

Numerical Solution of Singular Boundary Value Problems by Invariant Imbedding

MOHAN K. KADALBAJOO AND K. S. RAMAN

Department of Mathematics, Indian Institute of Technology, Kanpur 208016, India

Received February 2, 1983; revised August 25, 1983

An invariant imbedding method is proposed for numerically solving singular boundary value problems with a regular singular point at one end of the interval. The singular problem is first reduced to a regular boundary value problem by using series solution in the vicinity of the singular point to subtract out the singularity. The regular boundary value problem is then solved by employing invariant imbedding method. Some numerical examples have been included to demonstrate the efficiency of the method.

1. INTRODUCTION

Consider a second-order linear differential equation

$$f_0(x)y'' + f_1(x)y' + f_2(x)y = 0 \tag{1}$$

where $f_0(x)$, $f_1(x)$ and $f_2(x)$ are analytic at some point $x = x_0$ (say), then $x = x_0$ is said to be an ordinary point in the sense that the solution of (1) can be represented by a power series in powers of $(x - x_0)$. If for some point $x = x_0$, $f_0(x_0) = 0$, then x_0 is called a singular point of Eq. (1). In such a case rewriting Eq. (1) in the form

$$y'' + F_1(x)y' + F_2(x)y = 0 \tag{2}$$

where $F_i(x) = f_i(x)/f_0(x)$, $i = 1, 2$, we see that the coefficients $F_1(x)$ and $F_2(x)$ fail to be analytic at $x = x_0$. Singularities have been divided into two kinds; regular singular points and irregular points. The point $x = x_0$ is said to be regular singular point of (2) if $(x - x_0)F_1(x)$ and $(x - x_0)^2 F_2(x)$ are analytic at x_0 ; otherwise $x = x_0$ is an irregular singularity. We now consider our method for finding the solution of singular boundary value problem given by

$$L(y) = y'' + F_1(x)y' + F_2(x)y = Q(x), \quad x_0 < x \leq b \tag{3}$$

subject to boundary conditions

$$y(x_0) = \alpha \tag{4}$$

$$y(b) = \beta. \tag{5}$$

Singular boundary value problems of the above type have been studied by several authors. To mention a few, Jamet [1] has discussed existence and uniqueness of solutions and presented finite difference method for numerically solving such problems. Gustafsson [2] has treated the problem by first writing the series solution in the neighbourhood of the singularity and employing several compact and non-compact difference schemes in the remaining part of the interval. Cohen and Jones [3] have used an economized expansion to overcome the slow convergence of the Taylor series solution for the problems and employed deferred correction outside the range of economized expansion. Reddien [4] has studied collocation method for the numerical solution of such problems.

Scott [5] has considered sufficient conditions for existence of two different versions of invariant imbedding for linear second-order equations having a regular singular point. The work of Scott constitutes a significant extension of earlier results of Banks and Kurowski [6]. Elder [7] has described an invariant imbedding method for calculating the smallest eigenlength of a singular two-point boundary value problem with the singularity at the origin. Nelson [8] has adapted the approach of Elder to the solution of homogeneous two-point boundary value problems with a singularity of the first kind.

In this paper the invariant imbedding is proposed for numerically solving singular boundary value problems. The singular problem (3)–(5) over the interval $[x_0, b]$, x_0 a regular singularity, is first reduced to a regular boundary value problem over $[\delta, b]$, $\delta > x_0$; this is done by making use of series solution in the vicinity of the singularity and obtaining boundary condition at the point δ . The method of invariant imbedding is then developed for solving the resulting regular boundary value problem by reducing it to a sequence of initial value problems. These initial value problems are solved numerically by efficient initial value procedures. Some numerical examples have been solved to demonstrate the efficiency of the method.

2. REMOVAL OF SINGULARITY

In order to remove the singularity at the point $x = x_0$ for the problem given by (3)–(5), we make use of series expansion at a small interval near $x = x_0$ in $[x_0, \delta]$, so that Eq. (3) has a solution of the form

$$y(x) = (x - x_0)^p \sum_{k=0}^{\infty} a_k (x - x_0)^k, \quad a_0 \neq 0. \tag{6}$$

Differentiating (6) and substituting in (3) and comparing the coefficients of the powers of $(x - x_0)$ on both sides, the values of p as the roots of indicial equation and the recurrence relations for the coefficients a_k are obtained. Depending upon the nature of the roots of the indicial equation, the general solution of (3) can be written as

$$y(x) = \sum_{i=1}^m \alpha_i R_i(x) + R_{s+1}(x), \quad m \leq 2 \tag{7}$$

for $x \in [x_0, \delta]$, where $R_1(x)$ and $R_2(x)$ are two linearly independent solutions of homogeneous equation corresponding to (3) and $R_{s+1}(x)$ is the particular solution to (3). The derivation of $R_i(x)$ in general is treated in Coddington and Levinson [9]. The basic theoretical results about these series expansions about a singular point have been reviewed by Keller [10]. The series solution may be valid for the entire interval $[x_0, b]$, but we need the series expansion in the interval $[x_0, \delta]$ only.

We now transform the problem (3)–(5) to a regular boundary value problem over the interval $[\delta, b]$, where δ is any point in the interval (x_0, b) . We thus have to derive the boundary condition at the point δ . To do this, we have

$$\alpha_1 R_1(\delta) + \alpha_2 R_2(\delta) = y(\delta) - R_{s+1}(\delta) \quad (8)$$

$$\alpha_1 R_1'(\delta) + \alpha_2 R_2'(\delta) = y'(\delta) - R_{s+1}'(\delta) \quad (9)$$

where the primes denote the differentiation, which can be solved for α_1 and α_2 as

$$\alpha_1 = \frac{[y(\delta) - R_{s+1}(\delta)] R_2'(\delta) - [y'(\delta) - R_{s+1}'(\delta)] R_2(\delta)}{R_1(\delta) R_2'(\delta) - R_2(\delta) R_1'(\delta)} \quad (10)$$

and

$$\alpha_2 = \frac{[y'(\delta) - R_{s+1}'(\delta)] R_1(\delta) - [y(\delta) - R_{s+1}(\delta)] R_1'(\delta)}{R_1(\delta) R_2'(\delta) - R_2(\delta) R_1'(\delta)} \quad (11)$$

Also, we have from Eqs. (4) and (7)

$$\alpha_1 R_1(x_0) + \alpha_2 R_2(x_0) = y(x_0) - R_{s+1}(x_0). \quad (12)$$

Using the expansion (10), (11) and (12) we have

$$\begin{aligned} & \frac{g(\delta) R_2'(\delta) - g'(\delta) R_2(\delta)}{h(\delta)} R_1(x_0) \\ & + \frac{g'(\delta) R_1(\delta) - g(\delta) R_1'(\delta)}{h(\delta)} R_2(x_0) = \alpha - R_{s+1}(x_0) \end{aligned} \quad (13)$$

where $g(x) = y(x) - R_{s+1}(x)$ and $h(x) = R_1(x) R_2'(x) - R_2(x) R_1'(x)$. Equation (13) can be conveniently written as

$$\begin{aligned} & [R_2'(\delta) R_1(x_0) - R_1'(\delta) R_2(x_0)] g(\delta) + [R_1(\delta) R_2(x_0) - R_2(\delta) R_1(x_0)] g'(\delta) \\ & = h(\delta) [\alpha - R_{s+1}(x_0)] \end{aligned} \quad (14)$$

(or)

$$Ay(\delta) + By'(\delta) = C \quad (15)$$

where

$$\begin{aligned} A &= [R_2'(\delta) R_1(x_0) - R_1'(\delta) R_2(x_0)] \\ B &= [R_1(\delta) R_2(x_0) - R_2(\delta) R_1(x_0)] \end{aligned} \tag{15a}$$

and

$$C = h(\delta)[a - R_{s+1}(x_0)] + AR_{s+1}(\delta) + BR'_{s+1}(\delta).$$

Thus the regular boundary value problem over $[\delta, b]$ is given by Eq. (3) subject to boundary condition (15) and $y(b) = \beta$.

3. INVARIANT IMBEDDING

In this section we discuss the method of invariant imbedding for solving the regular boundary value problem derived in the previous section. We use Scott's version of imbedding [11] to reduce the regular boundary value problem into a sequence of initial value problems which are solved numerically by well-known initial value procedures. To be specific, we write Eq. (3) as a system of two first-order equations in the form

$$u'(x) = v(x), \tag{16}$$

$$-v'(x) = F_1(x)v(x) + F_2(x)u(x) - Q(x), \quad x \in [\delta, b]. \tag{17}$$

With the boundary conditions given by

$$Au(\delta) + Bv(\delta) = C \tag{18}$$

$$u(b) = \beta. \tag{19}$$

We now discuss the invariant imbedding method for a more general second-order system of the form

$$u'(x) = a(x)u(x) + b(x)v(x) + e(x), \tag{20}$$

$$-v'(x) = c(x)u(x) + d(x)v(x) + f(x), \quad x \in [\delta, b] \tag{21}$$

with all functions $a(x)$, $b(x)$, $c(x)$, $d(x)$, $e(x)$ and $f(x)$ be continuous and subject to the boundary conditions given by (18) and (19).

Using Scott's version of invariant imbedding [11], we have

$$u(x) = S_1(x)v(x) + S_2(x)u(\delta) + S_3(x), \tag{22}$$

$$v(\delta) = Q_1(x)v(x) + Q_2(x)u(\delta) + Q_3(x), \quad x \in [\delta, b]. \tag{23}$$

It can be easily verified that the coefficients $S_i(x)$, $i = 1, 2, 3$, satisfy the following differential equations:

$$S'_1(x) = b(x) + [a(x) + d(x)] S_1(x) + c(x) S_1^2(x) \quad (24)$$

$$S'_2(x) = [a(x) + c(x) S_1(x)] S_2(x) \quad (25)$$

$$S'_3(x) = [a(x) + c(x) S_1(x)] S_3(x) + f(x) S_1(x) + e(x) \quad (26)$$

with suitable initial conditions given as

$$S_1(\delta) = 0; \quad S_2(\delta) = 1, \quad S_3(\delta) = 0. \quad (27)$$

Similarly, the differential equations for the coefficients Q_i are

$$Q'_1(x) = [d(x) + c(x) S_1(x)] Q_1(x) \quad (28)$$

$$Q'_2(x) = c(x) Q_1(x) S_2(x) \quad (29)$$

$$Q'_3(x) = [c(x) S_3(x) + f(x)] Q_1(x) \quad (30)$$

subject to the suitable initial conditions given by

$$Q_1(\delta) = 1, \quad Q_2(\delta) = 0, \quad Q_3(\delta) = 0. \quad (31)$$

4. COMPUTATIONAL ALGORITHM

In order to compute the solution u , the computation is performed sequentially as under the following:

Step (i) Integrate the initial value problems given by Eqs. (24)–(31), using efficient initial value routines, from $x = \delta$ to $x = b$ to obtain the S_i and Q_i profiles and store them.

Step (ii) Find the values of A , B and C from Eqs. (15a).

Step (iii) Evaluate Eqs. (22)–(23) at $x = b$ using the values $S_i(b)$ and $Q_i(b)$ ($i = 1, 2, 3$) from step (i), and $u(b)$ from the boundary condition. The resulting equations would contain the unknowns $u(\delta)$, $v(\delta)$ and $v(b)$.

Step (iv) Combine the equations resulting from Step (iii), with Eq. (15), and solve these three equations for the unknowns $u(\delta)$, $v(\delta)$ and $v(b)$.

Step (v) Compute $v(x)$ and $u(x)$ for any $x \in (\delta, b)$ using the values of $u(\delta)$ and $v(\delta)$ from Step (iv), and the stored values of S_i and Q_i from Step (i).

It may be noted that Step (i), which incidentally involves maximum computer time in the entire computational procedure, need not be repeated if one has to solve different boundary value problems given by the same differential equation (3) but with different boundary conditions (4)–(5), but that only Steps (ii)–(v) need be repeated for each set of boundary conditions, using the stored values of S_i and Q_i from Step (i), in each case.

5. NUMERICAL EXAMPLES AND RESULTS

In this section we shall illustrate the use of the algorithm we have derived by applying it to several examples. In our examples all corresponding initial value problems (24)–(31) were solved using a fourth- to fifth-order Runge–Kutta–Fehlberg scheme designed to estimate the local error and to control the step size for the accuracy requirements [12]. All computations were carried out in single precision on a DEC-1090 computer system with a relative and absolute error of 10^{-5} and 10^{-13} , respectively.

EXAMPLE 1. We consider the linear two-point boundary value problem

$$u''(x) + \frac{\sigma}{x} u'(x) - \tau u(x) = 0, \quad 0 < \sigma < 1, \quad \tau > 0$$

with boundary conditions

$$u(0) = 1, \quad u(1) = 0.$$

This problem has been studied earlier by Jamet [1].

See Tables I–IV.

TABLE I
Numerical Results for Example 1 ($\sigma = 0.5, \tau = 1$)

x	$\delta = 0.2$	$\delta = 0.4$	$\delta = 0.5$
0.2	0.5080600	—	—
0.4	0.3221206	0.3221289	—
0.5	0.2520316	0.2520420	0.2520425
0.9	0.0424309	0.0424321	0.0424322

TABLE II
Comparison of Numerical Results for Example 1
($\sigma = 0.5, \tau = 1, x = 0.5$)

$N = 1/h$	Jamet's method	Reddien's method	Invariant imbedding method ^a
8	0.29038211	0.25305	0.25204250
16	0.27825809	0.25223	—
32	0.27009658	—	—
128	0.26077219	—	—
512	0.25633371	—	—

^a The step size h has no direct relevance to invariant imbedding solution and refers only to Jamet's and Reddien's solutions.

TABLE III
 Numerical Results for Example 1
 ($\delta = 0.05, \sigma = 0.5, \tau = 1$)

x	u
0.05	0.75006408
0.10	0.64846210
0.15	0.57142780
0.20	0.50806241
0.50	0.25204202
0.80	0.08773196
0.90	0.04243212

TABLE IV
 Numerical Results for Example 1
 ($\delta = 0.125, \sigma = 0.5, \tau = 1$)

x	u
0.125	0.60761680
0.250	0.45343930
0.375	0.34147399
0.500	0.25204244
0.625	0.17697532
0.750	0.11175222
0.875	0.53454321
1.000	0.00000000

EXAMPLE 2. Next we make the numerical experiments on the equation

$$u''(x) + \frac{\sigma}{x} u'(x) = -x^{1-\sigma} \cos x - (2 - \sigma) x^{-\sigma} \sin x, \quad 0 < \sigma < 1$$

with boundary conditions

$$u(0) = 0, \quad u(1) = \cos 1.$$

This example has been taken from Gustafsson [2] and has the exact solution $u(x) = x^{1-\sigma} \cos x$.

See Tables V and VI.

EXAMPLE 3. We solve $2x(1+x)y'' + (1+5x)y' + y = 0$ with boundary conditions $y(0) = 1.0, y(1.5) = 1.0$. This problem was solved earlier by Cohen and Jones [3] and has the exact solution given by $y(x) = (1 + \sqrt{x})/(1+x)$.

See Table VII.

TABLE V
Numerical Results for Example 2 ($\sigma = 0.5$)

x	$\delta = 0.1$	$\delta = 0.2$	$\delta = 0.4$
0.1	0.31464841	—	—
0.2	0.43829967	0.43829892	—
0.3	0.52326032	0.52325916	—
0.4	0.58253142	0.58252991	0.5825301
0.6	0.63930355	0.63930194	0.6393022
0.8	0.62315431	0.62315313	0.6231534
0.9	0.58971162	0.58971083	0.5897109

TABLE VI
Comparison of Maximum Errors^a

$N = 1/h$	δ	Gustafsson's solution	Invariant imbedding solution
40	0.1	1.5×10^{-5}	4.4×10^{-8}
80		7.2×10^{-7}	
160		4.0×10^{-8}	
40	0.2	7.9×10^{-7}	1.8×10^{-8}
80		4.4×10^{-8}	
160		2.6×10^{-9}	
40	0.4	3.7×10^{-8}	7.4×10^{-9}
80		2.1×10^{-9}	
160		1.3×10^{-10}	

^a The step size h refers only to Gustafsson's case.

TABLE VII
Numerical Results for Example 3 with $\delta = 0.5$

x	Invariant imbedding solution	Cohen's solution	Exact solution
0.5	1.243902	1.243964	1.244017
0.6	1.217836	1.217871	1.217927
0.7	1.190924	1.190939	1.190997
0.8	1.640782	1.164078	1.164136
0.9	1.137794	1.137781	1.137840
1.0	1.112338	1.112319	1.112372
1.1	1.087842	1.087824	1.087868
1.2	1.064364	1.064348	1.064382
1.3	1.041912	1.041900	1.041924
1.4	1.020469	1.020462	1.020474
1.5	1.000000	1.000000	1.000000

6. DISCUSSION AND CONCLUSION

The numerical results for Example 1 for different values of δ are presented in Tables I–IV. The computed solutions at various values of x compare very well with the analytical solution (series solution). This example was solved earlier by Jamet (by finite difference method) and Reddien (by collocation method) and their computed solutions at $x = 0.5$ for different mesh sizes are given in Table II. This table also contains solution computed at $x = 0.5$ by invariant imbedding method using a Runge–Kutta–Fehlberg scheme with step size control to solve our initial value problems. Thus the step sizes h given in the table have no direct relevance to invariant imbedding solution. As is evident from the table, the invariant imbedding solution is much superior to the solution obtained by Jamet or Reddien for a very fine mesh. The behaviour of the solution when δ is very near to the singularity is shown in Tables III and IV. It has been observed here that a comparatively smaller step size is required (as expected) to achieve the desired accuracy in the solutions.

Tables V and VI give the numerical results for Example 2. This example, which corresponds to the non-homogeneous case of Jamet's equation, has been extensively studied by Gustafsson [2] using some compact and non-compact difference schemes of higher order. The computed solutions at different points with respect to several values of δ are presented in Table V. The comparison of maximum error incurred in the solutions obtained by our method and that of Gustafsson is made in Table VI. The maximum error shown here in the case of Gustafsson corresponds to a compact difference scheme of order 4. The superiority of our method in most of the cases is evident from the results.

Some more numerical experiments were done on an example solved earlier by Cohen and Jones [3]. The numerical results obtained by our method and the comparison of those solutions with Cohen's solutions are given in Table VII. Cohen and Jones used economized expansion of the power series on the interval $[0, \delta]$ as against a series solution by us on the same interval. In the remaining part of the interval $[\delta, b]$, Cohen and Jones used finite difference approximations with deferred corrections. The solutions obtained by our method compare well with Cohen's solutions and that of the exact solutions.

In conclusion, the invariant imbedding method is an efficient and powerful technique for solving singular boundary value problems.

ACKNOWLEDGMENTS

The authors sincerely thank the referees for their comments and suggestions.

REFERENCES

1. P. JAMET, *Numer. Math.* **14** (1970), 355.
2. B. GUSTAFSSON, *Numer. Math.* **21** (1973), 328.

3. A. M. COHEN AND D. E. JONES, *J. Inst. Math. Appl.* **13** (1974), 379.
4. G. W. REDDIEN, *Numer. Math.* **25** (1975), 427.
5. M. R. SCOTT, "An Introduction to Invariant Imbedding," Addison-Wesley, Reading, Mass., 1973.
6. D. O. BANKS AND G. J. KUROWSKI, *Math. Comp.* **22** (1968), 304.
7. I. T. ELDER, *J. Math. Anal. Appl.* **85** (1982), 360.
8. P. NELSON, *Appl. Math. Comput.* **9** (1981), 93.
9. E. A. CODDINGTON AND N. LEVINSON, "Theory of Ordinary Differential Equations," McGraw-Hill, New York, 1955.
10. H. B. KELLER, "Numerical Solution of Two Point Boundary Value Problems," SIAM Regional Conference Series in Applied Mathematics No. 24, 1976.
11. M. R. SCOTT, On the conversion of boundary value problems into stable initial value problems via several invariant imbedding algorithms, in "Numerical Solution of Boundary Value Problems in Ordinary Differential Equations" (A. K. Aziz, Ed.), Academic Press, New York, 1975.
12. G. E. FORSYTHE, MICHAEL A. MELCOM, AND B. M. CLEVE, "Computer Methods for Mathematical Computations," Prentice-Hall, Englewood Cliffs, N.J., 1977.