Isospectral Property of Hamiltonian Boundary Value Methods (HBVMs) and their connections with Runge-Kutta collocation methods

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Date: February 23, 2010.

Abstract One main issue, when numerically integrating autonomous Hamiltonian systems, is the long-term conservation of some of its invariants, among which the Hamiltonian function itself. Recently, a new class of methods, named Hamiltonian Boundary Value Methods (HBVMs) has been introduced and analysed [4], which are able to exactly preserve polynomial Hamiltonians of arbitrarily high degree. We here study a further property of such methods, namely that of having, when cast as a Runge-Kutta method, a matrix of the Butcher tableau with the same spectrum (apart from the zero eigenvalues) as that of the corresponding Gauss-Legendre method, independently of the considered abscissae. Consequently, HBVMs are always perfectly $A$-stable methods. This, in turn, allows to elucidate the existing connections with classical Runge-Kutta collocation methods.

Keywords polynomial Hamiltonian · energy preserving methods · Hamiltonian Boundary Value Methods · HBVMs · Runge-Kutta collocation methods

Mathematics Subject Classification (2000) 65P10 · 65L05 · 65L06 · 65L80 · 65H10

Work developed within the project “Numerical methods and software for differential equations”.

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1 Introduction

Hamiltonian problems are of great interest in many fields of application, ranging from the macro-scale of celestial mechanics, to the micro-scale of molecular dynamics. They have been deeply studied, from the point of view of the mathematical analysis, since two centuries. Their numerical solution is a more recent field of investigation, which has led to define symplectic methods, i.e., the simplicity of the discrete map, considering that, for the continuous flow, simplicity implies the conservation of $H(y)$. However, the conservation of the Hamiltonian and simplicity of the flow cannot be satisfied at the same time unless the integrator produces the exact solution (see [9] page 379). More recently, the conservation of energy has been approached by means of the concept of the discrete line integral, in a series of papers [11][12][13][14][15], leading to the definition of Hamiltonian Boundary Value Methods (HBVMs) [2][3][4][5], which is a class of methods able to preserve, for the discrete solution, polynomial Hamiltonians of arbitrarily high degree (and then, a practical conservation of any sufficiently differentiable Hamiltonian). In more details, in [4], HBVMs based on Lobatto nodes have been analysed, whereas in [5] HBVMs based on Gauss-Legendre abscissae have been considered. In the last reference, it has been actually shown that both formulae are essentially equivalent to each other, since the order and stability properties of the method turn out to be independent of the abscissae distribution, and both methods are equivalent, when the number of the so called silent stages tends to infinity. In this paper this conclusion is further supported, since we prove that HBVMs, when cast as Runge-Kutta methods, are such that the corresponding matrix of the tableau has the nonzero eigenvalues coincident with those of the corresponding Gauss-Legendre formula (isospectral property of HBVMs).

This property can be also used to further analyse the existing connections between HBVMs and Runge-Kutta collocation methods.

With this premise, the structure of the paper is the following: in Section 2 the basic facts about HBVMs are recalled; in Section 3 we state the main result of this paper, concerning the isospectral property; in Section 4 such property is further generalized to study the existing connections between HBVMs and Runge-Kutta collocation methods; finally, in Section 5 a few concluding remarks are given.

2 Hamiltonian Boundary Value Methods

The arguments in this section are worked out starting from the arguments used in [4][5] to introduce and analyse HBVMs. We consider canonical Hamiltonian problems in the form

$$\dot{y} = J\nabla H(y), \quad y(t_0) = y_0 \in \mathbb{R}^{2m}, \quad (2.1)$$

where $J$ is a skew-symmetric constant matrix, and the Hamiltonian $H(y)$ is assumed to be sufficiently differentiable. The key formula which HBVMs rely on, is the line integral and the related property of conservative vector fields:

$$H(y_1) - H(y_0) = h \int_0^1 \sigma(t_0 + \tau h)^T \nabla H(\sigma(t_0 + \tau h))d\tau, \quad (2.2)$$
for any $y_1 \in \mathbb{R}^{2m}$, where $\sigma$ is any smooth function such that
\[
\sigma(t_0) = y_0, \quad \sigma(t_0 + h) = y_1.
\] (2.3)

Here we consider the case where $\sigma(t)$ is a polynomial of degree $s$, yielding an approximation to the true solution $y(t)$ in the time interval $[t_0, t_0 + h]$. The numerical approximation for the subsequent time-step, $y_1$, is then defined by \(2.\).)

After introducing a set of $s$ distinct abscissae,
\[
0 < c_1,\ldots,c_s \leq 1,
\] (2.4)
we set
\[
Y_i = \sigma(t_0 + c_i h), \quad i = 1,\ldots,s,
\] (2.5)
so that $\sigma(t)$ may be thought of as an interpolation polynomial, interpolating the fundamental stages $Y_i$, $i = 1,\ldots,s$, at the abscissae \(1\). We observe that, due to \(2.\), $\sigma(t)$ also interpolates the initial condition $y_0$.

**Remark 1** Sometimes, the interpolation at $t_0$ is explicitly required. In such a case, the extra abscissa $c_0 = 0$ is formally added to \(2.\). This is the case, for example, of a Lobatto distribution of the abscissae \(1\).

Let us consider the following expansions of $\dot{\sigma}(t)$ and $\sigma(t)$ for $t \in [t_0, t_0 + h]$:
\[
\dot{\sigma}(t_0 + \tau h) = \sum_{j=1}^{s} \gamma_j P_j(\tau), \quad \sigma(t_0 + \tau h) = y_0 + h \sum_{j=1}^{s} \gamma_j \int_{0}^{\tau} P_j(x) \, dx,
\] (2.6)
where $\{P_j(t)\}$ is a suitable basis of the vector space of polynomials of degree at most $s - 1$ and the (vector) coefficients $\{\gamma_j\}$ are to be determined. We shall consider an orthonormal basis of polynomials on the interval $[0,1]$, i.e.:
\[
\int_{0}^{1} P_i(t) P_j(t) \, dt = \delta_{ij}, \quad i, j = 1,\ldots,s,
\] (2.7)
where $\delta_{ij}$ is the Kronecker symbol, and $P_i(t)$ has degree $i - 1$. Such a basis can be readily obtained as
\[
P_i(t) = \sqrt{2i - 1} \hat{P}_{i-1}(t), \quad i = 1,\ldots,s
\] (2.8)
with $\hat{P}_{i-1}(t)$ the shifted Legendre polynomial, of degree $i - 1$, on the interval $[0,1]$.

**Remark 2** From the properties of shifted Legendre polynomials (see, e.g., \(1\) or the Appendix in \(2\)), one readily obtains that the polynomials $\{P_j(t)\}$ satisfy the three-terms recurrence relation:
\[
P_j(t) \equiv 1, \quad P_2(t) = \sqrt{3}(2t - 1),
\]
\[
P_{j+2}(t) = (2t - 1) \frac{2j + 1}{j+1} \sqrt{\frac{2j + 3}{2j + 1}} P_{j+1}(t) - \frac{j}{j+1} \sqrt{\frac{2j + 3}{2j - 1}} P_j(t), \quad j \geq 1.
\]

\(^1\) The use of an arbitrary polynomial basis is also permitted and has been considered in the past (see for example \(15,12\)), however as was shown in \(5\), among all possible choices, the Legendre basis turns out to be the optimal one.
We shall also assume that \( H(y) \) is a polynomial, which implies that the integrand in (2.2) is also a polynomial so that the line integral can be exactly computed by means of a suitable quadrature formula. It is easy to observe that in general, due to the high degree of the integrand function, such quadrature formula cannot be solely based upon the available abscissae \( \{ c_i \} \): one needs to introduce an additional set of abscissae \( \{ \hat{c}_i \} \), distinct from the nodes \( \{ c_i \} \), in order to make the quadrature formula exact:

\[
\int_0^1 \sigma(t_0 + t h)^T \nabla H(\sigma(t_0 + t h)) dt = \sum_{i=1}^{s} \beta_i \sigma(t_0 + c_i h)^T \nabla H(\sigma(t_0 + c_i h)) + \sum_{i=1}^{r} \hat{\beta}_i \sigma(t_0 + \hat{c}_i h)^T \nabla H(\sigma(t_0 + \hat{c}_i h)),
\]

where \( \beta_i, i = 1, \ldots, s \), and \( \hat{\beta}_i, i = 1, \ldots, r \), denote the weights of the quadrature formula corresponding to the abscissae \( \{ c_i \} \cup \{ \hat{c}_i \} \), i.e.,

\[
\beta_i = \int_0^1 \left( \prod_{j=1, j \neq i}^{s} \frac{t - c_j}{c_i - c_j} \right) \left( \prod_{j=1}^{r} \frac{t - \hat{c}_j}{\hat{c}_i - \hat{c}_j} \right) dt, \quad i = 1, \ldots, s, \tag{2.10}
\]

\[
\hat{\beta}_i = \int_0^1 \left( \prod_{j=1, j \neq i}^{s} \frac{t - \hat{c}_j}{\hat{c}_i - \hat{c}_j} \right) \left( \prod_{j=1}^{r} \frac{t - c_j}{c_i - c_j} \right) dt, \quad i = 1, \ldots, r.
\]

**Remark 3** In the case considered in the previous Remark, i.e. when \( c_0 = 0 \) is formally added to the abscissae (2.4), the first product in each formula in (2.10) ranges from \( j = 0 \) to \( s \). Moreover, also the range of \( \{ \beta_i \} \) becomes \( i = 0, 1, \ldots, s \). However, for sake of simplicity, we shall not consider this case further.

**Definition 1** The method defined by the polynomial \( \sigma(t) \), determined by substituting the quantities in (2.6) into the right-hand side of (2.9), and by choosing the unknown coefficient \( \gamma_j \) in order that the resulting expression vanishes, is called Hamiltonian Boundary Value Method with \( k \) steps and degree \( s \), in short HBVM\((k,s)\), where \( k = s + r \).\[4\]

According to [14], the right-hand side of (2.9) is called discrete line integral associated with the map defined by the HBVM\((k,s)\), while the vectors

\[
\hat{Y}_i \equiv \sigma(t_0 + \hat{c}_i h), \quad i = 1, \ldots, r, \tag{2.11}
\]

are called silent stages: they just serve to increase, as much as one likes, the degree of precision of the quadrature formula, but they are not to be regarded as unknowns since, from (2.6) and (2.11), they can be expressed in terms of linear combinations of the fundamental stages (2.5).

In the sequel, we shall see that HBVMs may be expressed through different, though equivalent, formulations: some of them can be directly implemented in a computer program, the others being of more theoretical interest.
Because of the equality (2.9), we can apply the procedure described in Definition 1 directly to the original line integral appearing in the left-hand side. With this premise, by considering the first expansion in (2.6), the conservation property reads

\[ \gamma_j = \int_0^1 P_j(\tau)J\nabla H(\sigma(t_0 + \tau h))d\tau, \quad j = 1, \ldots, s. \]  
(2.12)

which, as is easily checked, is certainly satisfied if we impose the following set of orthogonality conditions:

\[ \gamma_j = \int_0^1 P_j(\tau)J\nabla H(\sigma(t_0 + \tau h))d\tau, \quad j = 1, \ldots, s. \]  
(2.12)

Then, from the second relation of (2.6) we obtain, by introducing the operator

\[ L(f; h)\sigma(t_0 + ch) = \sigma(t_0) + h \sum_{j=1}^s \int_0^c P_j(x)dx \int_0^1 P_j(\tau)f(\sigma(t_0 + \tau h))d\tau, \quad c \in [0, 1], \]  
(2.13)

that \( \sigma \) is the eigenfunction of \( L(J\nabla H; h) \) relative to the eigenvalue \( \lambda = 1 \):

\[ \sigma = L(J\nabla H; h)\sigma. \]  
(2.14)

**Definition 2** Equation (2.14) is the Master Functional Equation defining \( \sigma \) [5].

**Remark 4** From the previous arguments, one readily obtains that the Master Functional Equation (2.14) characterizes HBVM \( (k, s) \) methods, for all \( k \geq s \). Indeed, such methods are uniquely defined by the polynomial \( \sigma \), of degree \( s \), the number of steps \( k \) being only required to obtain an exact quadrature formula (see (2.9)).

To practically compute \( \sigma \), we set (see (2.5) and (2.6))

\[ Y_i = \sigma(t_0 + c_i h) = y_0 + h \sum_{j=1}^s a_{ij} \gamma_j, \quad i = 1, \ldots, s, \]  
(2.15)

where

\[ a_{ij} = \int_0^{c_i} P_j(x)dx, \quad i, j = 1, \ldots, s. \]

Inserting (2.12) into (2.15) yields the final formulae which define the HBVMs class based upon the orthonormal basis \( \{ P_j \} \):

\[ Y_i = y_0 + h \sum_{j=1}^s a_{ij} \int_0^1 P_j(\tau)J\nabla H(\sigma(t_0 + \tau h))d\tau, \quad i = 1, \ldots, s. \]  
(2.16)

For sake of completeness, we report the nonlinear system associated with the HBVM \( (k, s) \) method, in terms of the fundamental stages \( \{ Y_i \} \) and the silent stages \( \{ \hat{Y}_i \} \) (see (2.11)), by using the notation

\[ f(y) = J\nabla H(y). \]  
(2.17)
In this context, it represents the discrete counterpart of (2.16), and may be directly retrieved by evaluating, for example, the integrals in (2.16) by means of the (exact) quadrature formula introduced in (2.9):

\[ Y_i = y_0 + h \sum_{j=1}^{s} a_{ij} \left( \sum_{l=1}^{r} \beta_l P_j(c_l) f(Y_l) + \sum_{l=1}^{r} \hat{\beta}_l P_j(\hat{c}_l) f(\hat{Y}_l) \right), \quad i = 1, \ldots, s. \] 

(2.18)

From the above discussion it is clear that, in the non-polynomial case, supposing to choose the abscissae \( \{ \hat{c}_i \} \) so that the sums in (2.18) converge to an integral as \( r \equiv k - s \to \infty \), the resulting formula is (2.16).

**Definition 3** Formula (2.16) is named \( \infty \)-HBVM of degree \( s \) or HBVM(\( \infty, s \)) [5].

This implies that HBVMs may be as well applied in the non-polynomial case since, in finite precision arithmetic, HBVMs are undistinguishable from their limit formulae (2.16), when a sufficient number of silent stages is introduced. The aspect of having a practical exact integral, for \( k \) large enough, was already stressed in [2,4,5,11,14].

On the other hand, we emphasize that, in the non-polynomial case, (2.16) becomes an operative method only after that a suitable strategy to approximate the integrals appearing in it is taken into account. In the present case, if one discretizes the Master Functional Equation (2.13)–(2.14), HBVM(\( k, s \)) are then obtained, essentially by extending the discrete problem (2.18) also to the silent stages (2.11). In order to simplify the exposition, we shall use (2.17) and introduce the following notation:

\[ \{ \tau_i \} = \{ c_i \} \cup \{ \hat{c}_i \}, \quad \{ \omega_i \} = \{ \beta_i \} \cup \{ \hat{\beta}_i \}, \]

\[ y_i = \sigma(t_0 + \tau_i h), \quad f_i = f(\sigma(t_0 + \tau_i h)), \quad i = 1, \ldots, k. \]

The discrete problem defining the HBVM(\( k, s \)) then becomes,

\[ y_i = y_0 + h \sum_{j=1}^{s} \int_{0}^{\tau_i} P_j(x)dx \sum_{\ell=1}^{k} \omega_\ell P_j(\tau_\ell) f_\ell, \quad i = 1, \ldots, k. \] 

(2.19)

By introducing the vectors

\[ y = (y_1^T, \ldots, y_k^T)^T, \quad e = (1, \ldots, 1)^T \in \mathbb{R}^k, \]

and the matrices

\[ \Omega = \text{diag}(\omega_1, \ldots, \omega_k), \quad \mathcal{S}_s, \mathcal{P}_s \in \mathbb{R}^{k \times s}, \] 

(2.20)

whose \( (i, j) \)th entry are given by

\[ (\mathcal{S}_s)_{ij} = \int_{0}^{\tau_i} P_j(x)dx, \quad (\mathcal{P}_s)_{ij} = P_j(\tau_i), \] 

(2.21)

we can cast the set of equations (2.19) in vector form as

\[ y = e \otimes y_0 + h(\mathcal{S}_s \mathcal{P}_s^T \Omega) \otimes I_{2m} f(y), \]
with an obvious meaning of \( f(y) \). Consequently, the method can be regarded as a Runge-Kutta method with the following Butcher tableau:

\[
\begin{array}{c|c}
\tau_1 & \mathcal{I}_s \mathcal{T}_s \Omega \\
\vdots & \\
\tau_k & \\
\hline
\omega_1 & \ldots & \omega_k \\
\end{array}
\]

(2.22)

**Remark 5** We observe that, because of the use of an orthonormal basis, the role of the abscissae \( \{c_i\} \) and of the silent abscissae \( \{\hat{c}_i\} \) is interchangeable, within the set \( \{\tau_i\} \). This is due to the fact that all the matrices \( \mathcal{I}_s, \mathcal{T}_s, \) and \( \Omega \) depend on all the abscissae \( \{\tau_i\} \), and not on a subset of them, and they are invariant with respect to the choice of the fundamental abscissae \( \{c_i\} \).

In particular, when a Gauss distribution of the abscissae \( \{\tau_1, \ldots, \tau_k\} \) is considered, it can be proved that the resulting HBVM \((k, s)\) method [5]:

- has order \( 2s \) for all \( k \geq s \);
- is symmetric and perfectly \( A \)-stable (i.e., its stability region coincides with the left-half complex plane, \( \mathbb{C}^- \));
- reduces to the Gauss-Legendre method of order \( 2s \), when \( k = s \);
- exactly preserves polynomial Hamiltonian functions of degree \( \nu \), provided that

\[
k \geq \frac{\nu s}{2}.
\]

(2.23)

Additional results and references on HBVMs can be found at the HBVMs Home-page [7].

### 3 The Isospectral Property

We are now going to prove a further additional result, related to the matrix appearing in the Butcher tableau (2.22), corresponding to HBVM \((k, s)\), i.e., the matrix

\[
A = \mathcal{I}_s \mathcal{T}_s \Omega \in \mathbb{R}^{k \times k}, \quad k \geq s,
\]

(3.1)

whose rank is \( s \). Consequently it has a \((k-s)\)-fold zero eigenvalue. In this section, we are going to discuss the location of the remaining \( s \) eigenvalues of that matrix.

Before that, we state the following preliminary result, whose proof can be found in [10, Theorem 5.6 on page 83].

**Lemma 1** The eigenvalues of the matrix

\[
X_s = \begin{pmatrix}
\frac{1}{2} & -\xi_1 & & \\
\xi_1 & 0 & \ddots & \\
& \ddots & \ddots & -\xi_{s-1} \\
& & \xi_{s-1} & 0
\end{pmatrix},
\]

(3.2)
with
\[ \xi_j = \frac{1}{2\sqrt{(2j+1)(2j-1)}}, \quad j \geq 1, \quad (3.3) \]

coincide with those of the matrix in the Butcher tableau of the Gauss-Legendre method of order 2s.

We also need the following preliminary result, whose proof derives from the properties of shifted-Legendre polynomials (see, e.g., [1] or the Appendix in [4]).

Lemma 2 With reference to the matrices in (2.20)–(2.21), one has
\[ \mathcal{A}_s = \mathcal{P}_{s+1} \hat{X}_s, \]
where
\[ \hat{X}_s = \begin{pmatrix} \frac{1}{2} - \xi_1 \\ \xi_1 & 0 & \cdots \\ \cdots & \cdots & \cdots & -\xi_{s-1} \\ \xi_{s-1} & 0 & \cdots & 0 \\ -\xi_s & 0 & \cdots & \cdots \\ -\xi_1 & \cdots & 0 & \cdots & \cdots \end{pmatrix}, \]
with the \( \xi_j \) defined by (3.3).

The following result then holds true.

Theorem 1 (Isospectral Property of HBVMs) For all \( k \geq s \) and for any choice of the abscissae \( \{\tau_i\} \) such that the quadrature defined by the weights \( \{\omega_i\} \) is exact for polynomials of degree \( 2s - 1 \), the nonzero eigenvalues of the matrix \( A \) in (3.1) coincide with those of the matrix of the Gauss-Legendre method of order 2s.

Proof For \( k = s \), the abscissae \( \{\tau_i\} \) have to be the \( s \) Gauss-Legendre nodes, so that HBVM\((s,s)\) reduces to the Gauss Legendre method of order 2s, as outlined at the end of Section 2.

When \( k > s \), from the orthonormality of the basis, see (2.7), and considering that the quadrature with weights \( \{\omega_i\} \) is exact for polynomials of degree (at least) \( 2s - 1 \), one easily obtains that (see (2.20)–(2.21))
\[ \mathcal{P}_s^T \Omega \mathcal{P}_{s+1} = (I_s \; 0), \]

since, for all \( i = 1, \ldots, s \) and \( j = 1, \ldots, s + 1 \):
\[ (\mathcal{P}_s^T \Omega \mathcal{P}_{s+1})_{ij} = \sum_{l=1}^k \omega_l p_i(t_l)p_j(t_l) = \int_0^1 p_i(t)p_j(t)dt = \delta_{ij}. \]
By taking into account the result of Lemma 2, one then obtains:

\[
AP_{s+1} = JP_{s}^{T} = P_{s+1}X_{s}(I_{s} 0) = P_{s+1}(\hat{X}_{s} 0) = P_{s+1}(\hat{X}_{s} 0)
\]

\[
\begin{pmatrix}
\frac{1}{s} - \xi_1 \\
\xi_1 \\
\vdots \\
\xi_{s-1}
\end{pmatrix}
\begin{pmatrix}
0 \\
\cdot \\
\cdot \\
\cdot \\
0
\end{pmatrix} = P_{s+1}(\hat{X}_{s}),
\]

with the \(\{\xi_j\}\) defined according to (3.3). Consequently, one obtains that the columns of \(P_{s+1}\) constitute a basis of an invariant (right) subspace of matrix \(A\), so that the eigenvalues of \(\hat{X}_{s}\) are eigenvalues of \(A\). In more detail, the eigenvalues of \(\hat{X}_{s}\) coincide with those of \(X_{s}\), i.e., with the eigenvalues of the matrix defining the Gauss-Legendre method of order \(2s\).

4 HBVMs and Runge-Kutta collocation methods

By using the previous results and notations, now we further elucidate the existing connections between HBVMs and Runge-Kutta collocation methods. We shall continue to use an orthonormal basis \(\{P_j\}\), along which the underlying extended collocation polynomial \(\sigma(t)\) is expanded, even though the arguments could be generalized to more general bases, as sketched below. On the other hand, the distribution of the internal abscissae can be arbitrary.

Our starting point is a generic collocation method with \(k\) stages, defined by the tableau

\[
\begin{array}{c|c}
\tau_1 & \mathcal{A} \\
\vdots & \vdots \\
\tau_k & \omega_1 \ldots \omega_k \\
\end{array}
\]

where, for \(i, j = 1, \ldots, k\):

\[
\mathcal{A} = (\alpha_{ij}) \equiv \left( \int_0^{\tau_i} \ell_j(x)dx \right), \quad \omega_j = \int_0^{1} \ell_j(x)dx,
\]

\(\ell_j(\tau)\) being the \(j\)th Lagrange polynomial of degree \(k - 1\) defined on the set of abscissae \(\{\tau_i\}\).

Given a positive integer \(s \leq k\), we can consider a basis \(\{p_1(\tau), \ldots, p_s(\tau)\}\) of the vector space of polynomials of degree at most \(s - 1\), and we set

\[
P_s = \begin{pmatrix}
p_1(\tau_1) & p_2(\tau_1) & \cdots & p_s(\tau_1) \\
p_1(\tau_2) & p_2(\tau_2) & \cdots & p_s(\tau_2) \\
\vdots & \vdots & \ddots & \vdots \\
p_1(\tau_k) & p_2(\tau_k) & \cdots & p_s(\tau_k)
\end{pmatrix}_{k \times s}
\]
(note that \( \mathcal{P}_s \) is full rank since the nodes are distinct). The class of Runge-Kutta methods we are interested in is defined by the tableau

\[
\begin{array}{c|c}
\tau_1 & A \equiv \mathcal{A} \mathcal{P}_s A_s \mathcal{P}_s^T \Omega \\
\vdots & \\
\tau_k & \\
\omega_1 & \ldots \omega_k
\end{array}
\] (4.3)

where \( \Omega = \text{diag}(\omega_1, \ldots, \omega_k) \) (see (2.20)) and \( A_s = \text{diag}(\eta_1, \ldots, \eta_s) \); the coefficients \( \eta_j, j = 1, \ldots, s \), have to be selected by imposing suitable consistency conditions on the stages \( \{y_i\} \) (see, e.g., [5]). In particular, when the basis is orthonormal, as we shall assume hereafter, then matrix \( \mathcal{P}_s \) reduces to matrix \( \mathcal{P}_s \) in (2.20)–(2.21), \( A_s = I_s \), and consequently (4.3) becomes

\[
\begin{array}{c|c}
\tau_1 & A \equiv \mathcal{A} \mathcal{P}_s \mathcal{P}_s^T \Omega \\
\vdots & \\
\tau_k & \\
\omega_1 & \ldots \omega_k
\end{array}
\] (4.4)

We note that the Butcher array \( A \) has rank which cannot exceed \( s \), because it is defined by filtering \( \mathcal{A} \) by the rank \( s \) matrix \( \mathcal{P}_s \mathcal{P}_s^T \Omega \).

The following result then holds true, which clarifies the existing connections between classical Runge-Kutta collocation methods and HBVMs.

**Theorem 2** Provided that the quadrature formula defined by the weights \( \{\omega_i\} \) is exact for polynomials at least \( 2s - 1 \) (i.e., the Runge-Kutta method defined by the tableau (4.4) satisfies the usual simplifying assumption \( B(2s) \)), then the tableau (4.4) defines a HBVM \((k,s)\) method based at the abscissae \( \{\tau_i\} \).

**Proof** Let us expand the basis \( \{P_1(\tau), \ldots, P_s(\tau)\} \) along the Lagrange basis \( \{\ell_j(\tau)\} \), \( j = 1, \ldots, k \), defined over the nodes \( \tau_i \), \( i = 1, \ldots, k \):

\[
P_j(\tau) = \sum_{i=1}^{k} P_j(\tau_i) \ell_j(\tau), \quad j = 1, \ldots, s.
\]

It follows that, for \( i = 1, \ldots, k \) and \( j = 1, \ldots, s \):

\[
\int_0^\tau P_j(x)dx = \sum_{i=1}^{k} P_j(\tau_i) \int_0^\tau \ell_j(x)dx = \sum_{i=1}^{k} P_j(\tau_i) \alpha_{ij},
\]

that is (see (2.20)–(2.21) and (4.1)),

\[
\mathcal{A}_s = \mathcal{A} \mathcal{P}_s.
\] (4.5)

By substituting (4.5) into (4.4), one retrieves that tableau (2.22), which defines the method HBVM \((k,s)\). This completes the proof. \( \Box \)

The resulting Runge-Kutta method (4.4) is then energy conserving if applied to polynomial Hamiltonian systems (2.1) when the degree of \( H(y) \), is lower than or equal to a quantity, say \( v \), depending on \( k \) and \( s \). As an example, when a Gaussian distribution of the nodes \( \{\tau_i\} \) is considered, one obtains (2.23).
Remark 6 (About Simplicity) The choice of the abscissae \{τ_1, ..., τ_k\} at the Gaussian points in [0, 1] has also another important consequence, since, in such a case, the collocation method (4.1) is the Gauss method of order 2k which, as is well known, is a symplectic method. The result of Theorem 2 then states that, for any \(s \leq k\), the HBVM\((k,s)\) method is related to the Gauss method of order 2k by the relation:

\[
A = \mathcal{A}(\mathcal{P}_s \mathcal{P}_s^T \Omega),
\]

where the filtering matrix \((\mathcal{P}_s \mathcal{P}_s^T \Omega)\) essentially makes the Gauss method of order 2k “work” in a suitable subspace.

It seems like the price paid to achieve such conservation property consists in the lowering of the order of the new method with respect to the original one (4.1). Actually this is not true, because a fair comparison would be to relate method (2.22)–(4.4) to a collocation method constructed on \(s\) rather than on \(k\) stages, since the resulting nonlinear system turns out to have dimension \(s\), as shown in [4]. This computational aspect is fully elucidated in a companion paper [6], devoted to the efficient implementation of HBVMs, where the Isospectral Property of the methods is fully exploited for this purpose.

4.1 An alternative proof for the order of HBVMs

We conclude this section by observing that the order 2s of an HBVM\((k,s)\) method, under the hypothesis that (4.1) satisfies the usual simplifying assumption \(B(2s)\), i.e., the quadrature defined by the weights \(\{ω_i\}\) is exact for polynomials of degree at least \(2s-1\), may be stated by using an alternative, though equivalent, procedure to that used in the proof of [4, Corollary 2] (see also [5, Theorem 2]).

Let us then define the \(k \times k\) matrix \(\mathcal{P} \equiv \mathcal{P}_k\) (see (2.20)–(2.21)) obtained by “enlarging” the matrix \(\mathcal{P}_s\) with \(k-s\) columns defined by the normalized shifted Legendre polynomials \(P_j(τ), j = s+1, ..., k\), evaluated at \(\{τ_i\}\), i.e.,

\[
\mathcal{P} = \begin{pmatrix}
P_1(τ_1) & ... & P_k(τ_1) \\
... & & ...
\end{pmatrix}.
\]

By virtue of property \(B(2s)\) for the quadrature formula defined by the weights \(\{ω_i\}\), it satisfies

\[
\mathcal{P}^T \Omega \mathcal{P} = \begin{pmatrix}
I_s & \mathcal{O} \\
\mathcal{O} & R
\end{pmatrix}, \quad R \in \mathbb{R}^{k-s \times k-s}.
\]

This implies that \(\mathcal{P}\) satisfies the property \(T(s,s)\) in [10, Definition 5.10 on page 86], for the quadrature formula \(\{ω_i, τ_j\}_{i=1}^s\). Therefore, for the matrix \(A\) appearing in (4.4) (i.e., (2.22), by virtue of Theorem 2), one obtains:

\[
\mathcal{P}^{-1} A \mathcal{P} = \mathcal{P}^{-1} \mathcal{A}(\mathcal{P}_s^T \mathcal{P}_s) \begin{pmatrix}
I_s \\
\mathcal{O}
\end{pmatrix} = \begin{pmatrix}
\tilde{X}_s \\
\mathcal{O}
\end{pmatrix},
\]

(4.6)

where \(\tilde{X}_s\) is the matrix defined in (3.4). Relation (4.6) and [10, Theorem 5.11 on page 86] prove that method (4.4) (i.e., HBVM\((k,s)\)) satisfies \(C(s)\) and \(D(s-1)\) and, hence, its order is 2s.
5 Conclusions

In this paper, we have shown that the recently introduced class of HBVMs \((k,s)\), when recast as Runge-Kutta method, have the matrix of the corresponding Butcher tableau with the same nonzero eigenvalues which, in turn, coincides with those of the matrix of the Butcher tableau of the Gauss method of order \(2s\), for all \(k \geq s\) such that \(B(2s)\) holds.

Moreover, HBVM\((k,s)\) defined at the Gaussian nodes \(\{\tau_1, \ldots, \tau_k\}\) on the interval \([0,1]\) are closely related to the Gauss method of order \(2k\) which, as is well known, is a symplectic method.

An alternative proof of the order of convergence of HBVMs is also provided.

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