

A Simple Approach to a Sensitive Two-Point Boundary Value Problem

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A well-known sensitive two-point boundary value problem is solved by two very simple shooting methods. The origin of the problem and some properties of the solution are discussed.

1. INTRODUCTION

The numerical solution of the problem

$$y'' = C \sinh Cy \quad 0 \leq x \leq 1 \quad (1.1)$$

with the boundary conditions

$$y(0) = 0, \quad y(1) = 1, \quad (1.2)$$

has been considered repeatedly in the literature. It is an attractive problem, but it is interesting to note that it was never intended as a problem to be solved numerically. Indeed, in [1, p. 70] Keller poses it as an example to elucidate a certain feature appearing in more complicated situations. Although the problem is, in principle, a sensitive two-point boundary value problem, we will solve it here with the most unsophisticated shooting method (see Section 2). Some general properties of the solution are discussed in Section 3, and an alternate numerical approach is presented in Section 4. In the last section, the shooting method is applied to a problem where the integration cannot be carried to the end of the integration interval. The origin of Eq. (1.1) is discussed in the Appendix.

During the past years, the numerical solution of two-point boundary value problems has been pursued very vigorously and with great success (cf. the survey article by Keller [2]). Several methods have been developed and implemented in powerful and accurate programs, and these programs have been tested on a number of problems that are known to possess inherent difficulties. However, it can happen

that a test problem looks more difficult in the context of a general purpose approach than it really is. For instance, the solution of the problem discussed in this note is actually quite simple, as has been pointed out previously [3, 4, 5].

It seems still worthwhile to consider simple methods for two-point boundary value problems as long as the advanced general purpose routines are not as widely available and as sturdy as, for instance, the routines for initial value problems or for problems in linear algebra. When faced with a two-point boundary value problem, the physicist or engineer may prefer to try an elementary approach, like the shooting method, but then take full advantage of the intimate knowledge of his own particular problem. Since he is attempting to solve only a single problem, possibly for a set of parameters, the number of iterations and the machine time required are not as crucial as they are for a general purpose tool. Also, the accuracy requirements of the final solutions are not as stringent; a graph of the results is often all that is desired [6, p. 205].

2. NUMERICAL SOLUTION

The most elementary shooting method is used to solve the problem (1.1), (1.2). The integration routine is a direct implementation of the fourth-order Runge-Kutta formula [7, 25.5.18], with constant stepsize throughout the interval, and the problem is solved on a short-wordlength machine (the IBM 360/44, in single precision). The constant stepsize is chosen not so much for the (insignificant)

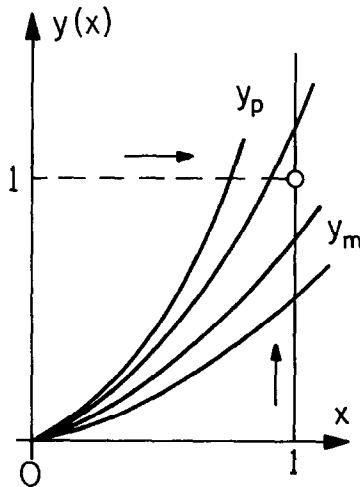


FIG. 1. The approach in the shooting method for Eq. (1.1).

TABLE I

Solution of $y'' = C \sinh Cy$, $y(0) = 0$, $y(1) = 1$

x	$C = 10$			
	$(h = 0.00125)$ $y(x)$	$y'(x)$	(extrapolated to $h = 0$) $y(x)$	$y'(x)$
0.0	0.0	0.3584E - 3	0.0	0.3583E - 3
0.2	0.1300E - 3	0.1348E - 2	0.1300E - 3	0.1348E - 2
0.4	0.9780E - 3	0.9787E - 2	0.9778E - 3	0.9785E - 2
0.6	0.7230E - 2	0.7231E - 1	0.7228E - 2	0.7230E - 1
0.8	0.5373E - 1	0.5438	0.5373E - 1	0.5437
0.9	0.1521	0.1672E + 1	0.1521	0.1672E + 1
0.95	0.2763	0.3729E + 1	0.2762	0.3728E + 1
1.0	1.0	0.1497E + 3	1.0	0.1471E + 3
$C = 12$				
0.0	0.0	0.4894E - 4	0.0	0.4891E - 4
0.2	0.2229E - 4	0.2720E - 3	0.2228E - 4	0.2718E - 3
0.4	0.2478E - 3	0.2973E - 2	0.2476E - 3	0.2972E - 2
0.6	0.2731E - 2	0.3278E - 1	0.2730E - 2	0.3276E - 1
0.8	0.3019E - 1	0.3642	0.3017E - 1	0.3640
0.9	0.1031	0.1318E + 1	0.1030	0.1317E + 1
0.95	0.2044	0.3115E + 1	0.2042	0.3112E + 1
1.0	1.0	0.4703E + 3	1.0	0.421E + 3
$C = 15$				
0.0	0.0	0.2450E - 5	0.0	0.2446E - 5
0.2	0.1636E - 5	0.2467E - 4	0.1634E - 5	0.2464E - 4
0.4	0.3295E - 4	0.4943E - 3	0.3291E - 4	0.4937E - 3
0.6	0.6618E - 3	0.9927E - 2	0.6610E - 3	0.9915E - 2
0.8	0.1330E - 1	0.1999	0.1329E - 1	0.1996
0.9	0.6059E - 1	0.9405	0.6052E - 1	0.9392
0.95	0.1370	0.2437E + 1	0.1368	0.2432E + 1
1.0	1.0	0.506E + 4	1.0	0.417E + 4

simplification, but because it seems preferable to be reliably and systematically in error than to be sporadically more accurate, when a short wordlength is used. Particularly for sensitive problems, the solution may depend in an undesirable way on the position where the stepsize is altered.

For the value of the constant C , we consider $C = 10, 12$, and 15 , since the results for smaller C have been reported repeatedly in the literature (starting with [8] in 1972).

The approach is divided into two parts, best described by referring to Fig. 1. A rough search is started with a small value for $y'(0)$; this value is increased until for one initial value, $y_p'(0)$, the solution $y_p(x)$ crosses the line $y = 1$, whereas for the previous initial condition, $y_m'(0)$, the solution satisfies $y_m(1) < 1$. There is only one precaution necessary: although the integration is stopped as soon as $y_p > 1$, the growth of $y(x)$ is so rapid that an exponential overflow may occur within one full Runge-Kutta step. In this case, an overflow trap is set to prevent the run from being terminated.

From y_p and y_m , the next guess $y'(0)$ is chosen as the average value, if $y_p(x)$ does not reach $x = 1$; otherwise, the next guess is computed by the secant method. The process is stopped when the accuracy consistent with the short wordlength is reached, and this is attained in fewer than 10 iterations. This is a more elementary approach than Newton's method (or, in more difficult cases, Powell's method) which has been used in [3], although the general approach is quite similar, including the device of stopping the integration when the solution is clearly about to diverge to infinity.

The computation is carried out for a stepsize of $h = 1/800$ and four larger stepsizes, and the results extrapolated to stepsize zero. The solutions are listed in Table I. For $C = 10$, they agree within a small fraction of a percent with the accurate results in [9, 10]. For $C = 15$, the results can be expected to be of the same accuracy, with the exception of $y'(1)$. This exception does not affect the shape of the curve $y(x)$, and very accurate values for $y'(1)$ follow anyway from the considerations discussed in the next section. Results for $C > 10$ are also reported in [4, 5] and will be compared in Section 4 below.

3. ANALYSIS OF THE PROBLEM

For the problem (1.1), the closed form solution has been obtained by Weibel and independently by Stoer and Bulirsch [11] in the form of elliptic functions. Nevertheless, certain well-known properties can be deduced in an elementary way.

If the equation is integrated once, we obtain

$$y'^2 = 2 \cosh Cy + c_0 \quad (3.1)$$

where the constant c_0 is related to the initial condition by

$$y'^2(0) = 2 + c_0,$$

so that

$$y'(1) = (2 \cosh C - 2 + y'^2(0))^{1/2}. \quad (3.2)$$

Next we compare the solution $y(x)$ with the solution $z(x)$ of the linearized problem (cf. [11])

$$\begin{aligned} z'' &= C^2 z, \\ z(0) &= 0, \quad z(1) = 1, \end{aligned}$$

i.e., with

$$z(x) = \sinh(Cx)/\sinh C. \quad (3.3)$$

This solution $z(x)$ must lie above $y(x)$ for $0 < x < 1$. Clearly, $y'(0) < z'(0)$, since for a particular ordinate $y'' \geq z''$, and if the curve $y(x)$ were to intersect $z(x)$, it would stay strictly above it for larger x values. Therefore

$$y(x) < \sinh(Cx)/\sinh C, \quad \text{for } 0 < x < 1,$$

and

$$0 < y'(0) < \beta, \quad (3.4)$$

where $\beta = C/\sinh C$.

A considerably better approximation for the initial slope is obtained from the estimate in [12] (cf. also [1]); if we assume that C is so large that the singularity

TABLE II
Eigenvalues λ of the Jacobian Matrix and Approximations to $y'(0)$ and $y'(1)$

C	$\pm\lambda$	$y'(0)$	$y'(0)e^{C/8}$	$\alpha < y'(1) < (\alpha^2 + \beta^2)^{1/2}$	
0	0.0	1.0	0.125	—	—
5	43.1	0.4575E - 1	0.849	12.10041	12.10060
6	85.2	0.1795E - 1	0.9052	20.03574	20.03576
10	1049.4	0.3583E - 3	0.9866	148.4064212	
12	3423.2	0.4891E - 4	0.9950	403.4263147	
15	19177.2	0.2444E - 5	0.9989	1808.041861	

of the solution occurs at x_s slightly above $x = 1$ and use $x_s = 1$ as an approximation, then

$$y'(0) \doteq 8e^{-C}. \quad (3.5)$$

The numerical results in Table II show that this approximation represents a quite accurate upper bound for $y'(0)$ (see also [11], where higher-order terms can be obtained from the closed-form solution).

Upper and lower bounds for $y'(1)$ are easily obtained from Eqs. (3.2) and (3.4)

$$\alpha < y'(1) < (\alpha^2 + \beta^2)^{1/2}, \quad (3.6)$$

where

$$\alpha^2 = 2 \cosh C - 2 = 4 \sinh^2(C/2).$$

The values in Table II show that these bounds are quite sharp. The Table II also lists the eigenvalues of the Jacobian matrix at $x = 1$ [9], $\lambda = C (\cosh C)^{1/2}$.

It might be mentioned that the maximum curvature and its ordinate can also be obtained rather easily. We simply state that for large C , the maximum curvature is

$$k \doteq C/1.51749,$$

and the corresponding ordinate y_0 and slope y_0'

$$y_0 \doteq (1/C) \cosh^{-1}((1/2)(13^{1/2} - 1)) \doteq 0.7598/C,$$

and

$$y_0' \doteq (13^{1/2} - 3)^{1/2} \doteq 0.7782.$$

For $C \rightarrow \infty$, the radius of curvature goes to zero and the solution curve makes a corner at y_0 , as y_0 also tends to zero. Since the initial slope y_0' (cf. Eq. (3.5)) approaches zero and $y'(1)$ (cf. Eq. (3.6)) approaches infinity, for $C \rightarrow \infty$ the solution curve follows the x -axis to $x = 1$, and then continues vertically to the point $x = 1, y = 1$.

4. AN ALTERNATE NUMERICAL SOLUTION

From the general shape of the solution curve it follows that the arclength s is a more suitable independent variable,

$$(ds)^2 = (dx)^2 + (dy)^2.$$

This choice of independent variable seems advantageous in any problem where the

TABLE III

Some Iterations in the Solution of Eqs. (4.1) for $C = 15$

Iteration 1, $s_0 = 1.5, y'(0) = 1.0$		
s/s_0	x	y
0.0	0.0	0.0
0.2	0.12542	0.26487
0.4	0.14183	0.56425
0.6	0.14356	0.86424
0.8	0.14375	1.16424
1.0	0.14377	1.46424
Iteration 4, $s_0 = 1.87276, y'(0) = 0.14142E - 5$		
0.0	0.0	0.0
0.2	0.37455	0.12983E - 4
0.4	0.74906	0.35734E - 2
0.6	1.00977	0.21576
0.8	1.03495	0.58896
1.0	1.03646	0.96350
Iteration 7, $s_0 = 1.87277, y'(0) = 0.24421E - 5$		
0.0	0.0	0.0
0.2	0.37455	0.22420E - 4
0.4	0.74897	0.61631E - 2
0.6	0.97978	0.25161
0.8	0.99891	0.62538
1.0	1.00007	0.99993
Iteration 8, $s_0 = 1.87277, y'(0) = 0.244450E - 5$		
0.0	0.0	0.0
0.2	0.37455	0.22442E - 4
0.4	0.74897	0.61691E - 2
0.6	0.97972	0.25167
0.8	0.99885	0.62545
1.0	1.00000	1.00000

solution curve has very flat and very steep segments. In our case, it can be expected that the solution for large C is close to the limit for $C \rightarrow \infty$, i.e.,

$$\begin{aligned} x(s) &\doteq s, \quad y(s) \doteq 0, & \text{for } 0 \leq s \doteq 1, \\ x(s) &\doteq 1, \quad y(s) \doteq s - 1, & \text{for } 1 \doteq s \doteq 2. \end{aligned}$$

If we set $f(y) = 4 \sinh^2(Cy/2)$, the problem is transformed to

$$\begin{aligned} dx/ds &= \{f(y) + 1 + y'(0)^2\}^{-1/2}, \\ dy/ds &= \{(f(y) + y'(0)^2)/(f(y) + 1 + y'(0)^2)\}^{1/2}. \end{aligned} \tag{4.1}$$

The functions now cannot grow faster than linearly. The value of $y'(0)$ could be altered until $x(s)$ and $y(s)$ reach unity for some $s_0 < 2$: $x(s_0) = y(s_0) = 1$. However, in the implementation, s_0 is scaled out, so that the integration interval is fixed and s_0 is improved in the course of the iterations together with $y'(0)$. The results of some iterations are shown in Table III. Rather poor initial guesses have been chosen, since with the approximation (3.5) for $y'(0)$ and $s_0 = 2$ convergence is already achieved in the third iteration. The results in Table IV show that there is good agreement with previously published results in [4, 5, 9]. The arclength s_0 is also listed; it appears to approach the limit $s_0(C = \infty) = 2$ with a deviation proportional to $1/C$.

TABLE IV
Initial slope $y'(0)$ and Arclength s_0 for Different C Values

C	$y'(0)$ using Eq. (4.1)	$y'(0)$ in [4, 5, 9]	s_0	$(2 - s_0)C$
5.00	0.45750E - 1	0.4575046E - 1[9]	1.65077	1.7461
6.00	0.17951E - 1	0.1795095E - 1[9]	1.69822	1.8107
10.00	0.35834E - 3	0.3583378E - 3[9]	1.81039	1.8961
10.01	0.35480E - 3	0.356 E - 3[4]	1.81057	1.8962
12.00	0.48910E - 4		1.84128	1.9046
12.003	0.48764E - 4	0.4878 E - 4[5]	1.84132	1.9046
13.59	0.10001E - 4	0.1 E - 4[4]	1.85965	1.9073
13.997	0.66600E - 5	0.6667 E - 5[5]	1.86371	1.9077
15.00	0.24445E - 5		1.87277	1.9084
15.89	0.10042E - 5	0.1 E - 5[4]	1.87987	1.9088

By analyzing the trend in the numerical results, the following expression is obtained

$$y'(0) = 8e^{-C}(1 - 2e^{-C/2} + 2e^{-C}). \tag{4.2}$$

For $C \geq 10$ it agrees with the numerical result within a relative error of less than 10^{-5} .

5. A SECOND EXAMPLE

It might be assumed that the shooting method must fail if the integration cannot be carried to the end of the integration interval for a particular guess of the initial conditions. This is not necessarily the case, as the following simple example shows:

$$y'' = C \sinh Cy + x^4\{1 - x - |1 - y|/(4 \sinh(C/2))\}^{1/2}, \tag{5.1}$$

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

It is impossible to shoot beyond the straight lines b (cf. Fig. 2): $x = 1 - |1 - y|/(4 \sinh(C/2))$, because y'' is no longer a real function. Nevertheless, the true solution can be approached in the same way as in Section 2, except that the approach now follows the arrows.

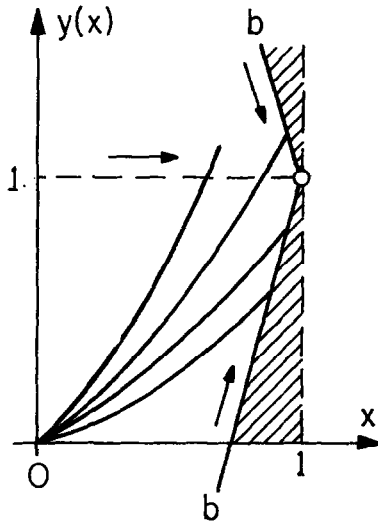


FIG. 2. The approach in the shooting method for Eq. (5.1).

For $C = 5$ and a constant stepsize of $h = 0.005$, the solution was obtained in single precision on the IBM 360/44, as given in Table V.

TABLE V
Solution of Eq. (5.1)

x	$y(x)$	$y'(x)$
0.0	0.0	0.044072
0.2	0.01036	0.06807
0.4	0.03210	0.1678
0.6	0.09000	0.4626
0.8	0.2562	1.389
0.9	0.4539	2.811
0.95	0.6346	4.702
1.0	1.0000	12.11

APPENDIX: THE ORIGIN OF THE PROBLEM

The differential equation $y'' = C \sinh Cy$ can be interpreted as a drastic simplification of more than one physical situation (cf. [12]). Here, we will trace its origin to a system of ordinary differential equations derived and solved by Weibel, who considers the following system, in natural units, in [13, Eqs. (14–28)]:

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{dE_0}{dr} \right) + \left(\omega^2 - \frac{e^2 N}{M} - \frac{e^2 n}{m} \right) E_0 = 0,$$

$$\frac{1}{r} \frac{d}{dr} (r E_r) = e(N - n),$$

$$E_r = - \frac{dU}{dr},$$

$$n(r) = n_0 \exp \left(- \frac{eU}{kT} - \frac{e^2 E_0^2}{4m\omega^2 kT} \right),$$

$$N(r) = N_0 \exp \left(- \frac{eU}{kT} - \frac{e^2 E_0^2}{4M\omega^2 kT} \right).$$

The difficulty in the numerical solution stems from the large ratio of two lengths of physical significance, namely the skin depth and the Debye length. If the equa-

tions are considered in cartesian, rather than polar coordinates, and if, in addition, E_0 is assumed to be negligibly small, then the system reduces to

$$\begin{aligned}dE/dx &= N(x) - n(x), \\E(x) &= -dU/dx, \\n(x) &= n_0 \exp(CU), \\N(x) &= N_0 \exp(-CU),\end{aligned}$$

up to constant factors. This can be written as a second-order equation

$$d^2U/dx^2 = N_0 \exp(-CU) - n_0 \exp(CU).$$

The additional simplifying assumption $N_0 = n_0 = N^*$, and setting $U = -y$, then leads to

$$y'' = 2N^* \sinh Cy.$$

However, the proper boundary conditions from the original problem, which are actually meaningful only if $E_0 \neq 0$, would be

$$y'(0) = 0, \quad y'(1) = 0,$$

with only the trivial solution $y(x) = 0$ for this oversimplified version.

The physically realistic parameters are $N^* = 50$ and $C = 60$. Therefore, it turns out that the problem with the artificial boundary conditions $y(0) = 0$, $y(1) = 1$ becomes quite trivial; the graph is very close to the limit for $C \rightarrow \infty$ described in Section 3. The initial and final slope are well approximated by Eqs. (3.5) and (3.6). But this solution bears no relation to the physical problem since it is known that, for nonvanishing E_0 , the derivative of $y(x)$ is never very large.

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