

Collocation Methods for Boundary Value Problems with an Essential Singularity^{*}

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Abstract. We investigate collocation methods for the efficient solution of singular boundary value problems with an essential singularity. We give numerical evidence that this approach indeed yields high order solutions. Moreover, we discuss the issue of a posteriori error estimation for the collocation solution. An estimate based on the defect correction principle, which has been successfully applied to problems with a singularity of the first kind, is less robust with respect to an essential singularity than a classical strategy based on mesh halving.

1 Introduction

We consider boundary value problems with an *essential singularity* (or *singularity of the second kind*),

$$t^\alpha z'(t) = f(t, z(t)), \quad t \in (0, 1], \quad (1)$$

$$g(z(0), z(1)) = 0, \quad (2)$$

$$z \in C[0, 1], \quad (3)$$

where $\alpha > 1$. f and g are smooth functions of dimension n and p , respectively. In general, $p < n$ holds and condition (3) provides the additional $n-p$ relations that guarantee the well-posedness of the problem. Analytical results for problems of this type have been discussed in detail in [1]. For the numerical treatment, we assume that an isolated solution of (1)–(3) exists.

Boundary value problems with an essential singularity are frequently encountered in applications. In particular, problems posed on infinite intervals are often transformed to this problem class. Here, we would like to mention a problem in foundation engineering discussed in [2], which is of use for the design of oil rigs above the ocean floor (see also Example 1 below). Models from fluid dynamics are another source for the problems we are interested in: The Blasius equation describes the laminar boundary layer on a flat plate, see for example [3]. The von Karman swirling flows result from the Navier-Stokes equations for a stationary, axisymmetric flow of a viscous incompressible fluid occupying the half space over an infinite rotating disk, cf. [4]. Finally, one approach to the classical

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electromagnetic self-interaction problem ([5]) leads to a boundary value problem with a singularity of the first kind ($\alpha = 1$ in (1)) at $t = 0$ and a singularity of the second kind due to the formulation on an infinite interval.

In this paper, we investigate numerical methods which may be successfully applied to obtain high-order solutions for boundary value problems of the type (1)–(3). Particularly, in §2 we examine the empirical convergence order of collocation methods at either equidistant or Gaussian points. These methods work satisfactorily when they are applied to boundary value problems with a singularity of the first kind, see [6]. Moreover, collocation has been implemented in the MATLAB code `sbvp` for the latter class of problems, see [7]. This code also uses an a posteriori error estimate based on defect correction, which has been analyzed for singularities of the first kind in [8]. In §3, we show that this estimate does not work for problems with an essential singularity. A modification of this idea is not satisfactory either, as demonstrated in §3.2. However, a strategy based on mesh halving is shown to be a promising candidate for an asymptotically correct error estimate for the collocation solution of (1)–(3), see §3.3.

2 Convergence of Collocation Methods

In this section, we discuss polynomial collocation with maximal degree $m \in \mathbb{N}$ for problems on grids $\Delta := \{t_{i,j} = t_i + \rho_j h, i = 0, \dots, N-1, j = 0, \dots, m\} \cup \{t_N\}$, where $h := 1/N$, $t_i := hi$ and $0 = \rho_0 < \rho_1 < \dots < \rho_m < 1$. This means that we approximate the analytical solution by a continuous collocating function $p(t) := p_i(t)$, $t \in [t_i, t_{i+1}]$, $i = 0, \dots, N-1$, where p_i is a polynomial of maximal degree m , which satisfies the differential equation (1) at the *collocation points* $t_{i,j}$, $i = 0, \dots, N-1$, $j = 1, \dots, m$, and the boundary conditions. In this setting, a convergence order of $O(h^m)$ can be guaranteed for regular problems with appropriately smooth data. However, when the collocation points are suitably chosen (*Gaussian points*) even a (super-) convergence order $O(h^{2m})$ holds at the mesh points t_i , see [9].

For problems with an essential singularity, we observed that the convergence order is at least $O(h^m)$, for numerical evidence see [10]. We illustrate this convergence behavior in Table 1. The results were computed for the problem from foundation engineering specified in [2],

Example 1

$$z'(t) = \frac{1}{t^2} \begin{pmatrix} -z_2(t) \\ -z_3(t) \\ -z_4(t) \\ 1 - e^{-z_1(t)/2} \end{pmatrix}, \quad (4)$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} z(1) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad (5)$$

where collocation at four equidistant points $\rho_j = j/5$, $j = 1, \dots, 4$ was applied. All computations in this paper were performed using MATLAB 6.1 in IEEE double precision with relative machine precision $\text{EPS} \approx 1.11\text{e-}16$. In Table 1, h denotes the step size, δ denotes the maximal global error at the grid Δ (computed with respect to a reference solution which was determined for $h = 1/320$), and p is the empirical convergence order determined from the values of δ for two consecutive step sizes. $\hat{\delta}$ and \hat{p} denote the respective quantities computed for the error at the mesh points t_i , $i = 0, \dots, N$, only. Note that for our choice of collocation points, no superconvergence effects are to be expected.

Table 1. Convergence order of collocation at four equidistant points for Example 1

h	δ	p	$\hat{\delta}$	\hat{p}
1/10	2.06e-17		2.06e-17	
1/20	4.26e-18	2.27	4.26e-18	2.27
1/40	1.65e-19	4.69	1.65e-19	4.69
1/80	6.22e-21	4.73	6.22e-21	4.73
1/160	3.84e-22	4.02	3.74e-22	4.06

Collocation at Gaussian points is affected by order reductions as compared to the classical superconvergence order. We demonstrate this observation using a simple test example,

Example 2

$$z'(t) = \frac{1}{t^\alpha} z(t) + e^t - \frac{e^t}{t^\alpha}, \quad (6)$$

$$z(1) = e, \quad (7)$$

with the exact solution $z(t) = e^t$. We conjecture that in general, the convergence order for Gaussian points is $m + \gamma$, where $0 < \gamma = \gamma(\alpha) < 1$, and γ decreases with increasing α . Table 2 shows the results for $\alpha = 3$ and collocation at four Gaussian points. Note that the maximal error is assumed throughout at mesh points, which implies that the convergence order \hat{p} is no higher than the uniform convergence order p .

Remark 2.1. The analysis of the box scheme given in [11] implies that its order of convergence is $1 + \gamma$, where $0 < \gamma < 1$. Since the box scheme is equivalent to collocation at Gaussian points with $m = 1$, this is consistent with the above conjecture.

3 A Posteriori Error Estimation

Here, we discuss several error estimation strategies for the numerical solution computed by collocation. First of all, we present the results obtained with our

Table 2. Convergence order of collocation at four Gaussian points for Example 2

h	δ	p	$\hat{\delta}$	\hat{p}
1/10	2.12e-09		2.12e-09	
1/20	9.07e-11	4.55	9.07e-11	4.55
1/40	3.92e-12	4.53	3.92e-12	4.53
1/80	1.71e-13	4.52	1.71e-13	4.52
1/160	5.99e-15	4.84	5.99e-15	4.84

MATLAB code `sbvp`. The graphs in Figure 1 demonstrate that the error estimate implemented in `sbvp`, see §3.1 below, is completely unreliable for Example 2 with $\alpha = 3$. The value of the error estimate (denoted by “`sbvp`”) is of the order of magnitude of 10^{60} , while the value of the exact global error (“`exact`”) is of the order of magnitude of the round-off error.

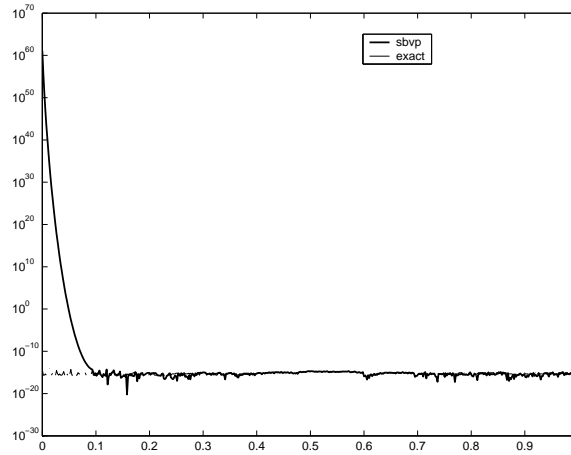


Fig. 1. Exact global error and the error obtained by `sbvp` for Example 2

3.1 Defect Correction Using the Backward Euler Method

The error estimation routine implemented in `sbvp` is based on the defect correction principle and uses the backward Euler method as an auxiliary scheme. This estimate was introduced in [6] and has been analyzed for problems with a singularity of the first kind in [8]. The numerical solution $p(t)$ obtained by collocation is used to define a “neighboring problem” to (1)–(3). The original and the neighboring problem are solved using the backward Euler method at the

points $t_{i,j}$, $j = 1, \dots, m$ and $t_{i,m+1} := t_{i+1}$, $i = 0, \dots, N-1$. This yields the grid vectors $\xi_{i,j}$ and $\pi_{i,j}$ as the solutions of the respective schemes

$$\frac{\xi_{i,j} - \xi_{i,j-1}}{t_{i,j} - t_{i,j-1}} = \frac{1}{t_{i,j}^\alpha} f(t_{i,j}, \xi_{i,j}), \quad \text{and} \quad (8)$$

$$\frac{\pi_{i,j} - \pi_{i,j-1}}{t_{i,j} - t_{i,j-1}} = \frac{1}{t_{i,j}^\alpha} f(t_{i,j}, \pi_{i,j}) + \bar{d}_{i,j}, \quad (9)$$

where $\bar{d}_{i,j}$ is a defect term defined by

$$\bar{d}_{i,j} := \frac{p(t_{i,j}) - p(t_{i,j-1})}{t_{i,j} - t_{i,j-1}} - \sum_{k=1}^{m+1} \alpha_{j,k} \frac{1}{t_{i,k}^\alpha} f(t_{i,k}, p(t_{i,k})). \quad (10)$$

Here, the coefficients $\alpha_{j,k}$ are chosen in such a way that the quadrature rules given by

$$\frac{1}{t_{i,j} - t_{i,j-1}} \int_{t_{i,j-1}}^{t_{i,j}} \varphi(\tau) d\tau \approx \sum_{k=1}^{m+1} \alpha_{j,k} \varphi(t_{i,k})$$

have precision $m+1$. The quantities $\xi_{i,j} - \pi_{i,j}$ serve as estimates for the global error of the collocation solution at the grid points, which is $O(h^m)$ in general. For regular problems and for a certain class of problems with a singularity of the first kind, this error estimate was shown to satisfy $\max_{i,j} |(z(t_{i,j}) - p(t_{i,j})) - (\xi_{i,j} - \pi_{i,j})| = O(h^{m+1})$, cf. [6] and [8].

The failure of this error estimate for problems with an essential singularity can clearly be attributed to the fact that the backward Euler method does not work for this problem class. It is clear from Table 3 that the method applied to Example 2 with $\alpha = 3$ is rapidly divergent.

Table 3. Numerical results for the backward Euler method for Example 2

h	δ	p	$\hat{\delta}$	\hat{p}
1/10	7.20e+00		7.20e+00	
1/20	5.93e+01	-3.04	5.93e+01	-3.04
1/40	1.73e+05	-11.5	1.73e+05	-11.5
1/80	8.70e+09	-15.6	8.70e+09	-15.6
1/160	5.99e+17	-26.0	5.99e+17	-26.0

The failure of the backward Euler method for Example 2 is apparently due to the instability of the numerical integration for this terminal value problem. For the solution of the associated difference scheme, terms of the form $(1 - h/t_i^\alpha)$ are accumulated. For $\alpha > 1$, these terms are unbounded for $t_i \rightarrow 0$. This possibly explains why this scheme works perfectly well for the cases where $\alpha = 1$, but fails for an essential singularity. An additional drawback of the backward Euler

scheme is the condition number of the associated system of linear algebraic equations, which becomes intolerably large for decreasing step size h . In Table 4 the condition number with respect to the maximum norm, “cond”, and its order of growth, “ p cond” are recorded. The norm of the system matrix “norm” is $O(h^{-3}) = O(h^{-\alpha})$, while the norm of the inverse “norm inv” increases very rapidly.

Table 4. Conditioning of the backward Euler method for Example 2

h	cond	p cond	norm	p norm	norm inv
1/10	6.99e+05		1.00e+03		6.99e+02
1/20	3.28e+09	−12.2	8.00e+03	−3.00	4.09e+05
1/40	1.55e+15	−18.9	6.40e+04	−3.00	2.42e+10
1/80	9.60e+23	−29.2	5.12e+05	−3.00	1.88e+18
1/160	5.10e+37	−45.6	4.10e+06	−3.00	1.25e+31

3.2 Defect Correction Based on the Box Scheme

When comparing the observations for the backward Euler method in §3.1 with the results for collocation, see §2, we may conjecture that a possible remedy for the observed instability could be to use symmetric schemes. In Table 5, we give the condition numbers “cond” for the box scheme which have the growth order p cond = $-\alpha$. This is the same as for the norm “norm” of the system matrices (not displayed). In contrast to the backward Euler scheme, the inverses are bounded in this case, see “norm inv”.

Thus, we propose the following alternative to the error estimate described in §3.1: Instead of solving the original and the neighboring problems using the backward Euler method, we use the box scheme to compute the quantities $\xi_{i,j}$ and $\pi_{i,j}$.¹ Unfortunately, the result is not fully satisfactory either. The error of the error estimate seems to have the order $m + \gamma$, where again γ decreases for growing α . We illustrate this observation in Table 5, where again Example 2 with $\alpha = 3$ is discussed. The underlying numerical method is collocation at four equidistant points, and we consider the error at the mesh points only. The error of the error estimate “ δ err” decreases faster than the error of the basic method $\hat{\delta}$ (which is $O(h^4)$), but the difference in the asymptotic orders is not sufficiently large to guarantee a reliable error estimate.

3.3 Error Estimate Based on Mesh Halving

The negative results for error estimation strategies based on the defect correction principle are the motivation to consider a computationally more expensive error

¹ For this purpose we use the defect $\bar{d}_{i,j}$ from (10) for the evaluation of the right-hand side at the point $(t_{i,j-1} + t_{i,j})/2$.

Table 5. Error of the error estimate based on the box scheme for collocation at four equidistant points and conditioning of the auxiliary scheme for Example 2

h	$\hat{\delta}$	$\hat{\delta}$ err	\hat{p} err	cond	p cond	norm	norm inv
1/10	1.11e-08	5.35e-09		2.28e+03		8.00e+03	2.85e-01
1/20	7.02e-10	2.26e-10	4.47	1.68e+04	-2.88	6.40e+04	2.62e-01
1/40	4.38e-11	1.02e-11	4.55	1.28e+05	-2.93	5.12e+05	2.50e-01
1/80	2.73e-12	4.42e-13	4.53	9.98e+05	-2.96	4.10e+06	2.44e-01
1/160	1.72e-13	1.90e-14	4.54	7.89e+06	-2.98	3.28e+07	2.41e-01

estimate based on mesh halving. In this approach, we compute the collocation solution at m equidistant points on a grid Δ with step size h and denote this approximation by $p_{\Delta}(t)$. Subsequently, we choose a second mesh Δ_2 with step size $h/2$. On this mesh, we compute the numerical solution based on the same collocation scheme to obtain the collocating function $p_{\Delta_2}(t)$. Using these two quantities, we define

$$\mathcal{E}(t) := \frac{2^p}{1 - 2^p} (p_{\Delta_2}(t) - p_{\Delta}(t)) \quad (11)$$

as an error estimate for the approximation $p_{\Delta}(t)$. Assume that the global error $\delta(t)$ of the collocation solution can be expressed in terms of the principal error function $e(t)$,

$$\delta(t) = e(t)h^m + O(h^{m+1}), \quad (12)$$

where $e(t)$ is independent of h . Then obviously the quantity $\mathcal{E}(t)$ satisfies $\mathcal{E}(t) - \delta(t) = O(h^{m+1})$. Consequently, for collocation at an even number of equidistant points, this error estimate is asymptotically correct. The convergence results for collocation methods, see §2, suggest that this is a promising approach.

However, numerical results given in [10] indicate that the higher order term in (12) is rather $O(h^{m+\gamma})$ with $\gamma < 1$ in case of an essential singularity. Here, we only give² the numerical results for the simple test problem Example 2, and refer the reader to [10] for further results. In Table 6, the error of the error estimate “ δ err” is given together with its asymptotic order “ p err”, where the underlying numerical solution is computed by collocation at four equidistant points. We can see that, similarly as for the box scheme (Table 5), the error of the error estimate has order $m + \gamma$ with $\gamma \approx 0.5$. However, the absolute quality of the error estimate is slightly better than for the box scheme. The error of the error estimate should be compared with the exact global error δ at the whole grid and at the mesh points ($\hat{\delta}$).

² For problems where a reference solution has to be used to compute the “exact” global error, the empirical orders observed are negatively affected by the influence of the error introduced by this latter approximation. Consequently, the asymptotic results for these examples may be less clear.

Table 6. Global error for collocation at four equidistant points and error of the error estimate based on mesh halving for Example 2

h	δ	$\hat{\delta}$	δ err	p err	$\hat{\delta}$ err	\hat{p} err
1/2	8.80e−06	8.80e−06	2.90e−07		1.61e−07	
1/4	5.41e−07	4.65e−07	1.16e−08	4.65	1.16e−08	3.80
1/8	3.02e−08	2.77e−08	3.75e−10	4.95	3.75e−10	4.95
1/16	1.82e−09	1.71e−09	1.61e−11	4.54	1.61e−11	4.54
1/32	1.11e−10	1.07e−10	6.93e−13	4.54	6.93e−13	4.54

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