USING THE SHERMAN-MORRISON-WOODBURY FORMULA TO SOLVE THE SYSTEM OF LINEAR EQUATIONS FROM THE STANDARD MULTIPLE SHOOTING METHOD FOR A LINEAR TWO POINT BOUNDARY-VALUE PROBLEM IS A BAD IDEA

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Abstract. We use the standard multiple shooting method to solve a linear two point boundary-value problem. To ensure that the solution obtained by combining the partial solutions is continuous and satisfies the boundary conditions, we have to solve a system of linear equations. Our idea is to first solve a bidiagonal system related to the original system of linear equations, and then update it with the Sherman-Morrison-Woodbury formula. We study the feasibility, the numerical stability and the running time of this method. The results are: The method described above has the same stability problems like the well known Condensing method. The running time analysis shows that the new method is slower than the Condensing method. Therefore we recommend not to use the method described in this article.

1. Introduction

We solve the linear two point boundary-value problem

\[ \mathcal{L} \mathbf{x}(t) := \dot{\mathbf{x}}(t) - A(t) \mathbf{x}(t) = \mathbf{r}(t), \quad t \in [a, b] \]

\[ \mathcal{B} \mathbf{x}(t) := B_a \mathbf{x}(a) + B_b \mathbf{x}(b) = \mathbf{\beta} \]

with the standard multiple shooting method, where \( \mathbf{x}(t), \mathbf{r}(t) : [a, b] \to \mathbb{R}^n, \mathbf{\beta} \in \mathbb{R}^n, A(t) : [a, b] \to \mathbb{R}^{n \times n} \) and \( B_a, B_b \in \mathbb{R}^{n \times n} \). We divide the interval \([a, b]\) with the shooting points

\[ a = \tau_0 < \tau_1 < \ldots < \tau_{m-1} < \tau_m = b \]

into \( m \) segments \([\tau_j, \tau_{j+1}]\). We use the principle of superposition on each segment to find the solution

\[ \mathbf{x}_j(t) = \mathbf{X}(t; \tau_j) \mathbf{c}_j + \mathbf{v}(t; \tau_j), \]

where \( \mathbf{c}_j \) is a constant vector. \( \mathbf{X}(t; \tau_j) \) is a fundamental system which fulfills the IVP

\[ \mathcal{L} \mathbf{X}(t; \tau_j) = \mathbf{0}, \quad t \in [\tau_j, \tau_{j+1}], \quad \mathbf{X}(\tau_j; \tau_j) = \mathbf{I}. \]

\( \mathbf{v}(t; \tau_j) \) is an inhomogeneous solution of the ODE and fulfills

\[ \mathcal{L} \mathbf{v}(t; \tau_j) = \mathbf{r}(t), \quad t \in [\tau_j, \tau_{j+1}], \quad \mathbf{v}(\tau_j; \tau_j) = \mathbf{0}. \]

The problem now consists in determining the vectors \( \mathbf{c}_j \) in such a way, that

1. the function \( \mathbf{x}(t) \) pieced together by the \( \mathbf{x}_j(t) \) is continuous and
2. satisfies the boundary conditions.

We define \( \mathbf{X}_j := \mathbf{X}(\tau_{j+1}; \tau_j) \) and \( \mathbf{v}_j := \mathbf{v}(\tau_{j+1}; \tau_j) \). To satisfy the boundary conditions we focus on \( \mathcal{B} \mathbf{x}(t) = \mathbf{\beta} \):

\[ B_a \mathbf{c}_0 + B_b \mathbf{X}_{m-1} \mathbf{c}_{m-1} = \mathbf{\beta} - B_b \mathbf{v}_{m-1}. \]

To ensure that \( \mathbf{x}(t) \) is a continuous function we need

\[ \mathbf{x}_{k-1}(\tau_k) = \mathbf{x}_k(\tau_k), \quad k = 1, \ldots, m - 1, \]

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which yields to the conditions
\[ c_k - X_{k-1}c_{k-1} = v_{k-1}, \quad k = 1, \ldots, m - 1. \]

Now we collect equation (1) and the \( m-1 \) equations (2) in the following system of linear equations:
\[ Mc = q, \]

where we define \( Y_j := -X_j \) and
\[
M := \begin{bmatrix}
Y_0 & I & I \\
Y_1 & I & I \\
& \ddots & \ddots \\
Y_{m-2} & I & I \\
B_a & B_b & X_{m-1}
\end{bmatrix}, \quad c := \begin{pmatrix}
c_0 \\
c_1 \\
\vdots \\
c_{m-1}
\end{pmatrix}, \quad q := \begin{pmatrix}
v_0 \\
v_1 \\
\vdots \\
v_{m-2} \beta - B_b v_{m-1}
\end{pmatrix}.
\]

Note that \( c, q \in \mathbb{R}^{mn} \) and \( M \in \mathbb{R}^{mn \times mn} \). It is known that \( M \) is regular if we assume that the BVP has an unique solution. In this case
\[ N := B_a + B_b X(b; a) \]
is regular, too. (see [2, Satz 8.1 (Theorem 8.1)])

2. THE AIM OF THIS WORK

There exists the well known method Condensing to solve the system (3) (see Section 6). Because of the special structure of \( M \) it is pretty obvious to try to find the solution in the following way: First solve the bidiagonal system from (6) and then update the solution with the Sherman-Morrison-Woodbury formula. In this paper we study the feasibility, the numerical stability and the running time of this method.

3. THE SHERMAN-MORRISON-WOODBURY FORMULA

Let \( A \) be a regular \( \ell \times \ell \) matrix and \( U \) and \( V \) be two \( \ell \times p \) matrices. If \( I_p + V^T A^{-1} U \) is regular, then
\[ (A + UV^T)^{-1} = A^{-1} - A^{-1} U (I_p + V^T A^{-1} U)^{-1} V^T A^{-1}. \]
holds.

4. IS IT POSSIBLE TO USE THE SHERMAN-MORRISON-WOODBURY FORMULA TO SOLVE \( Mc = q \)?

First, we have to split \( M \) into two matrices \( M = \mathcal{M} + \mathcal{U} \), where \( \mathcal{U} \) can be written in the form \( \mathcal{U} = UV^T \) with \( U, V \in \mathbb{R}^{mn \times n} \). For this we define
\[
U = \begin{bmatrix}
0, \ldots, 0, B_a^T
\end{bmatrix}^T \quad \text{and} \quad V^T = [I_n, 0, \ldots, -L],
\]
where \( L := X_0^{-1} \cdots X_{m-2}^{-1} \). Therefore we have
\[
\mathcal{U} = UV^T = \begin{bmatrix}
0 & \cdots & 0 \\
& \ddots & \ddots \\
B_a & -B_a L
\end{bmatrix},
\]
and
\[
\mathcal{M} = M - \mathcal{U} = \begin{bmatrix}
Y_0 & I & I \\
Y_1 & I & I \\
& \ddots & \ddots \\
& & Y_{m-2} & I \\
B_a & B_b & X_{m-1}
\end{bmatrix},
\]
where \( B := B_b X_{m-1} + B_a L \).
Now we have to check that $\mathcal{M}$ is regular. Because of
\[
\det \mathcal{M} = \det B \prod_{j=0}^{m-2} \det Y_j,
\]
it follows that $\det \mathcal{M} \neq 0$ iff $\det B \neq 0$, because the $Y_j$ are fundamental systems. But $B = NL$ and $N$ and $L$ are both regular. This follows from
\[
X(b; a) = \prod_{j=1}^{m} X_{m-j}.
\]
This shows that $\mathcal{M}$ is regular.

Finally we have to check that $I_n + V^T \mathcal{M}^{-1} U$ is regular. First we need an auxiliary result:

**Lemma.** Given $m$ regular $n \times n$ matrices $D_i$. Then, the matrix
\[
\Delta := \begin{bmatrix}
D_0 & I_n & I_n & \cdots & I_n \\
D_1 & D_0^{-1} & \cdots & \cdots & \cdots \\
& \ddots & \ddots & \ddots & \ddots \\
D_{m-2} & I_n & \cdots & \cdots & D_{m-1}
\end{bmatrix}
\]
is regular and
\[
\Delta^{-1} = \begin{bmatrix}
D_0^{-1} & -(D_1 D_0)^{-1} & (D_2 D_1 D_0)^{-1} & \cdots & (-1)^{m-1} (D_{m-1} \cdots D_0)^{-1} \\
D_1^{-1} & -(D_2 D_1)^{-1} & \cdots & \cdots & \cdots \\
& \ddots & \ddots & \ddots & \ddots \\
D_{m-2}^{-1} & -(D_{m-1} D_{m-2})^{-1} & \cdots & \cdots & D_{m-1}^{-1}
\end{bmatrix}
\]
holds.

**Proof.** It holds $\det \Delta = \prod_{j=0}^{m-1} \det D_j \neq 0$. $\Delta^{-1} = I_{mn}$ and $\Delta^{-1} \Delta = I_{mn}$ can easily be verified. \hfill $\square$

Now we go back to the matrix $I_n + V^T \mathcal{M}^{-1} U$. With $\mathcal{M}_j^{-1}$ we denote the $j$th column of $\mathcal{M}^{-1}$ and we write $\mathcal{M}_{ij}^{-1}$ for the $n \times n$ sub-matrix in the $i$th row and $j$th column of $\mathcal{M}^{-1}$. With the lemma above and the new notation we get
\[
V^T \mathcal{M}^{-1} U = [I_n, 0, \ldots, 0, -L][\mathcal{M}^{-1}_1 | \ldots | \mathcal{M}^{-1}_m][\{0, \ldots, 0, B_a^T\}^T \\
= [\mathcal{M}^{-1}_{i1} - L \mathcal{M}_{m1}^{-1} | \ldots | \mathcal{M}^{-1}_{im} - L \mathcal{M}_{mm}^{-1}][\{0, \ldots, 0, B_a^T\}^T \\
= \mathcal{M}^{-1}_{1m} B_a - L \mathcal{M}^{-1}_{mm} B_a.
\]
With the special structure of $\mathcal{M}^{-1}$ we can calculate the two sub-matrices $\mathcal{M}^{-1}_{1m}$ and $\mathcal{M}^{-1}_{mm}$ very easy: $\mathcal{M}^{-1}_{mm} = B^{-1}$ and
\[
\mathcal{M}^{-1}_{1m} = (-1)^{n-1} \left( B \prod_{j=2}^{m} Y_{m-j} \right)^{-1} = (-1)^{n-2} Y_0^{-1} \cdots Y_{m-2}^{-1} B^{-1} = X_0^{-1} \cdots X_{m-2}^{-1} B^{-1}.
\]
Now it follows that
\[
V^T \mathcal{M}^{-1} U = \mathcal{M}^{-1}_{1m} B_a - L \mathcal{M}^{-1}_{mm} B_a = LB^{-1} B_a - LB^{-1} B_a = 0.
\]
The result above shows that $I_n + V^T \mathcal{M}^{-1} U = I_n$ is regular and we can use the Sherman-Morrison-Woodbury formula to solve (9).
5. Solving $M c = q$ with the Sherman-Morrison-Woodbury formula

With (5) the solution of (3) can now be expressed as

$$c = M^{-1} q = (M + U)^{-1} q = M^{-1} q - M^{-1} U(I_n + V^T M^{-1} U)^{-1} V^T M^{-1} q$$

This gives us an algorithm to solve (3):

1. Solve $M \xi = q$.
2. Solve $M \zeta = U \xi$.
3. Calculate $c = \xi - \zeta$.

First we study the problem (1.) in detail. We have to solve

$$M \xi = q$$

Bulirsch. They solve (3) in the following way (see [1] or [4]):

We want to compare the new method above with the well known standard method from Stoer and Bulirsch. Therefore we only analyse the number of flops used by the two algorithms to compare them.

In the first step of our new algorithm from the section above we solve $B \xi_{m-1} = q_{m-1}$ and use recursion to find the other $\xi_j$:

$$Y_j \xi_j = q_j - \xi_{j+1}, \quad j = m - 2, \ldots, 0.$$  

We use the same method for our problem (2.). After we calculated

$$U \xi = \begin{bmatrix} 0 & \cdots & 0 \\ B_a & -B_a L \end{bmatrix} \begin{bmatrix} \xi_0 \\ \xi_{m-1} \end{bmatrix} = \begin{bmatrix} 0 \\ B_a(\xi_0 - L \xi_{m-1}) \end{bmatrix},$$

the resulting system of linear equations is

$$Y_0 I \begin{bmatrix} \xi_0 \\ \xi_1 \\ \vdots \\ \xi_{m-2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$  

Again we first solve $B \xi_{m-1} = B_a(\xi_0 - L \xi_{m-1})$ and then solve the remaining systems of linear equations with recursion:

$$Y_j \zeta_j = -\zeta_{j+1}, \quad j = m - 2, \ldots, 0.$$  

6. Condensing

We want to compare the new method above with the well known standard method from Stoer and Bulirsch. They solve (3) in the following way (see [1] or [4]):

1. Compute $E := B_a + B_b X_{m-1} \cdots X_0$ and $u := q_{m-1} - B_b X_{m-1}(q_{m-2} + X_{m-2} q_{m-3} + \cdots + X_{m-2} \cdots X_1 q_0)$.
2. Solve $E c_0 = u$.
3. Compute the remaining $c_j$ with recursion: $c_{j+1} = q_j + X_j c_j$.

In the first step of our new algorithm from the section above we solve $B \xi_{m-1} = q_{m-1}$. Notice that $B = NL$. But $N = E$ holds. This follows directly from (1) and (7). That means our new algorithm has the same stability problems like the Condensing method. See [1] and [3] for a detailed discussion.

Therefore we only analyse the number of flops used by the two algorithms to compare them.
We use LU-factorization to solve the systems of linear equations. We assume that this needs 2
\[ (m-1)(2n^3 - n^2) \]
M. Hermann
Condensing method. Therefore it is not recommendable to use the Sherman-Morrison-Woodbury
same stability problems like the Condensing method. Our new method is also slower than the
continuity conditions with the Sherman-Morrison-Woodbury formula. This new method has the
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method described above.

The running time of the Condensing method is analyzed in Table 1. For a running time analysis
of our new method see Table 2. The result is: The Condensing method is faster than the new
flops for a
\[ n \]


1 Solve \( M \xi = q \).

2 Solve \( Ec_0 = u \).

3 Compute the remaining \( c_j \) with recursion.

\( \sum = 2mn^3 + 3mn^2 - 4/3n^3 - 2n^2 + n \) flops

Table 2. Running time analysis of our new method.

| step  | description | flops |
|-------|-------------|-------|
| 1     | Solve \( M \xi = q \). | \( (m-2)(2/3n^3 + n) \) |
| 1.1   | \( B \xi_{m-1} = q_{m-1} \). | \( (m-2)(2n^3 - n^2) \) |
|       | Compute \( T := L^{-1} = X_{m-2} \cdots X_0 \). | \( 4n^3 - n^2 \) |
|       | Compute \( N := B_a + B_h X_{m-1} T \). | \( 2/3n^3 \) |
|       | Solve \( N s = q_{m-1} \). | \( 2n^2 - n \) |
|       | Compute \( \xi_{m-1} = B^{-1} q_{m-1} = L^{-1} N^{-1} q_{m-1} = T s \). | \( (m-2)(2/3n^3 + n) \) |
| 1.2   | Use recursion to find the other \( \xi_j \). | \( (m-2)(2/3n^3 + n) \) |
| 2     | Solve \( M \xi = t \xi \). | \( (m-2)(2n^3 - n^2) \) |
| 2.1   | \( B \xi_{m-1} = B_a(\xi_0 - L \xi_{m-1}) \). | \( 2/3n^3 \) |
|       | Solve \( T t = \xi_{m-1} \). | \( 2n^2 \) |
|       | Compute \( B_a(\xi_0 - t) \). | \( 2/3n^3 \) |
|       | Solve \( N s = B_a(\xi_0 - t) \). | \( 2n^2 - n \) |
|       | Compute \( \xi_{m-1} = T s \). | \( (m-2)(2/3n^3) \) |
| 2.2   | Use recursion to find the other \( \xi_j \). | \( (m-2)(2/3n^3) \) |
| 3     | Compute \( c = \xi - \xi \). | \( mn \) |
| \( \sum \) | \( = 10/3mn^3 - mn^2 + mn - 2/3n^3 + 7n^2 - 4n \) flops |

7. Running time analysis

We use LU-factorization to solve the systems of linear equations. We assume that this needs 2/3n^3
flops for a \( n \times n \) system.

The running time of the Condensing method is analyzed in Table 1. For a running time analysis
of our new method see Table 2. The result is: The Condensing method is faster than the new
method described above.

8. Conclusion

We found a new algorithm to solve the system of linear equations from the boundary and
continuity conditions with the Sherman-Morrison-Woodbury formula. This new method has the
same stability problems like the Condensing method. Our new method is also slower than the
Condensing method. Therefore it is not recommendable to use the Sherman-Morrison-Woodbury
formula in this case.

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