BS Linear Multistep Methods on Non-uniform Meshes

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Received 15 February, 2006; accepted in revised form 8 March, 2006

Abstract: BS methods are a special class of Linear Multistep Methods defined using B-spline functions. These methods are always convergent and have good stability properties when used as Boundary Value Methods. In addition, if \( k \) is the number of steps, a \( C^k \) spline of degree \( k + 1 \) can be computed with low computational cost and this serves as a continuous extension to the solution. It is shown that the continuous solution and the discrete solution both share the same order of convergence. In this paper we introduce this class of methods in the general case of a non-uniform mesh and we present numerical results showing their performance when dealing with some singularly perturbed Boundary Value Ordinary Differential Equations.

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Keywords: Boundary Value Problems, Ordinary Differential Equations, B-Splines, Spline Collocation, Boundary Value Methods.

Mathematics Subject Classification: 65L06, 65L10, 65D07

1 Introduction

We deal with the solution of the following Boundary Value Ordinary Differential Equation (BVODE):

\[
\begin{align*}
\{ & y'(x) = f(x, y(x)), \quad a \leq x \leq b, \\
& g(y(a), y(b)) = 0,
\end{align*}
\]

where \( y \in \mathbb{R}^d, d \geq 1 \) and \( f \) and \( g \) are sufficiently smooth functions. This class of problems arises in many applications and its most popular numerical solvers are based on Runge-Kutta schemes such as Mono Implicit Runge Kutta (MIRK) [5, 8], or on spline collocation [1]. Recently, a class of Linear Multistep Methods (LMMs), called Top Order Methods, has also been successfully used
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[13, 14]. For problems having different time scales, the numerical schemes need non-uniform meshes in order to be efficient. Moreover, in the case of nonlinear problems, when the mesh is changed the numerical solution has to be extended to off-mesh points in order to continue the process. In such cases the knowledge of an accurate continuous extension of the numerical solution is important. In [11] we have analyzed the BS methods, which are a class of LMMs based on B-Splines with distinct knots [4, 11] and can be interpreted as collocation methods. This means that, for a $k$-step BS method, a $k+1$ degree spline function, continuous up to the $k$-th derivative, can be associated with the numerical solution. In particular the convergence and the stability properties of the methods were analyzed and it was shown that the continuous extension gives an approximation of the solution with the same convergence order as the numerical scheme. Here we extend the BS methods to the case of a non-uniform mesh and we describe an accurate and relatively cheap algorithm to compute the coefficients of the methods.

After necessary preliminaries given in Section 2, in Section 3 we briefly describe the BS methods and their relation with B-spline functions in the uniform case. The non-uniform case is introduced in Section 4 while in Section 5 an efficient algorithm for computing the coefficients of the methods is presented. A special class of additional methods (corresponding to the not-a-knot spline condition) is then described in Section 6. Finally, some numerical results are reported in Section 7.

2 Preliminaries

Let $\{y_i, i = 0, \ldots, N\}$ be the numerical solution of (1) computed on the mesh $\pi = \{a = x_0 < x_1 < \ldots < x_N = b\}$ using a Linear Multistep Method (LMM). As is well known, a $k$-step LMM must be combined with $k_1$ additional and suitably chosen linear methods, in order to get the uniqueness of the associated numerical solution. These additional methods can be split into $k_1 - 1$ and $k_2 = k - k_1$ left and right methods, respectively. The appropriate value of $k_1$ depends on the class of LMMs considered. If $k_2 \neq 0$ this means that the LMM is used as a Boundary Value Method (BVM) [2, 3].

In the case of a uniform mesh with constant step size $h = \frac{b-a}{N}$, the numerical solution satisfies the following linear equations,

$$\sum_{j=-k_1}^{k_2} \alpha_{j+k_1} y_{i+j} = h \sum_{j=-k_1}^{k_2} \beta_{j+k_1} f_{i+j}, \quad i = k_1, \ldots, N - k_2,$$

(2)

where $\alpha := (\alpha_0, \ldots, \alpha_k)^T \in \mathbb{R}^{k+1}$ and $\beta := (\beta_0, \ldots, \beta_k)^T \in \mathbb{R}^{k+1}$, are the two coefficient vectors characterizing the method and $f_i := f(x_i, y_i)$.

In the general case of a non-uniform mesh, the equations (2) are replaced by

$$\sum_{j=-k_1}^{k_2} \alpha_{j+k_1}^{(i)} y_{i+j} = h_i \sum_{j=-k_1}^{k_2} \beta_{j+k_1}^{(i)} f_{i+j}, \quad i = k_1, \ldots, N - k_2,$$

(3)

with $h_i := x_i - x_{i-1}$ and $\alpha^{(i)}$ and $\beta^{(i)}$ depending on $i$.

The order condition $p \geq r$, which in the uniform case corresponds to a set of $r+1$ scalar linear conditions on the coefficient vectors $\alpha$ and $\beta$ (see for instance [3, 7]), can be briefly expressed by the following condition [3],

$$W^{(r)}_{i+k_1,k}(t) \alpha^{(i)} + h_i W^{(r)'}_{i+k_1,k}(t) \beta^{(i)} = 0, \quad i = k_1, \ldots, N - k_2,$$

(4)

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By using standard results on splines, it was proved that the values of the resulting spline at the knots could also be generated by a special class of LMMs that, for simplicity, we have called BS methods [11]. In the same papers such methods were used as Initial Value Methods and it was proved that their convergence is not guaranteed if $k \geq 3$. In [11] we have revisited them from the point of view of Boundary Value Methods, establishing their convergence and stability features. For the sake of clearness and completeness, we summarize here the results obtained.

Let $B(\cdot)$ denote the $\text{B}^{}$–spline of degree $(k + 1)$ with uniform integer active knots $0, 1, \ldots, k + 2$, (see e.g. [4]). By using the values of $B(\cdot)$ and $B'(\cdot)$ at the inner knots, we define the entries of the vectors $\alpha = (\alpha_0, \ldots, \alpha_k)^T$ and $\beta = (\beta_0, \ldots, \beta_k)^T$ as follows,

$$\begin{cases} \alpha_i := B'(k - i + 1), & i = 0, \ldots, k. \\ \beta_i := B(k - i + 1). \end{cases}$$

The $\alpha_i$ and $\beta_i$ in equation (6) are used as coefficients in (2) and the methods obtained are called BS methods. From the symmetry of $B(\cdot)$, it turns out that such methods are symmetric, that is

$$\alpha_i = -\alpha_{k - i}; \quad \beta_i = \beta_{k - i}, \quad i = 0, \ldots, k.$$ 

In particular, the trapezoidal and the Simpson rules are obtained for $k = 1, 2$, respectively. In Table 1 we report the normalized coefficients $\hat{\alpha}_i = \alpha_i / i!$ and $\hat{\beta}_i = \beta_i / (k + 1)!$, $i = 0, \ldots, \lfloor \frac{k}{2} \rfloor$ of the methods for all odd values of $k$, up to 9.

In [11] it was first proved that the $k$–step BS methods have convergence order $p \geq k + 1$. Choosing $k_1 = \lfloor \frac{k}{2} \rfloor$ (and, consequently, $k_2 = \lceil \frac{k}{2} \rceil$), it is then proved that they are always $0_{k_1,k_2}$–stable and $A_{k_1,k_2}$–stability (the concepts of $0_{k_1,k_2}$–stability and of $A_{k_1,k_2}$–stability are generalizations of 0–stability and $A$–stability, respectively, [2], [3]). Finally it was also proved that, if $k$ is odd, the $k$–step BS methods are also perfectly $A_{k_1,k_2}$–stable, (i.e. the $A$–stability region coincides with $\mathbb{C}^-$). This explains the use of odd values of $k$.

Table 1: uniform BS coefficients.

<table>
<thead>
<tr>
<th>$k$</th>
<th>$-\hat{\alpha}_0$</th>
<th>$-\hat{\alpha}_1$</th>
<th>$-\hat{\alpha}_2$</th>
<th>$-\hat{\alpha}_3$</th>
<th>$-\hat{\alpha}_4$</th>
<th>$\hat{\beta}_0$</th>
<th>$\hat{\beta}_1$</th>
<th>$\hat{\beta}_2$</th>
<th>$\hat{\beta}_3$</th>
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<td>1</td>
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<td>1</td>
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</tbody>
</table>
4 The BS methods on non-uniform meshes

In this section we introduce two sets of vectors $\alpha^{(i)}$ and $\beta^{(i)} \in \mathbb{R}^{k+1}, i = k_1, \ldots, N - k_2$ (with $k_1 = \lfloor \frac{K}{2} \rfloor$), satisfying (4) with $r = k + 1$ and reducing to the vectors $\alpha$ and $\beta$ given in (6) when the mesh is uniform. Their entries define the coefficients of the non-uniform BS methods defined in (3).

Let $S_{k,N}$ be the set of all $C^k$ polynomial splines of degree $k + 1$ defined in $[a, b]$ with knots $x_0, \ldots, x_N$ whose dimension is $N + k + 1$. We represent any $s \in S_{k,N}$ in the $k + 1$ degree B–spline basis $B_i(x), i = -(1 + k), \ldots, N - 1$ which can be defined after prescribing 2 sets of additional ($k + 1$) knots, $\{ x_i, i = -(1 + k), \ldots, -1 \}$ (left auxiliary knots), with $x_{-1-k} \leq \ldots \leq x_0$, and $\{ x_i, i = N+1, \ldots, N+k+1 \}$ (right auxiliary knots), with $x_N \leq x_{N+1} \leq \ldots \leq x_{N+k+1}$, [4]. Thus we can write $S_{k,N} = \langle B_{-(1+k)}, \ldots, B_{N-1} \rangle$.

Then, $\forall i = k_1, \ldots, N - k_2$, we can define the following matrix

$$G^{(i)} := \begin{bmatrix} A^{(i-k_1)}_1 & -h_i A^{(i-k_1)}_2 & \mathbf{e}_T \end{bmatrix},$$

with $\mathbf{e} := (1, \ldots, 1)^T \in \mathbb{R}^{k+1}$, and $A^{(j)}_1, A^{(j)}_2, j \in \mathbb{N}$, defined as,

$$A^{(j)}_1 := \begin{bmatrix} B_{j-k-1}(x_j), & \ldots, & B_{j-k-1}(x_j) \\ \vdots & \vdots & \vdots \\ B_{j-k-1}(x_{j+k}), & \ldots, & B_{j-k-1}(x_{j+k}) \end{bmatrix}_{(k+1) \times (2k+1)}$$

$$A^{(j)}_2 := \begin{bmatrix} B'_{j-k-1}(x_j), & \ldots, & B'_{j-k-1}(x_j) \\ \vdots & \vdots & \vdots \\ B'_{j-k-1}(x_{j+k}), & \ldots, & B'_{j-k-1}(x_{j+k}) \end{bmatrix}_{(k+1) \times (2k+1)}$$

The two vectors $\alpha^{(i)}$ and $\beta^{(i)} \in \mathbb{R}^{k+1}$ are defined as the solution of the following linear system,

$$G^{(i)} (\alpha^{(i)})^T, (\beta^{(i)})^T = \mathbf{e}_{2k+2},$$

where $\mathbf{e}_{2k+2} = (0, \ldots, 0, 1)^T \in \mathbb{R}^{2k+2}$. Note that the last equation in (9), $\sum_{j=0}^{k} \beta^{(i)}_j = 1$, is just a normalization condition. The non singularity of $G^{(i)}$ is proved in Corollary 1 reported in the Appendix.

In the following two Theorems we show that the vectors $\alpha^{(i)}$ and $\beta^{(i)}$ satisfy (4) with $r = k + 1$ and reduce to the vectors $\alpha$ and $\beta$ in the case of a uniform mesh.

**Theorem 1** The vectors $\alpha^{(i)}$ and $\beta^{(i)}$, which are the solutions of (9), satisfy the order condition (4) with $r = k + 1$.

**Proof:** Let us consider the following result concerning B–splines [15],

$$(t - x)^{k+1} = \sum_{i=-(1+k)}^{-1} \phi_i^{(k+1)}(t) B_i(x), \quad \forall x \in [a, b], \ \forall t \in \mathbb{R},$$

where $\phi_i^{(k+1)}(t) := \prod_{j=i+1}^{i+k+1} (t - x_j)$. Taking the derivatives of (10) $j$ times with respect to $t$ and differentiating once more with respect to $x$, ($j = 0, \ldots, k + 1$), the following expressions are obtained,

$$\begin{cases} (k + 1)^{(j)} (t - x)^{k+1-j} = \sum_{i=-(1+k)}^{-1} \frac{d^j \phi_i^{(k+1)}}{dt^j} (t) B_i(x), \\ j = 0, \ldots, k + 1 \\ -(k + 1)^{(j+1)} (t - x)^{k-j} = \sum_{i=-(1+k)}^{-1} \frac{d^j \phi_i^{(k+1)}}{dt^j} (t) B'_i(x). \end{cases}$$

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Thus, evaluating (11) at all \(x_i, l = i - \nu, \ldots, i + k - \nu\), the following relations are obtained,

\[
\begin{cases}
W^{(k+1)}_{i,\nu, k}(t) = \Delta_k Z^{(k+1)}_{i-\nu-k+1, 2k}(t) A^{(\nu)}_1 T,
-W^{(k+1)'}_{i,\nu, k}(t) = \Delta_k Z^{(k+1)}_{i-\nu-k+1, 2k}(t) A^{(\nu)}_2 T,
\end{cases}
\]

where \(\Delta_k := \text{diag}(\frac{1}{(k+\nu+1)}, \frac{1}{(k+\nu+2)}, \ldots, \frac{1}{(k+\nu+1)})\), \(W^{(k+1)}_{i,\nu, k}(t)\) is the Vandermonde matrix defined in (5), and

\[
Z^{(k+1)}_{j, s}(t) := \begin{bmatrix}
\frac{d^{k+1}}{dT^{k+1}} \phi_j^{(k+1)}(t) & \ldots & \frac{d^{k+1}}{dT^{k+1}} \phi_j^{(k+1)}(t) \\
\vdots & \ddots & \vdots \\
\phi_j^{(k+1)}(t) & \ldots & \phi_j^{(k+1)}(t)
\end{bmatrix}.
\]

Thus, (9), together with (12) used with \(\nu = k_1\), immediately implies (4) with \(r = k + 1\), that is the \(k\)-step BS method has order \(p \geq k + 1\).

**Theorem 2** Let \(h_1 = x_i - x_{i-1} = h, i = -k, \ldots, N + k + 1\). Then the vector \((\alpha^T, \beta^T)T\) with \(\alpha, \beta \in \mathbb{R}^{k+1}\) having entries defined in (6) is the solution of the linear system (9) \(\forall i = k_1, \ldots, N - k_2\).

**Proof**: In the uniform case the B-splines are scaled translations of the reference B-spline \(B(x)\) of degree \(k + 1\) with integer active knots \(0, \ldots, k + 2\),

\[
B_j(x) = B\left(\frac{x - x_j}{h}\right), j = -(1 + k), \ldots, N - 1.
\]

Thus, for all \(j\), \(A^{(j)}_1\) and \(A^{(j)}_2\) are bandwise Toeplitz matrices whose non zero elements in the first row are the first \((k + 1)\) entries and they are \(B(k + 1), \ldots, B'(k + 1)/h, \ldots, B'(1)/h\), respectively. Thus if \(\alpha, \beta \in \mathbb{R}^{k+1}\) are the two vectors defined in (6), it is easy to verify that both \(A^{(i-k_1+1)}_1\alpha\) and \(h A^{(i-k_1+1)}_2\beta\) are just their convolution and then they are equal. Considering that \(\epsilon^T\beta = 1\) because of the unity partition property of B-splines, we can conclude that, \((\alpha^T, \beta^T)^T\) is the solution of (9).

From a numerical point of view, it is convenient to re-write the linear system (9) in an equivalent but more structured form. This is done by introducing the following two permutation matrices \(P_{2r}\) and \(Q_{2r}\), where \(l = \left\lfloor \frac{k+1}{2} \right\rfloor\)

\[
\begin{cases}
P_{2r} := \begin{bmatrix}
e_{r+1}, e_1, \ldots, e_{r+1} - e_r, e_{r+1}, e_{r+1} - e_r, \ldots, e_r, e_{2r}\end{bmatrix}^T,
Q_{2r} := \begin{bmatrix}e_1, \ldots, e_r, e_{2r}, e_{r+1}, \ldots, e_{2r-1}\end{bmatrix}^T,
\end{cases}
\]

where \(e_s\) is the \(s\)-th unit vector of \(\mathbb{R}^{2r}\). Thus, by introducing the matrix,

\[
\tilde{G}^{(i)} := Q_{2(k+1)} G^{(i)} P_{2(k+1)}^T,
\]

(9) can be replaced with the following equivalent linear system, where \(l = \left\lfloor \frac{k+1}{2} \right\rfloor\)

\[
\tilde{G}^{(i)}(\beta_0^{(i)}, \alpha_0^{(i)}, \ldots, \beta_{l-1}^{(i)}, \alpha_{l-1}^{(i)}, \beta_{l}^{(i)}, \ldots, \alpha_k^{(i)}, \beta_k^{(i)})^T = e_{k+2}.
\]

Considering the B-spline properties, \(\tilde{G}^{(i)}\) turns out to be a \((2 \times 2)\)-block banded diagonal matrix with bandwidth equal to \(2\left\lfloor \frac{k+1}{2} \right\rfloor + 1\). More precisely we can say that, among all the square submatrices of \(\tilde{G}^{(i)}\) sharing with it the diagonal and antidiagonal \((2 \times 2)\)-blocks, the one having no zero block and maximum dimension has size \(2m \times 2m, m = k + 3 - 2\left\lfloor \frac{k+1}{2} \right\rfloor\) (see Figure 1).

Concerning the algebraic properties of \(\tilde{G}^{(i)}\), in Corollary 2 appearing in the Appendix it is proved that all the principal submatrices of \(\tilde{G}^{(i)}\) of order \(s, s \leq 2\left\lfloor \frac{k+1}{2} \right\rfloor\), are non singular and that this is also true for all the bottom-to-top principal submatrices (i.e. submatrices whose first diagonal element is any \(\tilde{G}^{(i)}_{j,j}\) and whose last diagonal element is \(\tilde{G}^{(i)}_{2k+2,2k+2}\)) of the same order.

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In this section we describe a symmetric bidirectional factorization algorithm for solving the linear system

\[ \hat{G} z = e_{k+2}, \]

where \( e_{k+2} \) is the \((k + 2)^{nd}\) unit vector of \( \mathbb{R}^{2k+2} \), \( z \in \mathbb{R}^{2k+2} \) and \( \hat{G} \) is any one of the matrices \( \hat{G}^{(i)} \) of size \( 2k + 2 \) (whose structure is represented in Figure 1).

Owing to the non singularity of all the principal and bottom-to-top principal submatrices of \( \hat{G}^{(i)} \) of order \( s, s \leq \lfloor \frac{k+1}{2} \rfloor \), (see corollary 2 in the appendix), we can introduce a simultaneous up-down and down-up Gaussian elimination algorithm which in \( l = k + 1 - m = 2(\lfloor \frac{k+2}{3} \rfloor - 1) \) steps defines a factorization of \( \hat{G} \), i.e. \( \hat{G} = S D T \). The algorithm works as follows,

\[ T^{(1)} := \hat{G}, T^{(j+1)} := S_j T^{(j)}, j = 1, \ldots, l \]

where \( S_j \) is the non singular matrix performing a bidirectional Gaussian elimination, that is,

\[ S_j := I_{2k+2} - c^{(j)} e_j^T, - r^{(j)} e_j^T, \]

with \( j^* := 2k + 3 - j \) and \( c^{(j)}, r^{(j)} \) denoting two vectors of length \( (2k + 2) \) defined as,

\[ c^{(j)} := \frac{1}{T_{j,j}}, r^{(j)} := \frac{1}{T_{j^*,j^*}} \]

In order to highlight the diagonal part of the final matrix, we define the diagonal matrix \( D \),

\[ D := \text{diag}(T_{1,1}^{(1)}, \ldots, T_{l,l}^{(l)}, T_{l+1,1}^{(l)}, \ldots, T_{2k+2,2k+2}^{(l)}), \]

and we define \( T := D^{-1} T^{(l+1)} \).

Finally, denoting by \( S = S_1^{-1} \cdots S_l^{-1} \), we get \( \hat{G} = S D T \) (observe that each \( S_j \) is non–singular and in particular that \( S_j^{-1} = I_{2k+2} + c^{(j)} e_j^T + r^{(j)} e_j^T \)). The final structure of \( T \) is,

\[ T = \begin{bmatrix} T_l & T_{lc} & 0 \\ 0 & T_c & 0 \\ 0 & T_{rc} & T_r \end{bmatrix}, \]
where \( T_l \) (\( T_r \)) is a \( l \times l \) upper (lower) triangular matrix (with diagonal entries all equal to 1) and \( T_c \) is a full matrix. It is easy to check that \( T^{-1} \) has the same block structure as \( T \) and that its diagonal blocks are the inverses of the corresponding blocks of \( T \) shown in (20). Thus, considering that \( T_l \) and \( T_r \) are triangular, the solution of a linear system having \( T \) as coefficient matrix requires only the factorization of the full matrix \( T_c \). This could be performed using a standard LU factorization with pivoting. Observe also that this symmetric factorization algorithm is particularly efficient when used to solve (17) because its right hand side remains unchanged when it is left multiplied by \( D^{-1} S^{-1} \). As a consequence, we can say that (17) is equivalent to the system

\[
T \mathbf{z} = \mathbf{e}_{k+2}.
\]

We conclude this section by giving a table where the conditioning number \( \kappa_2 \) (in the Euclidean norm) of \( G \) and of \( T \) are compared in the case of a uniform mesh for different values of \( k \). Looking at table 2, it is clear that when smooth non-uniform meshes are used, replacing (17) with the equivalent system (21) can increase the accuracy of the numerically computed BS coefficients.

<table>
<thead>
<tr>
<th>( k )</th>
<th>( 3 )</th>
<th>( 4 )</th>
<th>( 5 )</th>
<th>( 6 )</th>
<th>( 7 )</th>
<th>( 8 )</th>
<th>( 9 )</th>
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<tbody>
<tr>
<td>( \kappa_2(G) )</td>
<td>7.6 ( 10^1 )</td>
<td>6.4 ( 10^2 )</td>
<td>1.0 ( 10^4 )</td>
<td>1.9 ( 10^5 )</td>
<td>5.1 ( 10^6 )</td>
<td>1.7 ( 10^8 )</td>
<td>7.0 ( 10^9 )</td>
</tr>
<tr>
<td>( \kappa_2(T) )</td>
<td>5.7 ( 10^0 )</td>
<td>2.7 ( 10^1 )</td>
<td>2.6 ( 10^1 )</td>
<td>1.0 ( 10^2 )</td>
<td>4.2 ( 10^2 )</td>
<td>4.4 ( 10^2 )</td>
<td>1.7 ( 10^3 )</td>
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6 The additional methods

Similarly to what happens when fixing the additional conditions in spline interpolation, there are several possible choices of the additional \( k_1 - 1 = \lfloor \frac{k}{2} \rfloor - 1 \) left and \( k_2 = \lfloor \frac{k}{2} \rfloor \) right methods. In the general non-uniform case the left methods are expressed as follows,

\[
\sum_{j=-i}^{k-i} \alpha_{j+i}^{(i)} y_{i+j} = h_i \sum_{j=-i}^{k-i} \beta_{j+i}^{(i)} f_{i+j}, \quad i = 1, \ldots, k_1 - 1, \quad (22)
\]

and the right ones as

\[
\sum_{j=N-i-k}^{N-i} \alpha_{j-N+i+k}^{(i)} y_{i+j} = h_i \sum_{j=N-i-k}^{N-i} \beta_{j-N+i+k}^{(i)} f_{i+j}, \quad i = N - k_2 + 1, \ldots, N, \quad (23)
\]

where the coefficient vectors \( \alpha^{(i)}, \beta^{(i)}, \quad i = 1, \ldots, k_1 - 1 \text{ and } i = N - k_2 - 1, \ldots, N \) characterize the selected methods. In order to keep the approximation order equal to \( p \) (where \( p \) is the order of the main scheme) these additional methods must have order greater than \( p - 2 \) [3].

Considering the uniform case, in [11] we have proved that, if the numerical solution verifies (2) with coefficients defined as in (6), there is a unique (vector) spline \( \mathbf{s}_k(\cdot) = \sum_{i=-1-k}^{N-1} \mathbf{c}_i B_i(\cdot), \quad \mathbf{c}_i \in \mathbb{R}^d \), such that,

\[
\begin{cases}
\mathbf{s}_k(x_i) = \mathbf{y}_i \\
\mathbf{s}_k'(x_i) = \mathbf{f}_i 
\end{cases} \quad i = 0, \ldots, N.
\]

In the forthcoming paper [12], using a similar argument, we prove that this result can be extended to the case of non-uniform meshes. This spline extension verifies additional requirements which...
are a consequence of the additional methods (22) and (23) needed by the main method. This means that they can be interpreted in the BS setting as additional requirements to the associated collocation spline.

Considering for the sake of brevity the scalar case \( d = 1 \) and only the left methods, in this section we first derive the additional methods imposing the condition that the spline \( s_k(\cdot) \) verifies the not-a-knot condition at the knots \( x_i, i = 1, \ldots, k_1 - 1, \) that is \( s_k^{(k+1)}(x_i^-) = s_k^{(k+1)}(x_i^+) \) (in practice this condition removes the knot \( x_i \) from the spline knot set but not from the collocation point set). Then, in Theorem 4 we show that they have convergence order greater than \( k \).

By using the piecewise constant \((k+1)^{st}\)–derivative of the spline extension, we define the vector \( \mathbf{\delta} := (\delta_1, \ldots, \delta_N)^T \), where,

\[
\delta_i := s_k^{(k+1)}(x) / (k+1)!, \ x \in [x_{i-1}, x_i), \ i = 1, \ldots, N. \tag{25}
\]

Considering the recursive formula for B–spline derivatives [4], it can be proved that \( \mathbf{\delta} \) satisfies the following relation,

\[
\mathbf{\delta} = M_{k+1} \ldots M_1 \mathbf{c},
\]

where \( \mathbf{c} = (c_{-1-k}, \ldots, c_{N-1})^T \) is the vector of the spline coefficients in the B–spline basis and \( M_i \) is a bidiagonal rectangular matrix of size \((N + k + 1 - i) \times (N + k + 2 - i)\) defined as follows,

\[
M_i := \begin{bmatrix}
-1 & 1 & 0 & \ldots & 0 \\
\frac{1}{x_{i-1} - x_i} & \frac{1}{x_{i-1} - x_i} & \ddots & \ddots & \ddots \\
0 & \ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & \ldots & 1 & \frac{-1}{x_{N+k+1-i} - x_{N+i}} & \frac{1}{x_{N+k+1-i} - x_{N+i}}
\end{bmatrix}. \tag{26}
\]

As a consequence the not-a-knot condition at \( x_i \) becomes

\[
(e_i - e_{i+1})^T \mathbf{\delta} = (e_i - e_{i+1})^T M_{k+1} \ldots M_1 \mathbf{c} = 0, \tag{27}
\]

where \( e_i \) is the \( i^{th} \) unit vector in \( \mathbb{R}^N \). Thus, by setting

\[
\mathbf{\rho}_i := M_i^T \ldots M_{k+1}^T (e_i - e_{i+1}), \tag{28}
\]

the not a knot condition at \( x_i \) can be formulated as follows in terms of the vector \( \mathbf{c} \),

\[
\mathbf{\rho}_i^T \mathbf{c} = 0. \tag{29}
\]

Consider now for all \( i = 1, \ldots, k_1 - 1 \), the non singular linear system,

\[
\tilde{G}^{(k_1)} D_i (\mathbf{\alpha}^{(i)} T, \mathbf{\beta}^{(i)} T)^T = (\mathbf{\rho}_i^T, 0)^T, \tag{30}
\]

with

\[
\tilde{G}^{(k_1)} := \begin{bmatrix}
A_1^{(0)T} & -h_{k_1} A_2^{(0)T} \\
0^T & \mathbf{e}_{k+1}^T
\end{bmatrix},
\]

\[
D_i := \text{diag}(1, \ldots, 1, h_i/h_{k_1}, \ldots, h_i/h_{k_1}) \text{ and }
\]

\[
\tilde{\mathbf{\rho}}_i := [I_{2k+1}, 0_{2k+1, N-k}] \mathbf{\rho}_i. \tag{31}
\]

Then, the following theorem allows us to derive the coefficients of the left additional methods guaranteeing (29) for all \( i = 1, \ldots, k_1 - 1 \).
Theorem 3 Let \( \alpha^{(i)} \) and \( \beta^{(i)} \), \( 1 \leq i \leq k_1 - 1 \), be the solution of the linear system (30). Then if the numerical solution satisfies the \( i^{th} \) method in (22), the coefficient vector \( \mathbf{c} \) of the associated spline extension \( s_k(\cdot) \in S_{k,N} \) satisfies (29).

Proof: Owing to the bidiagonal structure of all the matrices \( M_j, j = 1, \ldots, k+1 \), \( \mathbf{p} \) can be block decomposed as \( \mathbf{p}_i = (\mathbf{p}_i^T, \mathbf{0}_{N-k_i}^T)^T, \forall i = 1, \ldots, k_1 - 1 \), with \( \mathbf{p}_i \in \mathbb{R}^{2k+1} \) defined in (31). This allows us to re-write (29) in the following way when \( i = 1, \ldots, k_1 - 1 \),

\[
\tilde{\mathbf{p}}_i^T (c_{-k-1}, \ldots, c_{k-1})^T = 0. \tag{32}
\]

Now, if \( \alpha^{(i)} \) and \( \beta^{(i)} \) are the solution of (30), then

\[
\tilde{\mathbf{p}}_i = A_1^{(0)} T \alpha^{(i)} - h_i A_2^{(0)} T \beta^{(i)}. \tag{33}
\]

On the other hand, considering the local support of B–splines and considering that (24) holds, it is possible to check that \( A_1^{(0)} (c_{-k-1}, \ldots, c_{k-1})^T = (y_{00}, \ldots, y_{k}) \) and \( A_2^{(0)} (c_{-k-1}, \ldots, c_{k-1})^T = (y_{0}, \ldots, y_{k}) \). Substituting (33) in (32), we prove that (29) is equivalent to the \( i^{th} \) method in (22).

In order to be sure that (22) does not destroy the convergence order of the main BS method, we need to check the order conditions. To do this, we first prove the following lemma,

Lemma 1 The vectors \( \tilde{\mathbf{p}}_i, i = 1, \ldots, k_1 - 1 \) defined in (28) and (31) belong to the null space of the matrix \( Z_{-1-k,2k}(t) \) defined in (13) (with \( j = -1, s = 2k \)).

Proof: With some easy manipulation it is possible to check that

\[
Z_{-1-k,2k}(t) \tilde{I} M_1^T = - \begin{bmatrix} 0_{1,2k} & L_1^{(1)} \\ Z_{-1-k,2k-1}(t) & L_2^{(1)} \end{bmatrix},
\]

where \( \tilde{I} := [I_{2k+1}, 0_{2k+1,N-k}] \) and where \( L_1^{(1)} \) and \( L_2^{(1)} \) are matrices with suitable dimension. Thus, using the same reasoning, we get

\[
Z_{-1-k,2k}(t) \tilde{I} M_1^T \cdots M_{k+1}^T = (-1)^{k+1} \begin{bmatrix} 0_{k+1,k} & L_1^{(k+1)} \\ Z_{0,k-1}(t) & L_2^{(k+1)} \end{bmatrix},
\]

where \( Z_{0,k-1}(t) \equiv \mathbf{e}^T \), with \( \mathbf{e} = (1, \ldots, 1)^T \in \mathbb{R}^k \). Thus, from (28) and (31) it follows that, \( \forall i = 1, \ldots, k_1 - 1 \),

\[
Z_{-1-k,2k}(t) \tilde{\mathbf{p}}_i = Z_{-1-k,2k}(t) \tilde{I} M_1^T \cdots M_{k+1}(\mathbf{e}_i - \mathbf{e}_{i+1}) = 0_{k+2}. \tag*{\blacksquare}
\]

Now, we are ready to prove the following theorem,

Theorem 4 If \( (\alpha^{(i)} T, \beta^{(i)} T)^T, 1 \leq i \leq k_1 - 1 \), is the solution of (30), then the order condition \( p \geq k + 1 \), holds true for the corresponding additional left method (22).

Proof: For the \( i^{th} \) additional left method (22) the order condition \( p \geq k + 1 \) can be expressed as follows in the general non-uniform case [3],

\[
W_{i,i,k}^{(k+1)}(t) \alpha^{(i)} + h_i W_{i,i,k}^{(p)}(t) \beta^{(i)} = 0. \tag{34}
\]
Now, the matrix relations (12) imply that \( W_{i,i,k}^{(k+1)}(t) = \Delta_k Z_{1-k,2k} A_1^{(0)} \) and \( W_{i,i,k}^{(k+1)'}(t) = -\Delta_k Z_{1-k,2k} A_2^{(0)} \), with \( \Delta_k \) denoting a non singular diagonal matrix. Then, using (33), (34) becomes
\[
Z_{1-k,2k} (A_1^{(0)} \alpha^{(i)} - h_i A_2^{(0)} \beta^{(i)}) = Z_{1-k,2k} \tilde{\rho}_i = 0.
\]

This allows us to conclude that (34) is an immediate consequence of the result proved in the previous lemma. □

7 Numerical Results

In order to test the non-uniform BS methods with \( k \) odd, a variable stepsize implementation of them has been used on some test problems [6] whose exact solution is known. This preliminary implementation, written in MATLAB, is very similar to the one presented in [13, 14] for the code TOM, especially concerning the stepsize variation strategy and the solution of the nonlinear equations. The coefficients of the methods are computed using the algorithm described in Section 5, the error estimation is done using a higher order method in the same class still with \( k \) odd. More precisely, the computed solution is accepted when,
\[
E_m(\tilde{y}) := \max_{i=0,\ldots,N} ||(y_i - \tilde{y}_i) /. \max(1, |\tilde{y}_i|)||_\infty < \text{tol},
\]
where \( \tilde{y} \) is the numerical solution provided by the higher order method ("/" is the pointwise division in the case of vector problems).

Observe that, when the test problem is a scalar differential equation of order greater than 1, it has been rewritten as a first order system before applying to it the numerical scheme. For the sake of brevity, further details concerning the implementation are skipped in this paper.

**Problem 1**
The first test problem is
\[
\begin{aligned}
\epsilon y''(x) &= y(x), \ x \in [0, 1], \ \epsilon > 0, \\
y(0) &= 1, \\
y(1) &= 0,
\end{aligned}
\]
whose exact solution is \( y(x) = \frac{\exp(-x/\sqrt{\epsilon}) - \exp(-(2-x)/\sqrt{\epsilon})}{1 - \exp(-2/\sqrt{\epsilon})} \). The solution has a boundary layer of width \( O(\sqrt{\epsilon}) \) at \( x = 0 \). The problem is solved using different values of both \( \epsilon \) and \( \text{tol} \) and the results are shown in Table 3, where \( N_{\text{max}} \) is the maximum number of mesh points used, \( h_{\text{max}}/h_{\text{min}} \) is the ratio between the largest and the smallest step size, \( E_m \equiv E_m(y) \), where \( y(x) \) is the exact solution.

The behavior of \( E_m \) is consistent with the order of the methods. For lower values of the tolerances higher order methods reach the solution using a smaller number of mesh points. As expected, the ratio \( h_{\text{max}}/h_{\text{min}} \) increases as \( \epsilon \) decreases.

**Problem 2**
The second test problem is
\[
\begin{aligned}
\epsilon y''(x) + xy'(x) &= -\epsilon^2 \pi^2 \cos(\pi x) - \pi x \sin(\pi x), \ x \in [-1, 1], \ \epsilon > 0, \\
y(-1) &= -2, \\
y(1) &= 0,
\end{aligned}
\]
whose exact solution is \( y(x) = \cos(\pi x) + \text{erf}(x/\sqrt{2})/\text{erf}(1/\sqrt{2}) \). The solution has a shock layer of width \( O(\sqrt{\epsilon}) \) near \( x = 0 \). We solve this problem using different values of \( \epsilon \) and different values of \( \text{tol} \). The results, reported in Table 4, are similar to those presented for the first example. The potential of the present schemes is even more evident when a much smaller value for \( \epsilon \) (e.g. \( \epsilon = 10^{-14} \)) with \( \text{tol} = 1e-6 \) is used. The order 4 BS method, which has \( k = 3 \), solves this problem using only 351 mesh points, with an error \( E_m = 3.8e - 6 \) and a value of \( h_{\text{max}}/h_{\text{min}} = 5.2e + 6 \).
Table 3: Test problem 1.

<table>
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<tr>
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Table 4: Test problem 2.

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<td>2.7e0</td>
<td>1.5e-09</td>
</tr>
</tbody>
</table>

Problem 3

The third test problem is a nonlinear one,

$$
\begin{align*}
  &\epsilon y''(x) = y(x) + y^2(x) - \exp(2x/\sqrt{\epsilon}), \quad x \in [0,1], \quad \epsilon > 0, \\
  &y(0) = 1, \quad y(1) = \exp(-1/\sqrt{\epsilon}),
\end{align*}
$$

whose exact solution is $y(x) = \exp(-x/\sqrt{\epsilon})$ and has a boundary layer of width $O(\sqrt{\epsilon})$ at $x = 0$. Table 5 reports the results showing that the behavior of the BS schemes on this nonlinear problem does not differ from that on linear ones.

8 Acknowledgement.

The authors are grateful to the referees for several helpful comments. This work was supported by G.N.C.S. (INdAM) and COFIN-PRIN 2004 (project “Metodi numerici e software matematico per le applicazioni”).

9 Appendix

In this section using the Witney–Schoenberg conditions for spline interpolation (e.g. see [4]) and their generalization to the case of osculatory spline interpolation originally proved in [16], we first
prove the non singularity of the matrix \( G^{(i)} \) defined in (7). Then we prove also that all the principal and bottom–to–top principal submatrices of \( G^{(i)} \) defined in (15), are non singular if they have order \( s \), with \( s \leq 2 \left[ \frac{k}{2} \right] \).

Let us start by reporting the Witney–Schoenberg conditions and the above mentioned result about osculatory spline interpolation in matrix form.

**Theorem 5 (Witney–Schoenberg)** Let \( \{ B_i(x), i = -1 - k, \ldots, N - 1 \} \) be the \( k + 1 \) degree B–spline basis with extended knot set \( X = \{ \xi_{-1-k}, \ldots, \xi_{N+k+1} \} \), where \( \xi_i \leq \xi_{i+1} \) and \( \xi_i < \xi_{i+k+2} \) (whose span has dimension \( N + k + 1 \)). Let \( T = \{ \tau_0, \ldots, \tau_{N+k} \} \) be a strictly increasing sequence of \( N + k + 1 \) abscissae. Then the matrix \( B := (B_j(\tau_i)) \) is non singular if and only if the following conditions hold,

\[
\xi_{j-k-1} < \tau_j < \xi_{j+1}, \quad \forall j = 0, \ldots, N + k. \tag{38}
\]

The previous result is relevant to spline interpolation of Lagrange type. For our purposes, the following generalization to osculatory spline interpolation is particularly significant.

**Theorem 6 (Karlin–Ziegler)** Let \( \{ B_i(x), i = -1 - k, \ldots, N - 1 \} \) be the \( k + 1 \) degree B–spline basis with extended knot set \( X = \{ \xi_{-1-k}, \ldots, \xi_{N+k+1} \} \), where \( \xi_i \leq \xi_{i+1} \) and \( \xi_i < \xi_{i+k+2} \) (whose span has dimension \( N + k + 1 \)). Let \( T = \{ \tau_0, \ldots, \tau_{N+k} \} \) be a non decreasing sequence of \( N + k + 1 \) abscissae such that \( \tau_i < \tau_{i+k+2} \). In addition, let us assume that \( \forall i = 0, \ldots, N + k \)

\[
\tau_i = \cdots = \tau_{i+q} = \xi_j = \cdots = \xi_{j+s} \quad \Longrightarrow \quad q + s \leq k. \tag{39}
\]

Then if (38) holds, the following matrix is non singular

\[
B := \begin{bmatrix}
B_{-1-k}^{(0)}(t_0) & \cdots & B_{N-1}^{(0)}(t_0) \\
\vdots & \ddots & \vdots \\
B_{-1-k}^{(m-1)}(t_0) & \cdots & B_{N-1}^{(m-1)}(t_0) \\
\vdots & \ddots & \vdots \\
B_{-1-k}^{(0)}(t_f) & \cdots & B_{N-1}^{(0)}(t_f) \\
\vdots & \ddots & \vdots \\
B_{-1-k}^{(m-1)}(t_f) & \cdots & B_{N-1}^{(m-1)}(t_f)
\end{bmatrix}, \tag{40}
\]
where $T = \{ t_0, \ldots, t_f \}$ is the set of all distinct abscissae in $T$ and $m_j$ denotes the multiplicity of $t_j$ in $T$ (thus, $\sum_{j=0}^{f} m_j = N + k + 1$).

The following two corollaries are useful for our purposes,

**Corollary 1** The square matrix $G^{(i)}$ defined in (7) is non singular.

**Proof:** Since the proof is analogous for all the indices $i$, without loss of generality we assume $i = k_1$ and $h_i = 1$. Then $G^{(k_1)T}$ becomes,

$$G^{(k_1)T} = \begin{bmatrix} A_1^{(0)} & \mathbf{0} \\ -A_2^{(0)} & \mathbf{e} \end{bmatrix}. \quad (41)$$

Now, first of all let us prove that the principal submatrix of $G^{(k_1)T}$ of order $2k+1$ is non singular. To show this, let us consider the $k+1$ degree B–splines with extended knot set $X = \{ x_{-1-k}, \ldots, x_{2k+1} \}$ (whose span has dimension $2k + 1$). The sequence $T = \{ x_0, x_0, \ldots, x_{k-1}, x_k \}$ verifies (39) and (38) with respect to $X$. As a consequence, the related matrix $B$ defined in (40) (where in this case $m_j = 2, \forall j = 0, \ldots, f - 1$ and $m_f = 1$ with $f = k$) is non singular. Considering that the principal submatrix of order $2k + 1$ of the matrix $G^{(k_1)T}$ reported in (41) is just a permutation of $B$, using Theorem 6 we can conclude that it is non singular, as well. Then, in order to prove that $G^{(k_1)T}$ is non singular, we have to show that its last column does not belong to the range of $A := [A_1^{(0)T} - A_2^{(0)T}]^T$. Let us assume that it belongs to such space. Then, relating again to the $k+1$ degree B–splines with extended knot set $X = \{ x_{-1-k}, \ldots, x_{2k+1} \}$, it should be possible to determine a non zero spline $s$ belonging to their span such that it vanishes at each knot $x_j, j = 0, \ldots, k$ and has unitary derivative value at all these knots. Thus, it should be possible to determine a set of $k$ additional abscissae $\eta_j \in (x_j, x_{j+1}), j = 0, \ldots, k - 1$ such that $s(\eta_j) = 0$. Considering that the sequence $T = \{ x_0, \eta_0, \ldots, x_{k-1}, \eta_{k-1}, x_k \}$ verifies (38) with respect to $X$, Theorem 5 implies a contradiction.

**Corollary 2** All the principal and bottom-to-top principal submatrices of $\hat{G}^{(i)}$ as defined in (15), are non singular if they have order $s$, with $s \leq 2\lfloor \frac{k}{2} \rfloor$.

**Proof:** Without loss of generality we can assume $i = k_1$ and $h_i = 1$. In addition, considering the structure of $G^{(k_1)}$, without loss of generality we can relate only to the principal submatrices. Let us consider the $k + 1$ degree B–splines with extended knot set $X = \{ x_{-1-k}, \ldots, x_{2k+1} \}$. For proving that the principal submatrix of order $s = 2r, r \leq \lfloor \frac{k}{2} \rfloor$, is non singular, let us introduce the following sequence of $2k + 1$ abscissae

$$T = \{ x_0, x_0, \ldots, x_{r-1}, x_{r-1}, x_{2r}, x_{2r}, \ldots, x_{k-1}, x_{k-1}, x_k, \ldots, x_k \}.$$

Since $T$ verifies (39) and (38) with respect to $X$, using Theorem 6 we can conclude that the associated matrix $B$ defined in (40) (where in this case $m_j = 2, j = 0, \ldots, f - 1, m_f = 2r$, with $f = k - r$) is non singular. Now, considering that each $B_j(\cdot)$ has local support $[x_j, x_{j+k+2}]$, we can observe that $B$ has the following block structure,

$$B = \begin{bmatrix} B_{1,1} & B_{1,2} \\ 0 & B_{2,2} \end{bmatrix},$$

where $B_{1,1}$ is of size $2r \times 2r$. Thus $B_{1,1}$ is non singular as well. Considering that $B_{1,1}$ comes out to be just the transpose of the principal submatrix of $\hat{G}^{(k_1)}$ of order $s = 2r$, the proof is completed. In the case $s = 2r - 1$ the proof is analogous, it is sufficient to choose...
\[
T = \{x_0, x_0, \ldots, x_0, x_{2r-2}, x_{2r-2}, x_{r-1}, x_{2r-1}, x_{2r}, x_{2r}, \ldots, x_{k-1}, x_{k-1}, x_k, \ldots, x_k\}.
\]

References


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