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Numerical methods for a singular boundary value problem with application to a heat conduction model in the human head

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Abstract

A class of singular boundary value problems modeling the heat conduction in the human head is studied. Suitable singular Cauchy problems are considered in order to determine one parameter families of solutions in the neighborhood of the singularities. These families are then used to construct stable shooting algorithms to the solution of the considered problems. A finite difference method is also introduced and, taking into account the behavior of the solution in the neighborhood of the singular points, a variable substitution is proposed to improve its convergence order. Numerical results are presented and discussed.

Key words: Singular boundary value problems, one-parameter families of solutions, shooting method, degenerate laplacian, finite difference
MSC 2000: 65L05

1 Introduction

In this paper we consider the following boundary value problem (BVP)

$$\left(\left|y'(x)\right|^{m-2} y'(x)\right)' + \frac{N-1}{x}\left|y'(x)\right|^{m-2} y'(x) = f(y), 0 < x < 1 \qquad (1)$$

$$y'(0) = 0, \qquad (2)$$

$$ay(1) + by'(1) = c, \qquad (3)$$

where we assume that $m > 1$ and $N \geq 1$, $a > 0$, $b \geq 0$ and $c \geq 0$. The source function f has the form

$$f(y) = -\alpha e^{-\beta y}, \quad \alpha > 0, \beta > 0. \qquad (4)$$

The motivation for studying problem (1)-(4) comes from a mathematical model for the distribution of heat sources in the human head. This model was originally described by U.Flesh [3] and B.Gray [4]. In [1], N. Anderson and A. Arthurs have analysed the same problem, which they describe in the form of the following BVP

$$y''(x) + \frac{2}{x} y'(x) + \frac{q(y)}{K} = 0, \qquad 0 < y < R; \tag{5}$$

$$y(0) - finite, \qquad -Ky'(R) = \beta(y(R) - \theta_a); \tag{6}$$

here q is the heat conduction rate per unit volume, y is the absolute temperature; x is the radial distance from the center; K is the termal conductivity (average) inside the head, β is a heat exchange coefficient and θ_a is the ambient temperature. The source function q has the form

$$q(y) = \alpha e^{-My/\alpha}, \tag{7}$$

where M and α are positive constants. In [1], the authors have used complementary variational principles to obtain approximate solutions of this problem. In [2], R.Duggan and A.M.Goodman have considered the same problem and computed lower and upper bounding functions (which in the literature also known as upper and lower solutions). In this way, they have obtained more accurate numerical results, which is verified by the closeness of the computed bounding functions. In [8] and [9] the authors have used a finite difference scheme to obtain the solution of a wider class of problems: instead of the linear differential operator $Ly = y''(x) + \frac{2}{x} y'(x)$ they have considered $\frac{(p(x)y'(x))'}{p(x)}$, where $p(x) = x^{b_0}$, with $b_0 \geq 1$. This operator reduces to Ly when $b_0 = 2$. They have also introduced the boundary condition $y'(0) = 0$, which in this case is equivalent to the condition that y is bounded at the origin. The problem (1)-(4), considered in the present paper, is also a generalization of (5), (6), where we replace the linear differential operator Ly by

$$x^{1-N} \left(x^{N-1} |y'(x)|^{m-2} y'(x) \right)',$$

which represents the radial part of the N-dimensional m-laplacian. As it can be easily seen, this operator reduces to Ly when $m = 2$ and $N = 3$. The physical meaning of introducing the m-laplacian in heat conduction problems is that we replace the usual Fourier law, according to which the module of the heat flux is proportional to the module of the temperature gradient, by a generalized Fourier law, which states that the module of the heat flux is proportional to a certain power $(m-1)$ of the module of the temperature gradient. This generalized Fourier law is usually applied to describe heat conduction in non-homogeneous media and therefore it seems reasonable to use it when modeling the human head.

The problem (1)-(3) is singular, in order to the independent variable, at $x = 0$ due to the division by zero on the second term of the right-hand side of (1), but also in order to the dependent variable whenever $m > 2$, due to the boundary condition (2).

Our main concern will be the study of the behavior of the solution in the neighborhood of this singular point. This is what we will do in the next section, where we determine one parameter families of solutions of the singular Cauchy problem (1), (2).

Based on that behavior, in section 3 we will introduce a stable shooting algorithm, using the same approach as we did in [6] and [7]; the family of solutions parameter is varied in order to satisfy condition (3). In section 4 we apply a finite difference scheme to solve the problem; in order to improve its convergence order, a variable substitution is introduced, which takes into account the asymptotic behavior of the solution.

2 Behavior of the solution in the neighborhood of the singularity $x = 0$

Consider the following singular initial value problem

$$\begin{aligned} \left(\left|y'(x)\right|^{m-2} y'(x)\right)' + \frac{N-1}{x}\left|y'(x)\right|^{m-2} y'(x) &= f(y), \quad x > 0 \qquad (8) \\ y(0) = y_0, \quad \lim_{x\to 0^+} xy'(x) &= 0, \qquad (9) \end{aligned}$$

where $f(y)$ is defined by (4).

Let us look for a solution of this problem in the form:

$$\begin{aligned} y(x) &= y_0 - Cx^k(1 + o(1)) \qquad (10) \\ y'(x) &= -Ckx^{k-1}(1 + o(1)) \\ y''(x) &= Ck(k-1)x^{k-2}(1 + o(1)), \quad x \to 0^+ \end{aligned}$$

where C is a positive constant and $k > 1$. If we substitute (10) in (8) we obtain

$$k = \frac{m}{m-1}, \quad k - 1 = \frac{1}{m-1} > 0, \text{and } C = \frac{1}{k}\left(\frac{\alpha e^{-\beta y_0}}{N}\right)^{k-1}. \qquad (11)$$

In order to improve representation (10) we perform the variable substitution

$$y(x) = y_0 - Cx^k(1 + g(x))$$

obtaining the Cauchy problem in the new unknown g:

$$\begin{aligned} \frac{m-1}{kN}\left[k(k-1)(1+g) + 2kxg' + x^2g''\right]\left[1 + g + \frac{x}{k}g'\right]^{m-2} + \\ + \frac{N-1}{N}\left[1 + g + \frac{x}{k}g'\right]^{m-1} &= e^{C\beta x^k(1+g)} \qquad (12) \\ g(0) = 0, \quad \lim_{x\to 0^+} xg'(x) &= 0. \qquad (13) \end{aligned}$$

Leu us seek for a particular solution of problem (12), (13) in the form

$$g_p(x, y_0) = \sum_{l=0,j=0,l+j\geq 1}^{+\infty} g_{l,j}\left(y_0\right) x^{l+j\frac{m}{m-1}}, \quad 0 \leq x \leq \delta\left(y_0\right), \ \delta\left(y_0\right) \geq 0. \qquad (14)$$

The coefficients $g_{l,j}$ depending on y_0 may be determined by formally inserting (14) in (12), resulting for $l = 0$ and $j = 1$:

$$g_{0,1} = \frac{CN\beta}{2(m - N + mN)}. \qquad (15)$$

We will now prove that the particular solution (14) is, in fact, the only solution of problem (12), (13).

Performing the variable substitutions $z_1 = g$, $z_2 = xg'$, the initial problem (12), (13) rewrites

$$\begin{aligned} xz' &= Az + F(x,z) + H(x) \\ z(0) &= 0 \end{aligned}$$

where $z = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$, $A = \begin{pmatrix} 0 & 1 \\ -\frac{mN}{(m-1)^2} & -\frac{m+N}{m-1} \end{pmatrix}$, $F(x,z) = \begin{pmatrix} 0 \\ f(x,z_1,z_2) \end{pmatrix}$, $H(x) = \begin{pmatrix} 0 \\ H(x) \end{pmatrix}$,

$f(x,z_1,z_2) = \frac{kN}{m-1} e^{Cx^k\beta} \left[\left(1 + z_1 + \frac{1}{k} z_2\right)^{2-m} e^{Cx^k\beta z_1} - 1 \right]$ and $H(x) = \frac{kN}{m-1}\left(e^{Cx^k\beta} - 1\right)$.

Since the eigenvalues of the matrix A are $\lambda_1 = -\frac{m}{m-1} < 0$ and $\lambda_2 = -\frac{N}{m-1} < 0$, theorem 5 of [5] states that problem (12), (13) has a unique solution. Therefore it has no other solution than g_p.

Returning to the initial variable we easily obtain the following result.

Theorem 1 *For each $y_0 > 0$, problem (8), (9) has, in the neighborhood of $x = 0$, a unique holomorphic solution that can be represented by*

$$y(x, y_0) = y_0 - Cx^k \left(1 + g_{0,1} x^k + o(x^k)\right),$$

where k, C and $g_{0,1}$ are given by (11) and (15), respectively.

3 A shooting algorithm

As we have done in previous works for different classes of boundary value problems (see, for example, [6] and [7]), in this section we implement a shooting algorithm basing us on the behavior of the solution in the neighborhood of the singular point $x = 0$.

In order to do that, we consider the following regular initial value problem

$$\begin{aligned} \left(|y'(x)|^{m-2} y'(x)\right)' &+ \frac{N-1}{x} |y'(x)|^{m-2} y'(x) = f(x,y), \\ y(\delta) &= y_0 - C\delta^k \left(1 + g_{0,1}\delta^k\right) \\ y'(\delta) &= \left[\frac{d}{dx}\left(y_0 - Cx^k \left(1 + g_{0,1} x^k\right)\right)\right]_{x=\delta} \end{aligned}$$

for a certain value of $y_0 > 0$ and δ small. This problem can be solved by any standard numerical method (in our case we have used the NDSolve package of *Mathematica*[10]). Starting with an initial value for y_0 (see Remark 2 below), this value is adusted by an iterative process, in order to make the solution of the initial value problem satisfy the boundary condition (3).

Remark 2 *The performance of the shooting method depends strongly on the choice of the initial value for* y_0*. In our case, such initial value can be obtained in a straightforward way. Consider an approximation of the solution of the Cauchy problem (8)-(9), whose form is given by Theorem 1 (retaining only the first two terms of the series):*

$$\bar{y}(x, y_0) = y_0 - Cx^k \left(1 + g_{0,1}x^k\right). \tag{16}$$

Replacing y *by* $\bar{y}$ *in the boundary condition (3), we obtain an equation that can be solved with respect to* y_0*. The value of* y_0 *obtained as the root of this equation has proved to be a good initial guess for the shooting method. (In all the cases considered in the present paper it gives an approximation of the exact value with 2-3 correct digits).*

In order to compare our results with the ones obtained by other authors, in our numerical experiments we have considered two test cases: 1) boundary condition (3) with $a = 1$, $b = 1$, $c = 0$; 2) boundary condition (3) with $a = 0.1$, $b = 1$, $c = 0$.

In table 1 and figure 1a) we display some numerical results for test case 1, with different values of m. The corresponding results for test case 2 are displayed in table 2 and figure 1b).

In all the cases, we have considered $N = 3$, $\alpha = \beta = 1$.

Comparing with the values presented in [9] (in the case $m = 2$) we verify that we have 6-7 coincident digits in all the results.

x	$y(x)$		
	$m = 1.5$	$m = 2$	$m = 3$
0.0	0.11966751	0.36751685	0.72268138
0.2	0.11943427	0.36289409	0.69859859
0.4	0.11779993	0.34894843	0.65405874
0.6	0.11335039	0.32544353	0.59538138
0.8	0.10462835	0.29197111	0.52437832
1.0	0.09008105	0.24792773	0.44175312

Table 1: Numerical solution of problem (1)-(4) when $N = 3$, $a = b = 1$, $c = 0$ and $\alpha = \beta = 1$ obtained with the shooting algorithm.

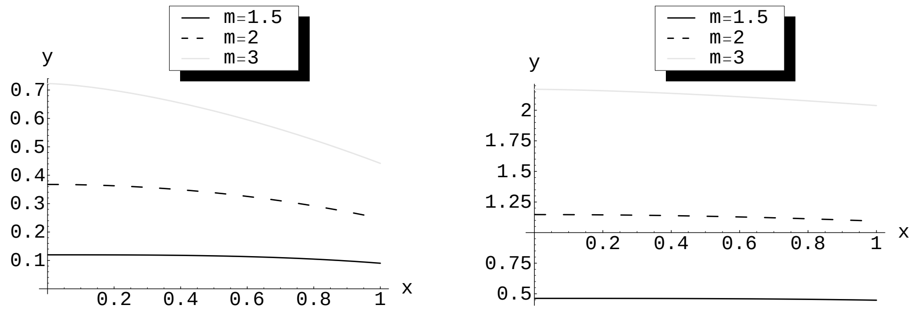
4 A finite difference scheme

Finite difference schemes are often used to obtain approximate solutions of boundary value problems, but it is known that the convergence order of such methods may decrease in the presence of singularities.

In order to discretize (1)-(4), we introduce in the interval $[0, 1]$ a uniform grid of stepsize $h = \frac{1}{n}$ defined by the gridpoints $x_i = ih$, $i = 0, \ldots, n$. At every point x_i, $i = 1, \ldots, n-1$, approximations for the first and second derivative of the solution are

x	$y(x)$		
	$m = 1.5$	$m = 2$	$m = 3$
0.0	0.46221338	1.14703907	2.17105340
0.2	0.46209582	1.14492055	2.15940415
0.4	0.46127247	1.13854877	2.13798668
0.6	0.45903426	1.12787477	2.11002292
0.8	0.45466122	1.11281554	2.07656772
1.0	0.44740965	1.09325196	2.03816311

Table 2: Numerical solution of problem (1)-(4) when $N = 3$, $a = 0.1$, $b = 1$, $c = 0$ and $\alpha = \beta = 1$ obtained with the shooting algorithm.



a) b)

Figure 1: Approximate solutions of problem (1)-(4) with $N = 3$, $b = 1$, $c = 0$, $\alpha = \beta = 1$ and a) $a = 1$, b) $a = 0.1$.

given by the first and second central differences formulas:

$$y'(x_i) \simeq \frac{y(x_{i+1}) - y(x_{i-1})}{2h} = y_i',$$
$$y''(x_i) \simeq \frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2} = y_i'',$$

respectively.

The derivatives at the endpoints $x = 0$ and $x = 1$ are approximated by the second order formulae

$$y'(0) = \frac{1}{2h}\left(-3y(0) + 4y(h) - y(2h)\right) + O(h^2)$$
$$y'(1) = \frac{1}{2h}\left(3y(1) - 4y(1-h) + y(1-2h)\right) + O(h^2).$$

In this way we obtain a discretized problem which is solved by the Newton method. As an initial approximation for the iterative process we have used the function $\bar{y}$, defined by (16), where y_0 is determined as described in Remark 2.

Some numerical results obtained by this finite difference method, with $h = \frac{1}{1000}$, are presented in table 3, for test case 1, and in table 4, for test case 2. In all the considered

x	$y(x)$		
	$m=1.5$	$m=2$	$m=3$
0.0	0.11966736	0.36751677	0.72268090
0.2	0.11943410	0.36289402	0.69859866
0.4	0.11779978	0.34894837	0.65405878
0.6	0.11335026	0.32544348	0.59538141
0.8	0.10462823	0.29197106	0.52437835
1.0	0.09008093	0.24792768	0.44175314

Table 3: Numerical solution of problem (1)-(4) with $N = 3$, $a = b = 1$, $c = 0$ and $\alpha = \beta = 1$ obtained with the finite difference scheme.

x	$y(x)$		
	$m=1.5$	$m=2$	$m=3$
0.0	0.46221308	1.14703897	2.17105331
0.2	0.46209552	1.14492045	2.15940433
0.4	0.46127218	1.13854870	2.13798684
0.6	0.45903397	1.12787471	2.11002307
0.8	0.45466093	1.11281547	2.07656787
1.0	0.44740937	1.09325190	2.03816325

Table 4: Numerical solution of problem (1)-(4) with $N = 3$, $a = 0.1$, $b = 1$, $c = 0$ and $\alpha = \beta = 1$ obtained with the finite difference scheme.

cases the number of iterations of the Newton method was never greater than four. We see that these numerical results are in good agreement with the ones obtained by the shooting method; they are also consistent with the results presented in [9]. In order to estimate the convergence order of the finite difference method at $x = 0$, we have carried out several experiments with different values of the step size h (see table 5) and used the formula

$$c_{y_0} = -\log_2 \frac{|y_0^{h_3} - y_0^{h_2}|}{|y_0^{h_2} - y_0^{h_1}|}, \tag{17}$$

where $y_0^{h_i}$ is the approximate value of y_0 obtained with stepsize h_i (the stepsizes satisfy the relation $h_i = \frac{h_{i-1}}{2}$, $i = 1, 2, 3, 4$. The results for test case 1 are presented in table 6.

The results of table 6 show that the convergence order estimates are very close to 2 when $m = 2$ and decrease when $m > 2$. This is not surprising if we take into account the behavior of the solution in the neighborhood of $x = 0$. When $m = 2$, according to Theorem 1, the solution behaves as the function $y_0 - Cx^2$, as x approaches zero. When $m < 2$, we have $k = \frac{m}{m-1} > 2$ and therefore the solution in the neighborhood of the origin behaves as $y_0 - Cx^\gamma$, $\gamma > 2$, so its second derivative vannishes at the origin.

The same can not be said whenever $m > 2$. As it can be easily seen, in this case the solution behaves near the as $y_0 - Cx^\gamma$, $\gamma < 2$, that is, the second derivative tends to infinity as x tends to 0. In order to overcome this problem, for $m > 2$ we introduce

	$h=\frac{1}{100}$	$h=\frac{1}{200}$	$h=\frac{1}{400}$	$h=\frac{1}{800}$
$m=1.5$	0.11965587	0.11966455	0.1196674	0.11966729
$m=2$	0.36751218	0.36751565	0.36751652	0.36751674
$m=3$	0.72266092	0.72267490	0.72267928	0.72268070
$m=4$	0.95008029	0.95015003	0.95017705	0.95018761
$m=5$	1.10780678	1.10793122	1.10798279	1.10800429
$m=6$	1.22384813	1.22400230	1.22406844	1.22409701

Table 5: Approximate solution of y_0 when $N=3$, $a=b=1$, $c=0$ and $\alpha=\beta=1$ for different values of h.

	$m=1.5$	$m=2$	$m=3$	$m=4$	$m=5$	$m=6$
$h_1=\frac{1}{200}$	1.99	1.98	1.62	1.36	1.26	1.21
$h_1=\frac{1}{100}$	1.99	2.00	1.67	1.37	1.27	1.22

Table 6: Estimates of the convergence order at $x=0$ when $N=3$, $a=b=1$, $c=0$ and $\alpha=\beta=1$ for different values of m.

the variable substitution

$$t=x^{\frac{k}{2}}, \quad k=\frac{m}{m-1}. \tag{18}$$

The solution in the new variable t always behaves as y_0-Ct^2 as t approaches zero (for any value of m). Therefore, the variable substitution (18) enables us to recover the second order of convergence. Some numerical results obtained by the finite difference method, using this variable substitution, are presented in table 7. The corresponding estimates of the convergence order are given in table 8. These results confirm the above arguments.

	$h=\frac{1}{100}$	$h=\frac{1}{200}$	$h=\frac{1}{400}$	$h=\frac{1}{800}$
$m=1.5$	0.11966680	0.11966730	0.11966743	0.11966746
$m=2$	0.36751218	0.36751565	0.36751652	0.36751674
$m=3$	0.72266938	0.72267838	0.72268064	0.72268121
$m=4$	0.95017870	0.95019052	0.95019349	0.95019423
$m=5$	1.10800242	1.10801543	1.10801870	1.10801951
$m=6$	1.22410108	1.22411444	1.22411779	1.22411863

Table 7: Approximate values of y_0 when $N=3$, $a=b=1$, $c=0$ and $\alpha=\beta=1$ for different step sizes of the finite difference scheme with variable substitution.

5 Conclusions

In this paper, for a class of singular boundary value problems arising in the modeling of heat conduction problems in the human head, numerical methods where implemented, based on the asymptotic behavior of the solution in the neighborhood of the singular

	$m = 1.5$	$m = 2$	$m = 3$	$m = 4$	$m = 5$	$m = 6$
$h_1 = \frac{1}{200}$	2.11	1.98	1.99	2.00	2.01	2.00
$h_1 = \frac{1}{100}$	1.94	2.00	1.99	1.99	1.99	2.00

Table 8: Estimates of the convergence order at $x = 0$ when $N = 3$, $a = b = 1$, $c = 0$ and $\alpha = \beta = 1$ of the finite difference scheme with variable substitution.

point $x = 0$: a shooting algorithm and a finite difference scheme, whose convergence order is increased by a simple variable substitution.

We remark that in the case $m = 2$ (which was also considered by the authors of [8] and [9]), our results suggest that second order convergence can be achieved even with a classical finite difference scheme (in spite of the singularity at $x = 0$). For the case $m > 2$, a classical finite difference scheme would not provide second order convergence, due to the behavior of the solution in the neighborhood of the origin. However, our numerical experiments suggest that second order convergence can be obtained even in this case, by introducing a variable substitution which makes the solution smooth near the origin.

In the future we intend to provide a detailed numerical analysis and, in particular, a theoretical justification for the convergence order of the considered method, when applied to this singular BVP. We are also planning to use extrapolation methods to accelerate the convergence.

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