d,2)|}{|x_{\min}(d,1)|} - 1 \right], \tag{76}
\]
where \( x_{\min}(d,1) \) and \( x_{\min}(d,2) \) are the lower end of the interval of stability of methods 1 and 2, respectively.
Table 3: Unscaled $|x_{\text{min}}|$ of HBO($d,k,p = [1.2d]$), $k = 2, 3$, series method and of Taylor series $T(d)$ method as a function of $d$ and $p$. The percentage stability gains of HBO($d,2,p$) and HBO($d,3,p$) methods over $T(d)$ are more than 16 % and 33 % respectively.

As an example, Table 3 lists bounds $|x_{\text{min}}|$ of unscaled intervals of stability $(x_{\text{min}},0)$ of CP HBO($d,k,p$) method, $k = 2, 3$, with $p = [1.2d]$, $d = 5, 6, \ldots, 12$ as a function of $d$ and $p$. Here, on the basis of $|x_{\text{min}}|$ averages and percentage stability gains, $|x_{\text{min}}|$ of CP HBO($d,k,p$) method, $k = 2, 3$, compare favorably with $|x_{\text{min}}|$ of $T(d)$ with the order of Taylor method $T(d)$ less than 87 % of the order of HBO method. It is also seen that HBO($d,3,p$) methods are generally more stable than HBO($d,2,p$) methods of the same order.

The values $|x_{\text{min}}|$ of CP HBO($d,3,p = [1.3d]$) method as a function of $d$ are depicted in Fig. 2. Similar to Barrio et al. [3], we use linear least square fits of $|x_{\text{min}}|$ as a function of $d$, the number of derivatives of the method. These linear least square fits give different positive slopes $\rho$ and $\sigma$ of $|x_{\text{min}}| = \rho d + \sigma$ depending on the values of $\eta$.

For a given formula of $p$ as a function of $d$, Table 4 lists slopes $\rho$ and $\sigma$ of a linear least square fit of $|x_{\text{min}}| = \rho d + \sigma$ for the listed methods. It is seen that HBO($d,k,p = [\eta d]$) series methods have slopes $\rho$ positive and non negligible up to $\eta = 1.4$ and compare favorably with $T(d)$ methods on the basis of $|x_{\text{min}}|$ averages and percentage stability gains. These $|x_{\text{min}}|$ averages and percentage stability gains increase with decreasing $\eta$.

Figure 2: Unscaled bounds $|x_{\text{min}}|$ of the intervals of absolute stability of HBO($d,3,p = [1.3d]$) methods as a function of $d$, number of their derivatives.

Table 4: Slope $\rho$ and $\sigma$ of a linear least square fit of $|x_{\text{min}}| = \rho d + \sigma$ for the HBO($d,3,p$) methods, $d = 4, 5, \ldots, 12$, corresponding $|x_{\text{min}}|$ averages and percentage stability gains (PSG) of HBO($d,3,p$) methods over $T(d)$.
6. Regions of absolute stability and principal error terms of two selected methods: HBO(9,2,13) and HBO(8,3,14)

Using the method described in Subsection 5.2, we obtain stability regions $R$ in the half-plane $\text{Im}(\hat{h}) > 0$ for two selected HBO methods: HBO(9,2,13) and HBO(8,3,14). These stability regions $R$ are depicted by the grey regions in Fig. 3.

![Figure 3: Grey unscaled regions of absolute stability, $R$, in the half-plane $\text{Im}(\hat{h}) > 0$ of two selected HBO methods with intervals of absolute stability ($-3.00, 0$) and ($-2.08, 0$).](image)

The unscaled intervals of stability of HBO(9,2,13) and HBO(8,3,14) are ($-3.00, 0$) and ($-2.08, 0$) respectively. The principal error terms of HBO(9,2,13) and HBO(8,3,14) are of the form

$$\left[ \delta_1 \{ f^p \} + \delta_2 \{ 2f^{p-1} \} \right] h^{p+1},$$

where $\{ f^p \}$ and $\{ 2f^{p-1} \}$ are elementary differentials defined in [4], [16] and [10] and $[\delta_1, \delta_2]$ are the principal local truncation error coefficients (PLTC) of the principal error term with $\ell_2$-norm $\| \text{PLTC} \|_2 = \sqrt{\delta_1^2 + \delta_2^2}$.

The principal local truncation error coefficients (PLTC) $[\delta_1, \delta_2]$ of HBO(9,2,13) and HBO(8,3,14) are listed in Table 5 together with their $\ell_2$-norm $\| \text{PLTC} \|_2$.

![Table 5: Principal local truncation error coefficients (PLTC) of HBO(9,2,13) and HBO(8,3,14) and their $\ell_2$-norm $\| \text{PLTC} \|_2$.](image)

7. Numerical results

Since HBO($d, k, p$) is not a one-step method, we must provide not only an initial value, i.e., $y_0$ but also $k - 1$ additional starting value, i.e., $y_1, y_2, \ldots, y_{k-1}$. The starting values for HBO($d, k, p$) are calculated by the one-step, 4-stage, Hermite–Birkhoff–Taylor method of order $d + 3$ using $y'$ to $y^{(d)}$ with appropriate small step sizes [19]. The $d$ derivatives, $y'$ to $y^{(d)}$, of the Taylor series are calculated at each integration step by known recurrence formulae (see, for example, [10, pp. 46–49], [17]).

The numerical performances of HBO(9,2,13), HBO(8,3,14) and Adams–Cowell of order 13 in PECE mode, denoted by AC(13), were compared on the problems mentioned in Subsections 7.1 and 7.2.

Computations were performed in C++ on a PC with the following characteristics: Memory: 5.8 GB, Processor 0,1, ...7: Intel(R) Core(TM) i7 CPU 920 @ 2.67GHz, Operating system: Ubuntu Release 11.04, Kernel Linux 2.6.38-12-generic, GNOME 2.32.1.
7.1. CPU time of HBO(9,2,13), HBO(8,3,14) and AC(13) after a 1000 periods integration of Kepler’s two-body problem

The relative energy error \( \text{EE}(t) \) at time \( t \) is defined as

\[
\text{EE}(t) = \left| \frac{E(t) - E(0)}{E(0)} \right|
\]

where \( E(t) \) is the energy at time \( t \).

Our first result is a comparison of the relative energy error \( \text{EE}(t) \) as a function of CPU time of HBO(9,2,13), HBO(8,3,14) and AC(13) after a 1000 periods integration of a Hamiltonian system (Huang and Innanen [13]). For this comparison, we used Kepler’s two-body problem with eccentricities of 0.3, 0.5 and 0.7 and an interval of integration of \([0, 2000\pi]\).

Fig. 4 depicts the graph of \( \log_{10}(\text{EE}) \) (vertical axis) as a function of CPU time in seconds (horizontal axis) for HBO(9,2,13), HBO(8,3,14) and AC(13) after a 1000 periods integration of Kepler’s two-body problem. It is seen, from Fig. 4, that HBO(9,2,13) and HBO(8,3,14) compare favorably with AC(13) at stringent tolerances.

Table 6 lists the CPU PEG of HBO(9,2,13) and HBO(8,3,14) over AC(13) after a 1000 periods integration of Kepler’s two-body problem with \( e = 0.3, e = 0.5 \) and \( e = 0.7 \), respectively, at stringent tolerances: \( 10^{-7} \) to \( 10^{-11} \).

Table 6: CPU PEG of HBO(9,2,13) and HBO(8,3,14) over AC(13) after a 1000 periods integration of Kepler’s two-body problem with \( e = 0.3, e = 0.5 \) and \( e = 0.7 \), respectively, at stringent tolerances: \( 10^{-7} \) to \( 10^{-11} \).

<table>
<thead>
<tr>
<th>HBO method</th>
<th>CPU PEG over AC(13) for two-body problem with:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>HBO(9,2,13)</td>
<td>( e = 0.3 )</td>
<td>( e = 0.5 )</td>
</tr>
<tr>
<td>HBO(8,3,14)</td>
<td>26 %</td>
<td>16 %</td>
</tr>
</tbody>
</table>

Figure 4: \( \log_{10}(\text{EE}) \) (vertical axis) as a function of CPU time (horizontal axis) after a 1000 periods integration of Kepler’s two-body problem. Left \( e = 0.3 \). Center \( e = 0.5 \). Right \( e = 0.7 \).
7.2. Error growth of HBO(9,2,13), HBO(8,3,14) and AC(13) on a 10000 periods integration of Kepler’s two-body problem

The relative positional error (\(RE(t)\)) at time \(t\) is defined as

\[
RE(t) = \frac{R_{\text{num}}(t) - R_{\text{true}}(t)}{R_{\text{true}}(t)},
\]

where \(R_{\text{true}}(t)\) is the norm of the true position at time \(t\) and \(R_{\text{num}}(t)\) is the norm calculated using the numerical solution.

In our second test, we compared the growth of relative positional error (\(RE(t)\)) and relative energy error (\(EE(t)\)) on a 10000 periods integration of Kepler’s two-body problem for different eccentricities.

![Graphs showing the growth in positional and energy error for different eccentricities](image)

Figure 5: The growth in the positional and energy error on a 10000 periods integration of Kepler’s two-body problem. Top row \(e = 0.3\). Middle row \(e = 0.5\). Bottom row \(e = 0.7\).

Fig. 5 gives the smoothed graph of \(RE(t)\) and \(EE(t)\) for \(e = 0.3\), \(e = 0.5\) and \(e = 0.7\) over an interval of 10000 periods. The smoothing removed the small amplitude high frequency oscillations in the original data and was done by using the MATLAB’s `filter` command with the window size of 20. The constant step size was chosen so that HBO(9,2,13), HBO(8,3,14) and AC(13) used the same CPU time.
### Table 7: Values of $C_1$ and $C_2$ of power law $C_1 t^{C_2}$ fitted to the graphs of $\log_{10}(RE(t))$ as a function of $\log_{10}(t)$ for a 10000 periods integration of Kepler’s two-body problem with $e = 0.3$, $e = 0.5$ and $e = 0.7$ respectively.

<table>
<thead>
<tr>
<th>Method</th>
<th>$e = 0.3$</th>
<th>$e = 0.5$</th>
<th>$e = 0.7$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HBO(9,2,13)</td>
<td>(6.99e-12, 0.311)</td>
<td>(3.74e-08, -0.496)</td>
<td>(2.61e-05, -1.420)</td>
</tr>
<tr>
<td>HBO(8,3,14)</td>
<td>(2.88e-15, 1.423)</td>
<td>(2.78e-11, 0.237)</td>
<td>(1.39e-12, 0.708)</td>
</tr>
<tr>
<td>AC(13)</td>
<td>(3.23e-13, 1.122)</td>
<td>(2.25e-11, 0.672)</td>
<td>(7.64e-14, 1.250)</td>
</tr>
</tbody>
</table>

### Table 8: Values of $C_1$ and $C_2$ of power law $C_1 t^{C_2}$ fitted to the graphs of $\log_{10}(EE(t))$ as a function of $\log_{10}(t)$ for a 10000 periods integration of Kepler’s two-body problem with $e = 0.3$, $e = 0.5$ and $e = 0.7$ respectively.

<table>
<thead>
<tr>
<th>Method</th>
<th>$e = 0.3$</th>
<th>$e = 0.5$</th>
<th>$e = 0.7$</th>
</tr>
</thead>
<tbody>
<tr>
<td>HBO(9,2,13)</td>
<td>(5.72e-14, 0.945)</td>
<td>(6.62e-14, 0.909)</td>
<td>(4.80e-13, 0.749)</td>
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<tr>
<td>HBO(8,3,14)</td>
<td>(3.31e-13, 0.999)</td>
<td>(1.96e-13, 1.009)</td>
<td>(3.68e-13, 1.041)</td>
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<tr>
<td>AC(13)</td>
<td>(7.17e-13, 0.988)</td>
<td>(5.07e-13, 1.005)</td>
<td>(1.03e-13, 1.206)</td>
</tr>
</tbody>
</table>

For $e = 0.3$, $e = 0.5$ and $e = 0.7$, the relative energy errors of HBO(9,2,13) and HBO(8,3,14) are generally less than the relative energy error of AC(13) across the interval of integration. These results are consistent with the CPU PEGs listed in Table 6 for two-body problem with $e = 0.3$, $e = 0.5$ and $e = 0.7$. It is seen, from Fig. 5, that HBO(9,2,13) and HBO(8,3,14) compare favorably with AC(13) on the basis of the growth of relative positional error and relative energy error over 10000 periods of integration.

We use linear least-squares to fit the power law $C_1 t^{C_2}$ to the graphs of Fig. 5 to obtain $C_1$ and $C_2$ shown in Table 7 and Table 8.

The values of $C_2$ of the relative positional errors of HBO(9,2,13) and HBO(8,3,14) are generally less than one and compare favorably with the value of $C_2$ of AC(13), listed in Table 7.

The values of $C_2$ of the relative energy errors of HBO(9,2,13), HBO(8,3,14) and AC(13), listed in Table 8, are in good agreement with the expected asymptotic value of one for non-symplectic methods.

### 8. Conclusion

This paper explores an alternative way to improve the stability and the order of predictor-corrector methods. We have used only $d = 2, 3, \ldots, 9$, Taylor coefficients, with $d < p$ to construct two series of optimal, contractivity-preserving (CP), $d$-derivative, 2- and 3-step, predictor-corrector, Hermite–Birkhoff–Obrechkoff methods of order $p$ up to 13 and 16, respectively, with nonnegative coefficients. It can be shown that HBO($d,k,p$) are absolutely stable for $d = 1$ to infinity. The stability regions of HBO($d,k,p$) have generally a good shape and grow with decreasing $p - d$. The lower ends $x_{\text{min}}$ of their intervals of stability are, in general, less than $x_{\text{min}} = -2$ of the most stable member of the predictor-corrector Adams–Bashforth–Moulton method family.

We compare the numerical performance of HBO(9,2,13), HBO(8,3,14) and AC(13) in solving Kepler orbit over an interval of 1000 periods. It is seen that HBO(9,2,13), HBO(8,3,14) use less CPU time than AC(13) at stringent tolerances. On the basis of the growth of relative positional error and relative energy error over 10000 periods of integration, these HBO methods also compare positively with AC(13) in solving standard N-body problems.
Acknowledgment

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References

Appendix A. Coefficients of two selected methods: HBO(9,2,13) and HBO(8,3,14)

Tables A.9 and A.10 of the appendix list the two selected CP HBO(d,k,p) methods: HBO(9,2,13) and HBO(8,3,14) with their c(HBO(d,k,p)), x_min (of the unscaled stability intervals (x_min, 0)), coefficients of stage formula P_2 and integration formula in modified Shu–Osher form (21).

Table A.9: c(HBO(d,k,p)), x_min and coefficients of stage formula P_2 of HBO(9,2,13), HBO(8,3,14) in modified Shu–Osher form (21).

<table>
<thead>
<tr>
<th>(d,k)</th>
<th>(9,2)</th>
<th>(8,3)</th>
</tr>
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<tbody>
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<td>c(HBO(d,p))</td>
<td>8.99927998631026862e-01</td>
<td>7.778297674144214e-01</td>
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<tr>
<td>x_min</td>
<td>-3.00</td>
<td>-2.08</td>
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<tr>
<td>c_2</td>
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Table A.10: Coefficients of the integration formulae of HBO(9,2,13), HBO(8,3,14) in modified Shu–Osher form (21).

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