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Collocation Schemes for Nonlinear Index 1 DAEs with a Singular Point

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Abstract. We discuss the convergence behavior of collocation schemes applied to approximate solutions of BVPs in nonlinear index 1 DAEs, which exhibit a critical point at the left boundary. Such a critical point of the DAE causes a singularity in the inherent nonlinear ODE system. In particular, we focus on the case when the inherent ODE system is singular with a *singularity of the first kind* and apply polynomial collocation to the *original DAE system*. We show that for a certain class of well-posed boundary value problems in DAEs having a sufficiently smooth solution, the global error of the collocation scheme converges in the collocation points with the so-called stage order. The theoretical results are supported by numerical experiments.

Keywords: Nonlinear differential-algebraic equations; Index 1; 0-critical points; Collocation methods; Convergence
PACS: 02.60.Lj; 02.70.Jn

In this paper we discuss the nonlinear boundary value problem for a system of DAEs given in the following form:

$$f((D(t)x(t))', x(t), t) = 0, \quad t \in (0,1], \quad B_0 D(0)x(0) + B_1 D(1)x(1) = \beta, \tag{1}$$

where $f(y,x,t) \in \mathbb{R}^m$, $D(t) \in \mathbb{R}^{n\times m}$, $y \in \mathbb{R}^n$, $x \in \mathscr{D}$, with $\mathscr{D} \subseteq \mathbb{R}^m$ open, $t \in [0,1]$, $n \leq m$. The data f, f_y, f_x, D are assumed to be at least continuous on their definition domains. Moreover, we require that

$$\ker f_y(y,x,t) = 0, \quad (y,x,t) \in \mathbb{R}^n \times \mathscr{D} \times (0,1], \tag{2}$$

$$\mathscr{R}(D(t)) = \mathbb{R}^n, \quad t \in [0,1]. \tag{3}$$

Conditions (2) and (3) guarantee that the matrix $D(t)$ has constant full row rank n on the closed interval while $f_y(y,x,t)$ has full column rank n on $\mathbb{R}^n \times \mathscr{D} \times (0,1]$, respectively. At $t = 0$ the matrix $f_y(y,x,t)$ may undergo a rank drop. This means that the system (1) has a properly stated leading term on $\mathbb{R}^n \times \mathscr{D} \times (0,1]$, cf. [1]. We consider solutions in the function space

$$C_D^1([0,1],\mathbb{R}^m) := \{x \in C([0,1],\mathbb{R}^m) : Dx \in C^1([0,1],\mathbb{R}^n)\}.$$

We now define

$$N_0(t) := \ker D(t), \quad t \in [0,1], \tag{4}$$

and note that owing to the properties of the leading term, cf. (2), (3),

$$\ker f_y(y,x,t)D(t) = N_0(t), \quad (y,x,t) \in \mathbb{R}^n \times \mathscr{D} \times (0,1].$$

Let us denote by Q_0 a continuous pointwise projector function onto $\ker D$, $Q_0(t)^2 = Q_0(t)$, $\mathscr{R}(Q_0(t)) = \ker D(t)$, $t \in [0,1]$, and let $P_0(t) := I - Q_0(t)$. Moreover, let us define

$$G_0(y,x,t) := f_y(y,x,t)D(t), \quad (y,x,t) \in \mathbb{R}^n \times \mathscr{D} \times [0,1], \tag{5}$$

$$G_1(y,x,t) := G_0(y,x,t) + f_x(y,x,t)Q_0(t), \quad (y,x,t) \in \mathbb{R}^n \times \mathscr{D} \times [0,1]. \tag{6}$$

In the following we discuss DAEs (1) which are regular with tractability index 1 on $\mathbb{R}^n \times \mathscr{D} \times (0,1]$. Consequently, $G_1(y,x,t)$ is nonsingular on $\mathbb{R}^n \times \mathscr{D} \times (0,1]$, see [2]. However, we permit a singular behavior of $G_1(y,x,t)$ for $t \to 0$, causing a singularity of the first kind in the associated *inherent ODE*. To this end, we assume that $tG_1(y,x,t)^{-1}$ has a continuous extension on $\mathbb{R}^n \times \mathscr{D} \times [0,1]$ [3]. The above assumptions result in the following form of the associated inherent ODE system:

$$u'(t) = \frac{1}{t}M(t)u(t) + h(u(t),t), \quad t \in (0,1], \quad B_0u(0) + B_1u(1) = \beta, \quad u \in C[0,1]. \tag{7}$$

Depending on the spectrum of the matrix $M(0)$, we generally encounter unbounded contributions to the solution manifold, such that $x \in C(0,1]$. However, irrespective of the eigenvalues of $M(0)$, by posing proper homogeneous initial conditions equivalent to $M(0)x(0) = 0$, we can ensure $x \in C[0,1]$. The system is then augmented by two-point boundary conditions to define a locally unique solution. If all the eigenvalues of $M(0)$ have negative real parts or are equal to zero, the boundary value problem can equivalently be posed as an initial value problem, making a shooting approach possible for both theoretical and practical purposes. Results on the extension of collocation techniques developed in the context of singular explicit ODEs to DAEs were first discussed for linear index 1 DAEs in [4].

Our decision to use polynomial collocation was motivated by its advantageous convergence properties for (7), while in the presence of a singularity other high order methods show order reductions and become inefficient. Convergence of collocation schemes applied to solve (7) with a singularity of the first kind was analyzed in [5, 6, 7]. It turns out that for k general interior collocation points, both the uniform convergence order and the order at the mesh points is equal to k. For the distribution of the collocation points such that superconvergence is observed for regular problems with smooth solutions, e.g. Gaussian points or an odd number of equidistant nodes, for problems with a singularity of the first kind the convergence order generally is $k+1$, both uniformly in t and at the mesh points. The usual high-order superconvergence at the mesh points does not hold in general for singular problems [5].

The open domain MATLAB code `bvpsuite` has been designed to solve general implicit systems of ODEs which may have arbitrary order including zero. In particular, algebraic constraints are permitted and therefore, DAEs are in the scope of the code. In [8, 9] numerical experiments and comparisons with existing software can be found. The additional difficulty in the case of DAEs is due to their *implicit nature*.

Much progress has been made concerning DAE theory and applications, but there are still many questions left open. In particular, the numerical treatment of critical points and singularities is just emerging. Encouraged by the positive results for the linear case [9], we approach here singular nonlinear index 1 DAE systems.

DAEs *with properly stated leading term* were introduced and studied for example in [1, 10, 2]. This concept enables a proper and natural description of the involved solution derivatives. To this end, one considers DAEs written in the form

$$f((D(t)x(t))', x(t), t) = 0, \quad t \in [a,b]. \tag{8}$$

One of the advantages of this precise description of the problem structure is that there exists an *inherent explicit regular ODE* uniquely determined by the problem data [1, 11]. Under mild assumptions, DAEs in standard form can be reformulated to have properly stated leading terms. For DAEs with properly stated leading terms arising in applications, see [1].

In [12], *linear DAEs* with properly stated leading term and type 0-critical points as well as type $1A$-critical points have been analyzed. This means that after decoupling the system using the matrix chain technique developed in [12] into the differential and algebraic components, the related inherent ODE exhibits a singularity of the first or second kind. The singularities discussed here are the counterparts to the 0-critical points for *nonlinear DAEs*.

We now use our so-called *decoupling function* $\omega : \mathscr{D}_\omega \times (0,1] \to \mathbb{R}^m$, where $\mathscr{D}_\omega \subseteq \mathbb{R}^n$ is an open set, to specify the inherent ODE associated with the nonlinear DAE (8). In order to apply the standard analysis for singular boundary value problems, cf. [13, 7], we assume that the decoupling function ω satisfies (7),

According to [4], for linear systems of DAEs with a singularity of the first kind and appropriately smooth problem data, the stage order of the collocation scheme is retained, provided that the so-called canonical projector remains bounded. This means that the global error of the collocation scheme with k collocation points is $O(h^k)$ uniformly in t, where h denotes the uniform mesh width. We observe order reductions if the canonical projector becomes unbounded. In this article we will formulate the respective convergence results for BVPs in nonlinear index 1 DAEs with a singularity of the first kind and bounded canonical projector. Clearly, the convergence results for polynomial collocation at inner collocation points presented here also hold for index 1 DAEs without singularities. We stress, that we aim to analyze known collocation schemes applied *directly to the DAE system in its original formulation*.

For the theoretical discussion of collocation methods, we define meshes $\Delta := (\tau_0, \tau_1, \ldots, \tau_N)$, and $h_i := \tau_{i+1} - \tau_i,\ i = 0, \ldots, N-1,\ \tau_0 = 0,\ \tau_N = 1$. For reasons of simplicity, we restrict the discussion to equidistant meshes, $h_i = h,\ i = 0, \ldots, N-1$. However, the results also hold for nonuniform meshes which have a limited variation in the stepsizes. For collocation, k distinct points $t_{i,j} := \tau_i + h_i\rho_j,\ j = 1,\dots,k$, are inserted in each subinterval (τ_i, τ_{i+1}). Since we want to focus on singular problems, we restrict ourselves to interior collocation points, where $\rho_1 > 0$ and $\rho_k < 1$.

Now, let us denote by $\mathscr{B}_k$ the Banach space of continuous, piecewise polynomial functions $q \in \mathbb{P}_k$ of degree $\leq k,\ k \in \mathbb{N}$, equipped with the maximum norm $\|\cdot\|_\infty$.

By $p \in \mathscr{B}_k$ we denote an approximation to the exact solution $x_\star$ of (8), and by $q \in \mathscr{B}_k$ an approximation to the exact solution $u_\star$ of the inherent ODE (7). As usual, to compute p and q, we set up the collocation equations augmented by the proper number of boundary conditions,

$$f(q'(t_{i,j}), p(t_{i,j}), t_{i,j}) = 0, \quad D(t_{i,j})p(t_{i,j}) - q(t_{i,j}) = 0, \quad B_0\, q(0) + B_1 q(1) = \beta, \tag{9}$$

where $j = 1,\dots,k$ and $i = 0,\dots,N-1$. By inspection of the number of unknowns ($(k+1)N(n+m)$ polynomial coefficients) and equations ($Nk(n+m)$ collocation conditions, $(N-1)(n+m)$ continuity conditions for p and q, n boundary conditions) we see that m further conditions will be necessary to close the system for the numerical treatment. Clearly, these additional conditions have to be consistent with the original DAEs. Various choices are possible, for details see [3].

It is possible to show that the collocation scheme for the DAE comprises exactly the same scheme applied to the inherent ODE. By applying the decoupling function to the resulting equations, it follows that the discretized inherent ODE together with boundary conditions form a classical collocation scheme for $q \in \mathscr{B}_k$. According to Theorem 3.1 in [7], there exists a unique collocation solution $q \in \mathscr{B}_k$ of this scheme under the assumptions that the underlying analytical problem is well-posed with sufficiently smooth data, and that the grid is sufficiently fine. Finally, $p \in \mathscr{B}_k$ is uniquely specified by the values of p at all collocation points.

The convergence result [7] for the inherent ODE carries over to the collocation solution of the full DAE:

Theorem: Let the nonlinear BVP (1) be well-posed and $x_\star \in C^{k+1}[0,1]$ be a solution, where (8) has a properly stated leading term and tractability index 1 on $\mathbb{R}^n \times \mathscr{D} \times (0,1]$. The matrix $G_1(y,x,t)$ may undergo a rank drop for $t \to 0$, causing a singularity of the first kind in the associated inherent ODE. To this end, let $tG_1(y,x,t)^{-1}$ have a continuous extension for $t \to 0$. Let the canonical projector function be bounded for $t \to 0$. The eigenvalues of the matrix $M(0)$ in (7) are assumed to have either negative real parts or to be zero. Moreover, the Jordan boxes associated with the zero eigenvalue are assumed to be diagonal. Then, for sufficiently fine grids, the collocation scheme provides a uniquely determined pair of collocation polynomials p and q such that at k interior collocation points

$$p(t_{ij}) - x_\star(t_{ij}) = O(h^k), \quad q(t_{ij}) - u_\star(t_{ij}) = O(h^k), \quad i = 0,\dots,N-1,\ \ j = 1,\dots,k,$$

holds.

As a numerical illustration of the convergence result, we consider the following problem:

$$A(t)(D(t)x(t))' + B(t)x(t) + h(x(t),t) = 0, \quad t \in (0,1], \quad n = 2,\ \ m = 4,\ \ D(t) = (I \quad 0),$$

$$A(t) = \begin{pmatrix} tI \\ 0 \end{pmatrix},\ \ B(t) = \begin{pmatrix} -11 & -18 & 3 & -1 \\ 12 & 19 & -2 & 1 \\ 1 & 1 & 1 & 0 \\ 2 & 3 & 0 & \frac{1}{5} \end{pmatrix},\ \ h(x,t) = t \begin{pmatrix} x_1 \sin(x_2) + x_3 e^{-x_1} \\ x_2 \cos(x_4) + x_4 \sin(x_1 + x_3) \\ x_1 x_2^3 + x_3 x_1 \\ x_1 x_2^2 + x_4 x_2^2 \end{pmatrix} + \beta(t),$$

where $x \in \mathscr{D} := \{x \in \mathbb{R}^4 : x_1 > -0.5\}$. The function $\beta(t)$ is such that $x_\star(t) = (t^2\sin(t), te^t, t\cos(t), \sin(t))^T$ is the exact solution and $\beta(0) = 0$ holds. The nonlinear inherent ODE is singular with a singularity of the first kind. We now augment the DAE system by the necessary number of boundary conditions given by

$$2x_1(0) + 3x_2(0) = 0,\ \ x_1(1) + x_2(1) = \sin(1) + e,\ \ x_1(0) + x_2(0) + x_3(0) = 0,\ \ 2x_1(0) + 3x_2(0) + 0.2x_4(0) = 0.$$

In the following table, we illustrate the convergence behavior of the collocation scheme. All calculations have been carried out with MATLAB. We report on the global error of the solution x and its differential $x_d = (x_1,x_2)^T$ and algebraic $x_a = (x_3,x_4)^T$ components. In the upper part of the table we illustrate the asymptotical properties of the differential components x_d with error at points τ_i defined as $\max_{\tau_i}\{\max\{|x_1(\tau_i)|, |x_2(\tau_i)|\}\}$. Similarly, the global error at the collocation points is given by $\max_{t_{ij}}\{\max\{|x_1(t_{ij})|, |x_2(t_{ij})|\}\}$. For the algebraic components the above quantities are specified in an analogous way. The order and the error constant are computed from two consecutive steps in the usual fashion. We can see that the observed order of convergence is k (since we are using an even number $k = 2$ of equidistant collocation points). In the lower part of the table we report on the asymptotical behavior of the whole solution vector. Here, we also observe the convergence of order $k = 2$.

uniform mesh		differential components x_d at points τ_i			differential components x_d at points $t_{i,j}$		
N	h	error	order	const.	error	order	const.
10	1.00e-01	2.172e-03			1.965e-03		
20	5.00e-02	5.252e-04	2.0	2.425e-01	5.004e-04	2.0	1.849e-01
40	2.50e-02	1.295e-04	2.0	2.231e-01	1.264e-04	2.0	1.913e-01
80	1.25e-02	3.216e-05	2.0	2.143e-01	3.179e-05	2.0	1.963e-01
160	6.25e-03	8.017e-06	2.0	2.099e-01	7.970e-06	2.0	1.998e-01
320	3.13e-03	2.001e-06	2.0	2.075e-01	1.995e-06	2.0	2.019e-01

uniform mesh		algebraic components x_a at points τ_i			algebraic components x_a at points τ_i		
N	h	error	order	const.	error	order	const.
10	1.00e-01	2.143e-02			1.808e-03		
20	5.00e-02	5.427e-03	2.0	2.055e+00	3.663e-04	2.3	3.631e-01
40	2.50e-02	1.361e-03	2.0	2.142e+00	8.308e-05	2.1	2.232e-01
80	1.25e-02	3.405e-04	2.0	2.169e+00	2.004e-05	2.1	1.607e-01
160	6.25e-03	8.515e-05	2.0	2.177e+00	4.935e-06	2.0	1.413e-01
320	3.13e-03	2.129e-05	2.0	2.179e+00	1.224e-06	2.0	1.339e-01

uniform mesh		solution x at points t_{ij}			solution x at 1000 uniform points		
N	h	error	order	const.	error	order	const.
10	1.00e-01	1.965e-03			2.143e-02		
20	5.00e-02	5.004e-04	2.0	1.849e-01	5.427e-03	2.0	2.055e+00
40	2.50e-02	1.264e-04	2.0	1.913e-01	1.361e-03	2.0	2.142e+00
80	1.25e-02	3.179e-05	2.0	1.963e-01	3.405e-04	2.0	2.169e+00
160	6.25e-03	7.970e-06	2.0	1.998e-01	8.515e-05	2.0	2.177e+00
320	3.13e-03	1.995e-06	2.0	2.019e-01	2.129e-05	2.0	2.179e+00

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