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ON A FINITE DIFFERENCE ANALOGUE OF A SINGULAR BOUNDARY VALUE PROBLEM

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Abstract. We consider a finite difference analogue for singularly perturbed boundary value problem obtained by the central difference scheme and the Hermite scheme on a special nonuniform mesh. The obtained systems of linear algebraic equations are solved using a method which is approximately three times faster than the usual method based on LU decomposition.

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1. Introduction

In this paper we shall consider numerical methods for solving a discrete analogue of nonlinear singularly perturbed boundary value problem

$$(1)\qquad \begin{gathered} -\varepsilon^2 u'' + c\,(x,u) = 0, \qquad x \in [0,1], \\ u\,(0) = u\,(1) = 0, \end{gathered}$$

where $\varepsilon \in (0, \varepsilon_0)$, $\varepsilon_0 \ll 1$, is a small perturbation parameter. Since under appropriate smoothness assumptions on c and the standard condition

$$(2)\qquad 0 < \gamma^2 \le c_u\,(x,u), \qquad x \in I, \qquad u \in \mathbf{R},$$

the solution u_ε to (1) has boundary layers at $x = 0$ and $x = 1$, it is necessary to use a special mesh discretization function which gives considerable amount of mesh points in these boundary layers. As a suitable mesh generating function we use the one from [6], and for approximation of $u''(x)$ at the mesh points we apply the standard central difference scheme and the Hermite scheme from [3].

In both cases, the corresponding discrete analogue can be written in the form

$$\begin{aligned} w_0 &= 0, \\ a_1\,(i)\,w_{i-1} + a_0\,(i)\,w_i + a_2\,(i)\,w_{i+1} &= b_1\,(i)\,c_{i-1} + b_0\,(i)\,c_i + b_2\,(i)\,c_{i+1}, \\ w_n &= 0, \end{aligned}$$

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where $i = 1, 2, \ldots, n-1$ and $c_i = c(x_i, w_i)$, $i = 1, 2, \ldots, n-1$. If we write this system of nonlinear equations as

$$Aw = H(w), \qquad A \in \mathbf{R}^{n-1,n-1}, \quad H : \mathbf{R}^{n-1} \to \mathbf{R}^{n-1},$$

its solution $w^* = [w_1, w_2, \ldots, w_{n-1}]^\top$ represents a numerical approximation to the solution u_ε of the problem (1). Using iterative method

$$Aw^{k+1} = H(w^k), \qquad k = 0, 1, \ldots,$$

with arbitrarily chosen w^0, the vectors $w^k = [w_1^k, w_2^k, \ldots, w_{n-1}^k]^\top$, $k = 0, 1, \ldots$, will be the approximations to the vector w^*.

Obviously, the next approximation w^{k+1} is obtained as a solution of the system of linear equations of the form $Az = d$. Sufficient conditions for the convergence of the sequence $\{w^k\}$ to the vector w^* can be found in [1]. In this paper we shall consider only calculation of the members of the sequence $\{w^k\}$, for a given w^0.

2. Mesh generating function and difference schemes

As a mesh generating function we shall use is the one from [6] given with

$$\text{(3)} \qquad \lambda(t) = \begin{cases} \mu(t) := \dfrac{a\varepsilon t}{q - t}, & t \in [0, \alpha], \\ \pi(t) := \mu(\alpha) + \mu'(\alpha)(t - \alpha), & t \in [\alpha, 0.5], \\ 1 - \lambda(1 - t), & t \in [0.5, 1], \end{cases}$$

where a and q are independent of ε, $q \in (0, 0.5)$, $a\varepsilon \leq q$. The value α represents the unique point from $(0, q)$, obtained from the condition $\pi(0.5) = 0.5$:

$$\alpha = \frac{q - \sqrt{aq\varepsilon(1 - 2q + 2a\varepsilon)}}{1 + 2a\varepsilon}.$$

Now, the discretization mesh is

$$I_h = \{x_i = \lambda(ih),\ i = 0, 1, \ldots, n\}, \qquad h = \frac{1}{n}.$$

As mentioned above, for approximation of $-\varepsilon^2 u''(x_i)$ we shall use the Hermite scheme with the coefficients

$$a_1(i) = \frac{2\varepsilon^2}{h_i(h_i + h_{i+1})}, \qquad a_0(i) = -\frac{2\varepsilon^2}{h_i h_{i+1}}, \qquad a_2(i) = -a_0(i) - a_1(i),$$

$$b_1(i) = -a_1(i)\,\frac{h_i^2 - h_{i+1}^2 + h_{i+1}h_i}{12}, \qquad b_0(i) = a_0(i)\,\frac{h_i^2 + h_{i+1}^2 + 3h_{i+1}h_i}{12},$$

$$b_2(i) = 1 - b_0(i) - b_1(i),$$

where $h_i = x_i - x_{i-1}$, $i = 1, 2, \ldots, n$. For the central difference scheme it holds

$$b_1(i) = b_2(i) = 0, \qquad b_0(i) = 1,$$

and the coefficinets $a_1(i)$, $a_0(i)$, $a_2(i)$ are the same as in the Hermite scheme.

3. Discrete analogue

For the vector w^k, let $d_i = H(w_i^k)$, $i = 1, 2, \ldots, n-1$, and

$$d = [d_1, d_2, \ldots, d_{n-1}]^\top .$$

The vector w^{k+1} can be obtained as a solution z of the system $Az = d$ with the tridiagonal matrix

$$A = \begin{bmatrix} a_0(1) & a_2(1) & & & & \\ a_1(2) & a_0(2) & a_2(2) & & & \\ & & \cdots & \cdots & \cdots & \\ & & & a_1(n-2) & a_0(n-2) & a_2(n-2) \\ & & & & a_1(n-1) & a_0(n-1) \end{bmatrix}.$$

This system can be solved using the well known LU decomposition

$$\begin{aligned} \alpha_1 &= a_0(1), \\ \beta_k &= \frac{a_1(k)}{\alpha_{k-1}}, \qquad \alpha_k = a_0(k) - \beta_k a_2(k-1), \qquad k = 2, 3, \ldots, n-1, \end{aligned}$$

$$\begin{aligned} f_1 &= d_1, \\ f_k &= d_k - \beta_k f_{k-1}, \qquad k = 2, 3, \ldots, n-1, \end{aligned}$$

$$\begin{aligned} z_{n-1} &= \frac{f_{n-1}}{\alpha_{n-1}}, \\ z_k &= \frac{f_k - a_2(k)\, z_{k+1}}{\alpha_k}, \qquad k = n-2, n-3, \ldots, 1. \end{aligned}$$

The coefficients of the matrix A are very complex since they depend on the parameters n, q, a and ε. This results in great use of the CPU time, where the total time for finding the vector z is a sum of the time needed for calculating the coefficients and the time for solving the corresponding linear system. The aim of our paper is to transform the system $Az = d$ into an equivalent system which can be solved much faster. Analyzing its structure, the matrix A can be represented as a product of two diagonal matrices and one matrix with constant coefficients. For this transformation we shall use very much the package *Mathematica 3.0.*

4. Block LU decomposition

For fixed n, q, a and ε, where n is an even number, first we calculate the parameter α, and then define $m = \lfloor n\alpha - 1 \rfloor$ and $k = n - 2m - 5$. We split the matrix A and the vector d into blocks in the following way:

$$\begin{bmatrix} A_1 & C_1 & & & & & \\ B_2 & A_2 & C_2 & & & & \\ & B_3 & A_3 & C_3 & & & \\ & & B_4 & A_4 & C_4 & & \\ & & & B_5 & A_5 & C_5 & \\ & & & & B_6 & A_6 & C_6 \\ & & & & & B_7 & A_7 \end{bmatrix}, \quad \begin{bmatrix} D_1 \\ D_2 \\ D_3 \\ D_4 \\ D_5 \\ D_6 \\ D_7 \end{bmatrix},$$

with the dimensions of the blocks

i	m_i	A_i	B_i	C_i	D_i
1	m	$m \times m$	$-$	$m \times 1$	$m \times 1$
2	1	1×1	$1 \times m$	1×1	1×1
3	1	1×1	1×1	$1 \times k$	1×1
4	k	$k \times k$	$k \times 1$	$k \times 1$	$k \times 1$
5	1	1×1	$1 \times k$	1×1	1×1
6	1	1×1	1×1	$1 \times m$	1×1
7	m	$m \times m$	$m \times 1$	$-$	$m \times 1$

For solving the system $Az = d$ we can also use the block LU decomposition which has the form

$$\begin{aligned} \alpha_1 &= A_1, \\ \beta_k &= B_k \alpha_{k-1}^{-1}, \quad \alpha_k = A_k - \beta_k C_{k-1}, \qquad k = 2, 3, \ldots, 7, \end{aligned}$$

$$\begin{aligned} f_1 &= D_1, \\ f_k &= D_k - \beta_k f_{k-1}, \qquad k = 2, 3, \ldots, 7, \end{aligned}$$

$$\begin{aligned} Z_7 &= \alpha_7^{-1} f_7, \\ Z_k &= \alpha_k^{-1}(f_k - C_k Z_{k+1}), \qquad k = 6, 5, \ldots, 1. \end{aligned}$$

The solution z is a vector with the block components $Z_1, Z_2, \ldots, Z_7$. Matrices α_1, α_4 and α_7 have the same dimensions as the matrices A_1, A_4 and A_7 respectively. This means that for calculating Z_1, Z_4 and Z_7 we have to find the inverses of α_1, α_4 and α_7, and of course, spend much more CPU time than when using LU decomposition described in the previous section.

5. Our method

Using *Mathematica*, after arranging very complex expressions for the elements of the matrix A, we obtain the following factorization

$$A = PWQ,$$

where $g = P^{-1}d = [G_1, G_2, \ldots, G_7]^{\top}$,

$$W = \begin{bmatrix} R_1 & T_1 & & & & & \\ S_2 & R_2 & T_2 & & & & \\ & S_3 & R_3 & T_3 & & & \\ & & S_4 & R_4 & T_4 & & \\ & & & S_5 & R_3 & S_3 & \\ & & & & T_2 & R_2 & T_6 \\ & & & & & S_7 & R_7 \end{bmatrix},$$

and R_1, R_4 and R_7 are the matrices with the dimensions $m \times m$, $k \times k$, $m \times m$ respectively, of the form

$$\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}.$$

The rest of the blocks are given with

$$\begin{aligned} S_2 &= [0, 0, \ldots 0, -1]_{1\times m}, \qquad T_3 = [-1, 0, \ldots, 0]_{1\times k}, \\ S_5 &= [0, 0, \ldots 0, -1]_{1\times k}, \qquad T_6 = [-1, 0, \ldots, 0]_{1\times m}, \\ T_1 &= S_2^{\top}, \qquad S_4 = T_3^{\top}, \qquad T_4 = S_5^{\top}, \qquad S_7 = T_6^{\top}. \end{aligned}$$

The elements of 1×1 matrices R_2, R_3, S_3 and T_2, can be calculated explicitly

$$\begin{aligned} \sigma &= hq - h^2m^2 - 3h^2m + 2\alpha hm - 2h^2 + 2\alpha h - \alpha^2, \\ R_2 &= \frac{2hq - h^2m^2 - 2h^2m + 2\alpha hm - \alpha^2}{\sigma}, \\ R_3 &= \frac{2hq - h^2m^2 - 4h^2m + 2\alpha hm - 3h^2 + 2\alpha h - \alpha^2}{\sigma}, \\ T_2 &= \frac{-h(q-\alpha)^2}{\sigma}, \quad S_3 = \frac{-h}{\sigma}. \end{aligned}$$

The matrices P and Q are diagonal matrices with the elements p_i and q_i respectively, given with

$$s_i = \begin{cases} q - ih, & i = 1, 2, \ldots, m+1, \\ 1, & i = m+2, m+3, \ldots, n/2, \end{cases}$$

$$p_i = \frac{1}{(aqh)^2}\begin{cases} s_{i-1}s_is_{i+1}, & i = 1,2,\ldots,m, \\ \frac{2(\alpha-q)^2 s_m s_{m+1}}{-h(m+1-n\alpha)^2+h+2(q-\alpha)}, & i = m+1, \\ \frac{2(\alpha-q)^4 s_{m+1}}{-h(m+2-n\alpha)^2+h+2(q-\alpha)}, & i = m+2, \\ (\alpha-q)^4, & i = m+3,\ldots,m+2+k, \\ p_{n-i}, & i = m+3+k,\ldots,n-1, \end{cases}$$

$$q_i = \begin{cases} s_i^{-1}, & i = 1,2,\ldots,m+1, \\ 1, & i = m+2,\ldots,m+3+k, \\ q_{n-i}, & i = m+4+k,\ldots,n-1. \end{cases}$$

Using the described factorization, the new system which is equivalent to $Az = d$ is $Wy = g$, where $y = Qz$ and $g = P^{-1}d$. It can be solved using block LU decomposition and the vector z is obtained from $z = Q^{-1}y$. The special structure of the matrix W makes it possible to avoid inverting of the matrices R_1, R_4 and R_7.

According to the formulae for block LU decomposition, we have

$$\begin{aligned} \alpha_1 &= R_1, \\ \beta_2 &= S_2R_1^{-1} = -[\alpha_{m1}, \alpha_{m2}, \ldots, \alpha_{mm}], \end{aligned}$$

where α_{ij} are elements of the matrix R_1^{-1}, (see [5]), given with

$$\alpha_{ij} = \frac{1}{m+1}\begin{cases} i(m+1-j), & i \le j, \\ j(m+1-i), & j \le i. \end{cases}$$

Further we have

$$\begin{aligned} \alpha_2 &= R_2 - \beta_2T_1 = R_2 - \alpha_{mm}, \\ \beta_3 &= \frac{S_3}{\alpha_2}, \qquad \alpha_3 = R_3 - \beta_3T_2, \\ \beta_4 &= \frac{1}{\alpha_3}S_4 = \left[-\alpha_3^{-1}, 0, \ldots, 0\right]^\top, \end{aligned}$$

$$\alpha_4 = R_4 - \beta_4\left[-1,0,\ldots,0\right]_{1\times k} = \begin{bmatrix} 2-\alpha_3^{-1} & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}_{k\times k},$$

$$\beta_5 = [0, \ldots 0, -1]_{1\times k}\, \alpha_4^{-1} = -\left[\gamma_{k1}, \gamma_{k2}, \ldots, \gamma_{kk}\right].$$

The elements γ_{ij} of the matrix α_4^{-1} can be calculated from the Sherman–Morrison–Woodbury formula, [4],

$$\left(A + uv^\top\right)^{-1} = A^{-1} - \frac{1}{1 + v^\top A^{-1} u} A^{-1} u v^\top A^{-1},$$

where u and v are vectors with dimensions equal to the order of the matrix α_4. In our case, $u = \beta_4$ and $v = [-1, 0, \ldots, 0]_{1\times k}$, hence

$$\gamma_{ij} = \frac{1}{k + 1 - kx} \begin{cases} (x\,(i-1) - i)\,(k+1-j), & i \le j, \\ (x\,(j-1) - j)\,(k+1-i), & j \le i, \end{cases}$$

with $x = \alpha_3^{-1}$. Finally

$$\alpha_5 = R_3 - \beta_5 \begin{bmatrix} 0 \\ \vdots \\ 0 \\ -1 \end{bmatrix}_{k\times 1} = R_3 - \gamma_{kk},$$

$$\beta_6 = \frac{T_6}{\alpha_5}, \qquad \alpha_6 = R_6 - \beta_6 S_3,$$

$$\beta_7 = \frac{1}{\alpha_6} \begin{bmatrix} -1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}_{m\times 1} = \begin{bmatrix} -\alpha_6^{-1} \\ 0 \\ \vdots \\ 0 \end{bmatrix}_{m\times 1},$$

$$\alpha_7 = R_7 - \beta_7 [-1, 0, \ldots, 0]_{1\times m} = \begin{bmatrix} 2 - \alpha_6^{-1} & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix}_{m\times m}.$$

Using the auxiliary vectors

$$\begin{aligned} f_1 &= G_1, \\ f_k &= G_k - \beta_k f_{k-1}, \qquad k = 2, 3, \ldots, 7, \end{aligned}$$

the components $y_1, y_2, \ldots, y_7$ of the block vector y can be easily obtained. First of all, applying LU decomposition to the $m \times m$ system $\alpha_7 y_7 = f_7$, we obtain the vector y_7. Let $y_7^{[1]}$ be the first component of y_7. Then

$$y_6 = \frac{f_6 + y_7^{[1]}}{\alpha_6}, \qquad y_5 = \frac{f_5 - S_3 y_6}{\alpha_5},$$

and the vector y_4 is the solution of the $k \times k$ system

$$\alpha_4 y_4 = F_4 = f_4 + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ y_5 \end{bmatrix}.$$

Further

$$y_3 = \frac{f_3 + y_4^{[1]}}{\alpha_3}, \qquad y_2 = \frac{f_2 - T_2 y_3}{\alpha_2},$$

where $y_4^{[1]}$ represents the first component of the vector y_4. Finally, solving the $m \times m$ system

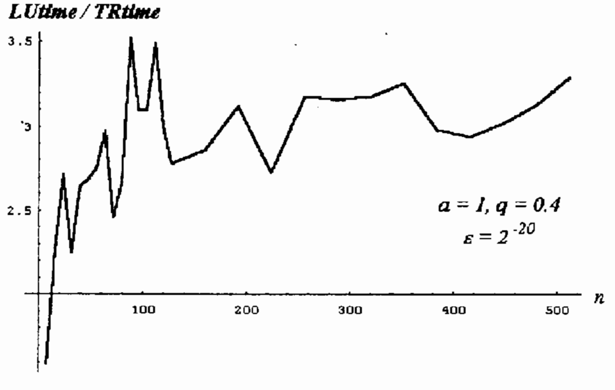
$$\alpha_1 y_1 = F_1 = f_1 + \begin{bmatrix} 0 \\ \vdots \\ 0 \\ y_2 \end{bmatrix},$$

we obtain the vector y_1. The dimension of the vector $y = [y_1, y_2, \ldots, y_7]^\top$ is $n-1$, and putting $z = Q^{-1}y$ we obtain the solution of the system $Az = d$.

6. Comparison of the methods

Let *LUtime* represents the CPU time needed for forming and solving the system $Az = d$ using the LU decomposition, and let *TRtime* be the CPU time needed for forming and solving the system $Wy = g$ and calculating the vector $z = Q^{-1}y$.

In the figure below is shown the ratio *LUtime/TRtime* as a function of dimension of the system $Az = d$. We can see that for solving the system $Az = d$ using direct LU decomposition requires approximately three times more CPU time than our method. The results were approximately equal when using the central difference scheme and the Hermite scheme, since the CPU time needed for forming the vector d in *Mathematica* alters only slightly.



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