Pseudospectral method for numerical solution of DAEs with an error estimation

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Abstract

In [E. Babolian, M.M. Hosseini, Reducing index, and pseudospectral methods for differential-algebraic equations, Appl. Math. Comput. 140 (2003) 77–90], numerical solution of linear differential-algebraic equations (DAEs) has been presented by pseudospectral method. In this paper, a new error estimation technique is proposed to pseudospectral method such that is well done for linear semi-explicit DAEs. When the DAEs has index 2, the obtained approximate solution can be improved by using the proposed error estimation technique. Furthermore, with providing some examples the proposed error estimation method is dealt with numerically.

Keywords: Differential-algebraic equations; Pseudospectral method

1. Introduction

It is well known that differential-algebraic equations (DAEs) can be difficult to solve when they have a higher index, i.e., an index greater than one [1]. Higher index DAEs are ill posed and an alternative treatment is the use of
index reduction methods [2,5,6,8,9,15]. In [4,11,12], a new reducing index method has been proposed which had not need to the repeated differentiation of the constraint equations. This method has been well applied for DAEs with and without constraint singularities and the $m+1$-index DAEs has been reduced to $m$-index DAEs problem. Also, for numerical solving, pseudospectral method has been used. In this paper, for this numerical solution, a new error estimation technique is proposed such that is well done for linear semi explicit DAEs. This technique can simply be extended to DAEs with constraint singularities (mentioned in [11,12]).

It is known that the eigenfunctions of certain singular Sturm–Liouville problems allow the approximation of functions in $C^\infty[a,b]$ where truncation error approaches zero faster than any negative power of the number of basic functions used in the approximation, as that number (order of truncation $N$) tends to infinity [7]. This phenomenon is usually referred to as “spectral accuracy” [10]. The accuracy of derivatives obtained by direct, term-by-term differentiation of such truncated expansion naturally deteriorates [7], but for low-order derivatives and sufficiently high order truncations this deterioration is negligible, compared to the restrictions in accuracy introduced by typical difference approximations (for more details, refer to [3,7,13]). Throughout, we are using first kind orthogonal Chebyshev polynomials \( \{T_k\}_{k=0}^\infty \) which are eigenfunctions of singular Sturm–Liouville problem:

\[
(\sqrt{1-x^2}T'(x))' + \frac{k^2}{\sqrt{1-x^2}}T_k(x) = 0.
\]

2. DAEs with and without constraint singularities

Consider a linear (or linearized) model problem:

\[
X^{(m)} = \sum_{j=1}^{m} A_j X^{(j-1)} + By + q, \quad \text{(1a)}
\]

\[
CX = r, \quad \text{(1b)}
\]

where $A_j$, $B$ and $C$ are smooth functions of $t$, $t_0 \leq t \leq t_f$, $A_j(t) \in R^{m\times n}$, $j = 1, \ldots, m$, $B(t) \in R^n$, $C(t) \in R^{1\times n}$, $n \geq 2$, and $CB$ is nonsingular (the DAE has index $m+1$) except possibly at a finite number of isolated points of $t$. For simplicity of exposition, let us say that there is one singularity point $t^*$, $t_0 \leq t^* \leq t_f$. The inhomogeneities are $q(t) \in R^n$ and $r(t) \in R$. Now, if $CB(t) \neq 0$, $t_0 \leq t \leq t_f$, then we say DAEs has not constraint singularity but DAEs has constraint singularities, if $CB(t) = 0$ at a finite number of isolated points of $t$, $t_0 \leq t \leq t_f$. 

In many methods which has been used for the linear model problem (1), the following accordingly are assumed [1],

H1: The matrix function \( P = B(CB)^{-1}C \) is smooth or, more precisely, \( P \) is continuous and \( P' \) is bounded near the singular point \( t^* \), where we define

\[
P(t_* = \lim_{t \to t_*} (B(CB)^{-1}C)(t).
\]

H2: The inhomogeneity \( r(t) \) satisfies \( r \in S \), where

\[
S = \{ w(t) \in \mathbb{R}^n : \text{there exist a smooth function } z(t) \text{ s.t. } Cz = w \}.
\]

We note that H1 and H2 are satisfied automatically if \( CB \) is nonsingular for each \( t \). We also indicate that here only need the continuity of \( P \).

3. Implementation of numerical method

Here, the implementation of pseudospectral method is presented for DAEs system (1), when \( m = 1 \) and \( n = 2 \). This discussion can simply be extended to general form (1) (with and without singularities). Now consider the DAEs system,

\[
\begin{align*}
X' - AX - By &= q, \quad (3a) \\
CX &= r(t), \quad (3b)
\end{align*}
\]

where

\[
X = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}, \quad A = \begin{bmatrix} a_{11}(t) & a_{12}(t) \\ a_{21}(t) & a_{22}(t) \end{bmatrix}, \quad B = \begin{bmatrix} b_1(t) \\ b_2(t) \end{bmatrix},
\]

\[
q = \begin{bmatrix} q_1(t) \\ q_2(t) \end{bmatrix}, \quad C = [c_1(t) \ c_2(t)],
\]

with boundary condition,

\[
x_1(t_0) + x_2(t_f) = \alpha, \quad (4)
\]

For an arbitrary natural number \( v \), we suppose that the approximate solution of DAEs system (3) is as below:

\[
x_1(t) = \sum_{i=0}^{v} a_i T_i(s), \quad (5a)
\]

\[
x_2(t) = \sum_{i=0}^{v} a_{v+i+1} T_i(s), \quad s \in [-1, 1], \quad (5b)
\]
\[ y(t) = \sum_{i=0}^{v} a_{2i+i+2} T_i(S), \quad (5c) \]

where
\[ t = h(s) = \frac{t_f - t_0}{2} s + \frac{t_f + t_0}{2}, \quad (6) \]

where \( a = (a_0, \ldots, a_{3v+2})^T \in R^{3v+3} \) and \( \{T_k\}_{k=0}^{v} \) is sequence of Chebyshev polynomials of the first kind. Here, the main purpose is to find \( a = (a_0, \ldots, a_{3v+2})^T \).

Now, by using the variation of variables (6) we rewrite system (3), as below,
\[
\frac{ds}{dt} x'_1 - a_{11}(h(s))x_1 - a_{12}(h(s))x_2 - b_1(h(s))y = q_1(h(s)),
\]
\[
\frac{ds}{dt} x'_2 - a_{21}(h(s))x_1 - a_{22}(h(s))x_2 - b_2(h(s))y = q_2(h(s)), \quad s \in [-1, 1], \quad (7a)
\]
\[
c_1(h(s))x_1 + c_2(h(s))x_2 = r(h(s)). \quad (7c)
\]

Substituting (5) into (7), implies that (for more details refer to [3,4]),
\[
\sum_{i=0}^{3v+2} a_i \Phi_i(s) = q_1(h(s)), \quad (8a)
\]
\[
\sum_{i=0}^{3v+2} a_i \overline{\Phi}_i(s) = q_2(h(s)), \quad (8b)
\]
\[
\sum_{i=0}^{3v+2} a_i \Gamma_i(s) = r(h(s)). \quad (8c)
\]

Now, by substituting Chebyshev–Guass–Lobato points [7],
\[
s_j = \cos \left( \frac{j\pi}{v+1} \right), \quad j = 0, 1, \ldots, v, \quad (9a)
\]
into (8a) and (8b), and
\[
s_j = \cos \left( \frac{j\pi}{v} \right), \quad j = 0, 1, \ldots, v - 1, \quad (9b)
\]

into (8c), a linear system with \( 3v + 2 \) equations and \( 3v + 3 \) unknowns is obtained. To construct the remaining 1 equations (by attending to boundary condition (4)), we put,
\[
x_1(-1) + x_2(1) = \alpha,
\]
to obtain 1 equations. In addition, according to boundary (or initial) conditions, the collocation points can be chosen by different manners in (9).
4. An error estimation technique for pseudospectral method

Suppose that DAE (3) is solved by pseudospectral method and

\[ x_1(t) = \sum_{i=0}^{v} a_i T_i(t), \]  
\[ x_2(t) = \sum_{i=0}^{v} a_{i+1} T_i(t), \]  
\[ y_v(t) = \sum_{i=0}^{v} a_{2v+i} T_i(t) \]

are obtained. So, we have,

\[ X'_v - AX_v - By_v \equiv q \]  
\[ CX_v \equiv r(t) \]

with boundary condition,

\[ x_1(t_0) + x_2(t_f) = \alpha. \]

Now, we define \( E_v(t) \) and \( F_v(t) \) as below:

\[ E_v(t) = X'_v - AX_v - By_v - q, \]
\[ F_v(t) = CX_v - r(t). \]

By considering (3) and (13), we have

\[ e'_{xy} - Ae_{xy} - Be_{yv} = -E_v(t), \]
\[ Ce_{xy} = -F_v(t), \]
\[ e_{xy}(t_0) + e_{yv}(t_f) = 0, \]

where \( e_{xy} = X - X_v, e_{yv} = y - y_v \).

Here, we call \( e_{xy}(t) \) and \( e_{yv}(t) \) as error functions. Now, if we put,

\[ \bar{e}_{xy}(t) = \sum_{i=0}^{v} \bar{a}_i T_i(t), \]
\[ \bar{e}_{x2v} = \sum_{i=0}^{v} \bar{a}_{i+1} T_i(t), \]
\[ \bar{e}_{yv}(t) = \sum_{i=0}^{v} \bar{a}_{2v+i} T_i(t), \]
(8) implies that,
\begin{align}
\sum_{i=0}^{3v+2} \bar{a}_i \bar{\Phi}_i(s) & \equiv -E_{1v}(h(s)), \\
\sum_{i=0}^{3v+2} \bar{a}_i \bar{\Psi}_i(s) & \equiv -E_{2v}(h(s)), \\
\sum_{i=0}^{3v+2} \bar{a}_i \Gamma_i(s) & \equiv -F_{v}(h(s)).
\end{align}

(16a) (16b) (16c)

Now we put
\begin{align}
\sum_{i=0}^{3v+2} \bar{a}_i \bar{\Phi}_i(s) & = -E_{1v}(h(s)), \\
\sum_{i=0}^{3v+2} \bar{a}_i \bar{\Psi}_i(s) & = -E_{2v}(h(s)), \\
\sum_{i=0}^{3v+2} \bar{a}_i \Gamma_i(s) & = -F_{v}(h(s)),
\end{align}

(17a) (17b) (17c)

\[ e_{x_{1v}}(-1) + e_{x_{2v}}(1) = 0. \]

(17d)

By substituting the collocation points (9) into (17) and with solving the obtained linear system, the \( \bar{e}_v(t) \) will be determined. But, in this manner, \( \bar{e}_v(t) \) cannot appropriately estimate the error function \( e_v(t) \), because we obtained \( X_v(t) \) and \( y_v(t) \) by substituting the collocation points (9) and again, we used of these points to compute \( E_v(t) \) and \( F_v(t) \). So the norm of obtained \( E_v(t) \) and \( F_v(t) \) will be very small and \( \bar{a} = (\bar{a}_1, \bar{a}_2, \ldots, \bar{a}_{3v+3}) \in \mathbb{R}^{3v+3} \), and consequently \( \bar{e}_v(t) \), will be approximately obtained as vanish (the similar result obtain when we use of the proposed algorithm mentioned in [14]). To remove this difficulty, we note to this fact, relation (13) is defined for every points belong to \([-1, 1]\), so, for computing \( \bar{e}_v(t) \), we can use of other appropriate points. For this reason, consider the \((v+1)\) zero points of \( T_{v+1}(x) \), i.e.,

\[ x_k = \cos \left( \frac{(2k+1)\pi}{2v+2} \right), \quad k = 0, 1, 2, \ldots, v, \]

(18a)

and the \( v \)-zero points of \( T_v(t) \), i.e.,

\[ x_k = \cos \left( \frac{(2k+1)\pi}{2v} \right), \quad k = 0, 1, 2, \ldots, v - 1. \]

(18b)
Here, every points of (18a) is exactly between two points of (9a) and every points of (18b) is exactly between two points of (9b) [7,10]. Now by substituting points (18) into (17) and with solving the obtained linear system, the obtained $e_m(\tau)$ will be appropriately estimated the error function $e(\tau)$. Here, we conclude that obtained approximate solution is not well if the $e_m(\tau)$ has a large norm value (specially occurred, when DAEs has index 2). In this case, if we introduce $X = X_m + e_x$ and $y = y_m + e_y$, the obtained solutions are more appropriate than $X$ and $y$. In Section 4 some examples are solved by above techniques and the presented discusses are numerically illustrated.

5. Numerical examples

Early in [4], some index 2 DAEs have been considered. They have been transformed to index 1 problem and solved by pseudospectral method. Here again, these problems are considered and proposed error estimation technique in Section 3, is applied for them. Furthermore for 2-index DAEs, since $e_m(\tau)$ has a large norm, the new approximate solutions $X = X_m + e_x$ and $y = y_m + e_y$ are computed and the results show that the $X$ and $y$ are quietly more appropriate than $X$ and $y$. In general, for 2-index DAEs and their reduced index DAEs, the proposed error estimation technique are applied and the results show the advantage using this technique for these problems. In this section $\lambda \geq 1$ is a parameter. Also the maximum norms are approximately obtained through their graphs and the pseudospectral method is performed by using Maple 8 with 20 digits precision.

Example 1 [4]. Consider for $0 \leq t \leq 1$,

$$x_1' = \left(\lambda - \frac{1}{2-t}\right)x_1 + (2-t)\lambda y + q_1(t),$$

$$x_2' = \frac{\lambda - 1}{2-t}x_1 - x_2 + (\lambda - 1)y + q_2(t),$$

$$0 = (t + 2)x_1 + (t^2 - 4)x_2 + r(t)$$

with $x_1(0) = 1$. The inhomogeneities $q$ and $r$ are chosen to be

$$q(t) = \left(\frac{3-t}{2-t}e^t\right), \quad r(t) = -(t^2 + t - 2)e^t,$$

so that the exact solution is $x_1(t) = e^t, \ x_2(t) = e^t, \ y(t) = -\frac{e^t}{2-t}$.

This problem has index 2. In Table 1, we record results of running pseudospectral method and the proposed error estimation technique, when $\lambda = 100$. 

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For this example, the obtained estimated error \( \tilde{e}_v(t) \) is quietly closed to exact error function \( e_v(t) \) and the new approximate solutions \( \tilde{X} = X_v + e_{Xv} \) and \( \tilde{y} = y_v + e_{Yv} \) are more appropriate than \( X_v \) and \( Y_v \), respectively. In addition the reducing index method (mentioned in [4,12]) is applied for this problem and the obtained 1-index DAEs is solved using pseudospectral method, Table 2.

Table 2 shows that the estimated errors which are obtained through proposed error estimation technique, are closed to exact errors.

Example 2. [4]. Consider for \( 0 \leq t \leq 1 \),

\[
\begin{align*}
    x'_1 &= (2 - t)\lambda y + q_1(t), \\
    x'_2 &= (\lambda - 1)y + q_2(t), \\
    0 &= (t + 2)x_1 + (r^2 - 4)x_2 + r(t)
\end{align*}
\]

with \( x_1(0) = 1 \). The inhomogeneities \( q \) and \( r \) are chosen to be

\[
q(t) = \begin{pmatrix}
    (1 - \lambda)e' \\
    (1 + \frac{\lambda}{2-t})e'
\end{pmatrix}, \\
R(t) = -(t^2 + t - 2)e',
\]

such that the exact solution is \( x_1(t) = e' \), \( x_2(t) = e' \), \( y(t) = -\frac{e'}{2-t} \).

This problem has index 2 and is solved by using pseudospectral method with \( \lambda = 1000 \), Table 3.

Also the above problem is transformed to 1-index problem by reducing index method (mentioned in [4,12]) and the obtained problem is solved by pseudospectral method, Table 4.
So, by using the proposed technique (mentioned in Section 3), it can appropriately be determined the degree of accuracy of the approximate solution.

References


