Symbolic Algorithm for Solving SLAEs with Heptadiagonal Coefficient Matrices

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Abstract

This paper presents a symbolic algorithm for solving band matrix systems of linear algebraic equations with heptadiagonal coefficient matrices. The algorithm is given in pseudocode. A theorem which gives the condition for the algorithm to be stable is formulated and proven.

1 Introduction

Systems of linear algebraic equations (SLAEs) with heptadiagonal coefficient matrices may arise after many different scientific and engineering problems, as well as problems of the computational linear algebra where finding the solution of a SLAE is considered to be one of the most important problems. For instance, a semi-implicit formulation for the discretization of the transient terms of the system of partial differential equations (PDEs) which models a multiphase fluid flow in porous media yields to a heptadiagonal system of pressure equations for each time step (see [1]). On the other hand, in [2] the 3D problem, simulating the incompressible blood flow in arteries with a structured mesh domain leads to a heptadiagonal SLAE.

A whole branch of symbolic algorithms for solving systems of linear algebraic equations with different coefficient matrices exists in the literature. [3] considers a tridiagonal matrix and a symbolic version of the Thomas method [4] is formulated. The authors of [5] build an algorithm in the case of a general bordered tridiagonal SLAE, while in [6] the coefficient matrix taken into consideration is a general opposite-bordered tridiagonal one. A pentadiagonal coefficient matrix is of interest in [7], while a cyclic pentadiagonal coefficient matrix is considered in [8]. The latter algorithm can be applied to periodic tridiagonal and periodic pentadiagonal SLAE either by setting the corresponding matrix terms to be zero.

A performance analysis of effective methods (both numerical and symbolic) for solving band matrix SLAEs (with three and five diagonals) being implemented in C++ and run on modern (as of 2018) computer systems is made by us in [9]. Different strategies (symbolic included) for solving band matrix SLAEs (with three and five diagonals) are explored by us in [11]. A performance analysis of effective symbolic algorithms for solving band matrix SLAEs with coefficient matrices with three, five and seven diagonals being implemented in both C++ and Python and run on modern (as of 2018) computer systems is made by us in [10]. Note that the algorithm for solving a SLAE with a heptadiagonal coefficient matrix considered in [10] is the one that is going to be introduced in the next Section.

After obtaining the algorithm independently, it has been found in the article [12] where it is applied for cyclic heptadiagonal SLAEs. Thus, we do not claim out priority to this algorithm. However, the novelties of this work are as follows: pure heptadiagonality, proved necessary requirements, classical Thomas expressions i.e. the algorithm’s formalism follows the form of expressions that are usually used in the Thomas algorithm for tridiagonal SLAE [3], that is, the solution is searched in the form: \( y_i = \alpha_{i+1} y_{i+1} + \beta_{i+1} \).
2 The Algorithm

Let us consider a SLAE $Ax = y$, where $A$ is a $N \times N$ heptadiagonal matrix, $A = \text{heptadiag}(c^*, b^*, a^*, d, a, b, c)$, $x$ and $y$ are vectors of length $N$:

$$
\begin{pmatrix}
(d_0, a_0, b_0, c_0, 0, \ldots, \ldots, 0) \\
(a_1, d_1, a_1, b_1, c_1, 0, \ldots, \ldots, 0) \\
b_2, a_2, d_2, a_2, b_2, c_2, 0, \ldots, 0 \\
c_3, b_3, a_3, d_3, a_3, b_3, c_3, 0, \ldots, 0 \\
\vdots \\
0, c_N, b_N, a_N, d_N, a_N, b_N, c_N, 0, \ldots, 0 \\
0, 0, c_{N-4}, b_{N-4}, a_{N-4}, d_{N-4}, a_{N-4}, b_{N-4}, c_{N-4}, 0 \\
0, \ldots, 0, c_{N-4}, b_{N-4}, a_{N-4}, d_{N-4}, a_{N-4}, b_{N-4}, c_{N-4}, 0 \\
0, \ldots, 0, c_{N-2}, b_{N-2}, a_{N-2}, d_{N-2}, a_{N-2}, b_{N-2}, c_{N-2}, 0 \\
0, \ldots, 0, c_{N-1}, b_{N-1}, a_{N-1}, d_{N-1}, a_{N-1}, b_{N-1}, c_{N-1}, 0 \\
end{pmatrix}
= 
\begin{pmatrix}
x_0 \\
x_1 \\
x_2 \\
x_3 \\
x_4 \\
x_N-4 \\
x_N-3 \\
x_N-2 \\
x_N-1 \\
y_0 \\
y_1 \\
y_2 \\
y_3 \\
y_4 \\
y_{N-4} \\
y_{N-3} \\
y_{N-2} \\
y_{N-1}
\end{pmatrix}.
$$

A symbolic algorithm for solving SLAEs with a heptadiagonal coefficient matrix is considered. It is based on LU decomposition in which the system $Ax = y$ is rewritten as $LUx = y$, where $L$ and $U$ are a lower triangular and an upper triangular matrices, respectively. The algorithm consists of two steps – the $LU$ decomposition together with the downwards sweep $Lz = y$ happen during the first step, leading us from $Ax = y$ to $Ux = z$, while the upwards sweep (solving $Ux = z$ for $x$) is done during the second step.

Remark: seems that the expression for $g_{i-2}$ is missing in the for loop on p. 435 of [12]. Also, the expression for $k_1$ on p. 435 of the same paper is not used anywhere, so it is probably a leftover from a previous algorithm.

Now we shall formulate a symbolic algorithm for solving such a SLAE.

Algorithm 1. Symbolic algorithm for solving a SLAE $Ax = y$.

Input: $c^*, b^*, a^*, d, a, b, c, y, \varepsilon$

Output: $x$

1. if $\text{det}(A) = 0$ then
   2. Exit.
   3. end if
4. bool flag = False
5. $\mu_0 := d_0$ ▷ Step 1.(0)
6. if $|\mu_0| < \varepsilon$ then
   7. $\mu_0 := \text{symb}; \text{flag} = \text{True}$
   8. end if
9. $\alpha_0 := \frac{a_0}{\mu_0}$; $\beta_0 := \frac{b_0}{\mu_0}$; $\gamma_0 := \frac{c_0}{\mu_0}$; $\delta_0 := 0.0$
10. $\delta_1 := a_1^* + \alpha_0 \delta_1$; $\mu_1 := d_1 - \alpha_0 \delta_1$ ▷ (1)
11. if !flag then
12. if $|\mu_1| < \varepsilon$ then
13. $\mu_1 := \text{symb}; \text{flag} = \text{True}$
14. end if
15. end if
16. $\alpha_1 := \frac{a_1 - \beta_0 \delta_1}{\mu_1}$; $\beta_1 := \frac{b_1 - \gamma_0 \delta_1}{\mu_1}$; $\gamma_1 := \frac{c_1}{\mu_1}$
17. $\delta_2 := a_2^* - \alpha_0 b_2^*$; $\mu_2 := d_2 - \alpha_1 \delta_2 - \beta_0 b_2^*$ ▷ (2)
18. if !flag then
19. if $|\mu_2| < \varepsilon$ then
20. $\mu_2 := \text{symb}; \text{flag} = \text{True}$
21. end if
22. end if
23. $\alpha_2 := \frac{a_2 - \beta_1 \delta_2 - \gamma_0 b_2^*}{\mu_2}$; $\beta_2 := \frac{b_2 - \gamma_1 \delta_2}{\mu_2}$; $\gamma_2 := \frac{c_2}{\mu_2}$

2
24: \( z_0 := \frac{y_0}{\mu_0} \); \( z_1 := \frac{y_1 - \delta_1 z_0}{\mu_1} \); \( z_2 := \frac{y_2 - \delta_2 z_1 - b_2^* z_0}{\mu_2} \)

25: \( \xi_0 := 0.0 \); \( \xi_1 := 0.0 \); \( \xi_2 := 0.0 \)

26: for \( i = 3, \ldots, N - 4 \) do \( \triangleright \) (i)

27: \( \delta_i := a_i^* - \alpha_i - 2b_i^* - c_i^* (\beta_{1;i-3} - \alpha_{1;i-3}) \)

28: \( \xi_i := b_i^* - \alpha_i - 3c_i^* \)

29: \( \mu_i := d_i - \alpha_i - 1\delta_i - \beta_i - 2\xi_i - \gamma_i - 3c_i^* \)

30: if \( \text{flag} = \text{True} \)

31: if \( |\mu_i| < \varepsilon \) then

32: \( \mu_i := \text{symb}; \text{flag} = \text{True} \)

33: end if

34: end if

35: \( \alpha_i := \frac{a_i - \beta_{i-1} - \gamma_{i-2} \xi_i}{\mu_i}; \beta_i := \frac{b_i - \gamma_{i-1} \delta_i}{\mu_i}; \gamma_i := e_i \)

36: \( z_i := \frac{y_i - \delta_i z_{i-1} - \xi_i z_{i-2} - c_i^* z_{i-3}}{\mu_i} \)

37: end for

38: \( \delta_N-3 := a_N^* - \alpha_N - 3\delta_{N-3} - c_N^*(\beta_N - 6 - \alpha_N - 6\alpha_{N-5}) \)

39: \( \xi_N-3 := b_N^* - \alpha_N - 6c_N^* \)

40: \( \mu_N-3 := d_N - \alpha_N - 4\delta_{N-3} - \beta_{N-5} \xi_{N-3} - \gamma_N - 6c_{N-3} \)

41: if \( \text{flag} = \text{True} \)

42: if \( |\mu_{N-3}| < \varepsilon \) then

43: \( \mu_{N-3} := \text{symb}; \text{flag} = \text{True} \)

44: end if

45: end if

46: \( \alpha_N-3 := \frac{a_N-3 - \beta_{N-4} \delta_{N-3} - \gamma_{N-5} \xi_{N-3}}{\mu_{N-3}} \)

47: \( \beta_N-3 := \frac{b_N-3 - \gamma_{N-4} \delta_{N-3}}{\mu_{N-3}} \)

48: \( z_N-3 := \frac{y_{N-3} - \delta_{N-4} z_{N-4} - \xi_{N-3} \xi_{N-5} - c_{N-3}^* z_{N-6}}{\mu_{N-3}} \)

49: \( \delta_{N-2} := a_{N-2} - \alpha_N - 4\delta_{N-2} - c_{N-2}^* (\beta_{N-5} - 5 - \alpha_N - 5\alpha_{N-4}) \)

50: \( \xi_{N-2} := b_{N-2} - \alpha_N - 5c_{N-2} \)

51: \( \mu_{N-2} := d_{N-2} - \alpha_{N-3} \delta_{N-2} - \beta_{N-4} \xi_{N-2} - \gamma_{N-5} c_{N-2}^* \)

52: if \( \text{flag} = \text{True} \)

53: if \( |\mu_{N-2}| < \varepsilon \) then

54: \( \mu_{N-2} := \text{symb}; \text{flag} = \text{True} \)

55: end if

56: end if

57: \( \alpha_{N-2} := \frac{a_{N-2} - \beta_{N-3} \delta_{N-2} - \gamma_{N-4} \xi_{N-2}}{\mu_{N-2}} \)

58: \( z_{N-2} := \frac{y_{N-2} - \delta_{N-2} z_{N-3} - \xi_{N-2} \xi_{N-4} - c_{N-2}^* z_{N-5}}{\mu_{N-2}} \)

59: \( \delta_{N-1} := a_{N-1} - \alpha_N - 3\delta_{N-1} - c_{N-1}^* (\beta_{N-4} - 4 - \alpha_N - 4\alpha_{N-3}) \)

60: \( \xi_{N-1} := b_{N-1} - \alpha_N - 4c_{N-4} \)

61: \( \mu_{N-1} := d_{N-1} - \alpha_{N-2} \delta_{N-1} - \beta_{N-3} \xi_{N-1} - \gamma_{N-4} c_{N-1}^* \)

62: if \( \text{flag} = \text{True} \)

63: if \( |\mu_{N-1}| < \varepsilon \) then

64: \( \mu_{N-1} := \text{symb}; \text{flag} = \text{True} \)

65: end if

66: end if

67: \( \xi_{N-1} := \frac{y_{N-1} - \delta_{N-1} z_{N-2} - \xi_{N-1} \xi_{N-4} - c_{N-1}^* z_{N-5}}{\mu_{N-1}} \)

68: \( z_{N-1} := \frac{y_{N-1} - \xi_{N-1} z_{N-2} - \delta_{N-1} z_{N-3} - c_{N-1}^* z_{N-4}}{\mu_{N-1}} \)

69: \( \xi_{N-2} := \frac{y_{N-2} - \delta_{N-2} z_{N-3} - \xi_{N-2} \xi_{N-4} - c_{N-2}^* z_{N-5}}{\mu_{N-2}} \)

70: \( z_{N-3} := \frac{y_{N-3} - \delta_{N-3} z_{N-4} - \xi_{N-3} \xi_{N-5} - c_{N-3}^* z_{N-6}}{\mu_{N-3}} \)

71: for \( j = N - 4, \ldots, 0 \) do

72: \( x_j := \frac{z_j - \alpha_j x_{j+1} - \beta_j x_{j+2} - \gamma_j x_{j+3}}{\mu_{j+3}} \)
73: end for
74: Cancel the common factors in the numerators and denominators of \( x \), making them coprime.

Substitute \( \text{symb} := 0 \) in \( x \) and simplify.

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**Remark:** If any \( \mu_i \) expression has been evaluated to be zero or numerically zero, then it is assigned to be a symbolic variable. We cannot compare any of the next \( \mu \) expressions with \( \varepsilon \), because any further \( \mu \) is going to be a symbolic expression. To that reason, we use a boolean flag which tells us if any previous \( \mu \) is a symbolic expression. In that case, comparison with \( \varepsilon \) is not conducted as being not needed.

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### 3 Stability of the Algorithm

Some observations on the stability of the proposed algorithm can be made. Firstly, assigning \( \mu_i, i = 0, N-1 \) to be equal to a symbolic variable, then it is going to appear in both the numerator and the denominator of the expression for the determinant and so it can be cancelled:

\[
\det(A) = \frac{\mu_0}{\mu_i} \cdot \frac{\mu_1}{\mu_i} \cdot \ldots \cdot \frac{\mu_{N-2}}{\mu_i} \cdot \frac{\mu_{N-1}}{\mu_i} = \prod_{i=0}^{N-1} \mu_i
\]

This formula could be used so as the nonsingularity of the coefficient matrix to be checked.\( \Box \)

#### Theorem 1

The only requirement to the coefficient matrix so as the algorithm to be stable is nonsingularity.

**Proof.** As a direct consequence of the transformations done so as the matrix \( A \) to be factorized and then the downwards sweep to be conducted, it follows that the determinant of the matrix \( A \) in the terms of the introduced notation is:

\[
\det(A) = \prod_{i=0}^{N-1} \mu_i|_{\text{symb}=0}.
\]

(1)

If \( \mu_i \) for any \( i \) is assigned to be equal to a symbolic variable, then it is going to appear in both the numerator and the denominator of the expression for the determinant and so it can be cancelled:

\[
\begin{align*}
\det(A) &= \prod_{i=0}^{N-1} \mu_i
\end{align*}
\]

(2)

**Remark:** If any \( \mu_i \) expression has been evaluated to be zero or numerically zero, then it is assigned to be a symbolic variable. We cannot compare any of the next \( \mu \) expressions with \( \varepsilon \), because any further \( \mu \) is going to be a symbolic expression. To that reason, we use a boolean flag which tells us if any previous \( \mu \) is a symbolic expression. In that case, comparison with \( \varepsilon \) is not conducted as being not needed.

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### Acknowledgements

The work is partially supported by the Russian Foundation for Basic Research under project \#18-51-18005.
4 Conclusions

A symbolic algorithm for solving band matrix SLAEs with heptadiagonal coefficient matrices was presented in pseudocode. Some notes on the stability of the algorithm were made.

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