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Qualitative behavior and computation of multiple solutions of singular nonlinear boundary value problems

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We consider boundary value problems of the form

$$y'' = -f(t, y), \quad y(0) = 0, \quad y(1) = 0,$$

motivated by examples where $f(t, y) = \phi(t)g(y)$ and $g(y)$ behave like $y^{-\lambda}$ ($\lambda > 0$) as $y \rightarrow 0^+$. We explore conditions under which such problems have multiple positive solutions, investigate qualitative behavior of these solutions, and discuss computational methods for approximating the solutions.

1. Introduction

The present work is a first attempt to understand singular boundary value problems with multiple solutions. As such, it seeks to combine research on singular boundary value problems having unique solutions that began with the paper of Taliaferro [1979] with work on nonsingular boundary value problems having multiple solutions that received impetus from the paper by Henderson and Thompson [2000] but dates back at least to work by Parter [1974]. The majority of later papers dealt with theoretical questions of existence, but a few, such as [Baxley 1995; Baxley and Thompson 2000; Ballard et al. 2006], have dealt with computational questions.

We shall focus here on two examples, which have the form

$$y'' = -f(t, y), \quad 0 < t < 1, \tag{1}$$

$$y(0) = 0, \quad y(1) = 0, \tag{2}$$

where the nonlinear function $f(t, y)$ is positive and singular as $y \rightarrow 0^+$ and may also be singular as $t \rightarrow 0^+$ or $t \rightarrow 1^-$.

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Taliaferro [1979] considered the case

$$f(t, y) = \frac{\phi(t)}{y^\lambda},$$

where $\lambda > 0$ and ϕ is continuous on $(0, 1)$. He proved the existence of a unique positive solution if

$$\int_0^1 t(1-t)\phi(t) dt < \infty.$$

He then described the asymptotic behavior at the endpoints of this solution $y(t)$. For example, if

$$\int_0^{1/2} \phi(t)t^{-\lambda} dt < \infty,$$

then the slope of the solution $y(t)$ is finite at $t = 0$. If this integral is infinite and, for example, $\phi(t) \sim t^\alpha$, as $t \rightarrow 0^+$, where $-2 < \alpha \leq \lambda - 1$, then the slope of the solution is infinite at $t = 0$ and Taliaferro [1979] provides the detailed asymptotic behavior. Note that for these results, the function $f(t, y)$ is decreasing in y for fixed t and tends to ∞ as $t \rightarrow 0^+$.

To compute the positive solution to such a problem, the papers [Baxley 1995; Baxley and Thompson 2000] took advantage of the known asymptotic behavior of the solution at the endpoints to design a shooting method. Basically, the interval $[0, 1]$ was replaced by a slightly smaller interval $[a, b]$ and the asymptotic knowledge was used to design an initial value problem at a and a terminal value problem at b , each depending on a parameter. These problems were solved using an initial value method such as that of Runge–Kutta–Fehlberg and parameters were adjusted by a modified Newton method until the solutions met at $t = 1/2$ with essentially the same slope and altitude.

Henderson and Thompson [2000] dealt with the problem (Equation (1), (2)) in the autonomous case $f(t, y) = f(y)$ with $f(y)$ continuous for $y \geq 0$. They gave conditions under which the problem has at least three positive solutions, and the behavior of $f(y)$ which triggered the multiple solutions was, in contrast to Taliaferro [1979], a tendency for $f(y)$ to increase. Specifically, they required that there be numbers $0 < a < b < 2b$ so that $f(y)$ is much larger on the interval $[b, 2b]$ than on the interval $[0, a]$.

Henderson and Thompson [2000] also provided qualitative information about the size of the three positive solutions, and this knowledge was used in [Ballard et al. 2006] to compute solutions to such nonsingular problems. Since this qualitative knowledge has a global character and gives no information about the behavior near endpoints, the problem was discretized on the interval $[0, 1]$ and an iterative method was used to obtain rough approximations to the solutions. The values of these approximations near the endpoints were then used to estimate slopes at the

endpoints and these estimates were used to seed a shooting method similar to that used earlier on the Taliaferro problems.

The last example discussed in [Ballard et al. 2006] is singular and was designed by modifying an example in [Baxley 1995] so that the singular nonlinearity $f(t, y)$ exhibited also the behavior required in [Henderson and Thompson 2000]. The solution of the original example has finite slope at both endpoints. The computational work indicates that the problem has three solutions, each having finite slopes at the endpoints.

2. Solutions with finite slopes at endpoints

We begin with a synopsis of the last example considered in [Ballard et al. 2006].

Example 2.1. For $0 < t < 1$, let

$$f(t, y) = \begin{cases} \frac{2\sqrt{t(1-t)}}{\sqrt{y}}, & 0 < y \leq 1, \\ 2\sqrt{(2-y)t(1-t) + 400(y-1)}, & 1 < y < 2, \\ 40, & 2 \leq y. \end{cases}$$

According to [Taliaferro 1979] (or see the generalization in [Baxley 1991]), we would expect solutions to exist and have finite slopes at the endpoints $t = 0$ and $t = 1$ since $f(t, \theta t)$ is integrable in a neighborhood of $t = 0$ and $f(t, \theta(1-t))$ is integrable in a neighborhood of $t = 1$, for each constant $\theta > 0$. Further, one easily verifies that $f(t, y)$ satisfies the Henderson–Thompson type estimates

$$\begin{aligned} f(t, y) &< 8a, & \alpha \leq y \leq \alpha + a, \\ f(t, y) &> 16b, & b \leq y \leq 2b, \\ f(t, y) &< 8c, & \alpha \leq y \leq \alpha + c, \end{aligned}$$

where $\alpha = 1/32$, $a = 1$, $b = 2$, $c = 6$, so one might hope that Equations (1) and (2) will have three positive solutions. Note that the theory in [Taliaferro 1979] and [Baxley and Thompson 2000; Henderson and Thompson 2000] cannot actually be applied to this example, but work in progress will extend the results of Taliaferro [1979] and Henderson and Thompson [2000] to such problems.

Our method, used in [Ballard et al. 2006], is basically a two-step procedure. Step 2 is a shooting method and for each solution $y(t)$, we need approximate values of $y'(0)$ and $y'(1)$ to seed the method. Then we can choose a slightly smaller subinterval $[a, b]$ of $[0, 1]$ and use the asymptotic formulas of Taliaferro [1979] to estimate the values of $y(a)$, $y'(a)$ and $y(b)$, $y'(b)$. Employing any dependable initial value solver, such as RKF45, we can then solve the resulting initial value problem on $[0, 1/2]$ and the terminal value problem on $[1/2, 1]$. The initial approximations of $y'(0)$, $y'(1)$ can then be adjusted by a modified Newton method until these two

solutions meet at $t = 1/2$ with essentially the same altitude and slope. Details of such a shooting method appear in [Baxley 1995; Baxley and Thompson 2000; Ballard et al. 2006].

Thus step 1 of our method is designed to produce reasonably good approximations for $y'(0)$ and $y'(1)$ for each of the three solutions. For this purpose, we discretize the problem by dividing the interval $[0, 1]$ into $n + 1$ equal parts at the mesh points $t_i = i/(n + 1)$ and seek to approximate $y(t_i)$, for $i = 1, 2, \dots, n$. We approximate the second derivative as usual with the central divided difference quotient

$$y''(t_k) \approx \frac{1}{h^2} \left(y(t_{k+1}) - 2y(t_k) + y(t_{k-1}) \right),$$

where $h = 1/(n + 1)$. Letting y_i be our approximation for $y(t_i)$ and Y be the n -dimensional column vector with components y_i , our discrete problem is

$$\frac{1}{h^2} AY = F(T, Y), \quad (3)$$

where T is the n -vector with components t_i , $F(T, Y)$ is the n -vector with components $f(t_i, y_i)$, and A is the matrix

$$A = \begin{bmatrix} -2 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -2 \end{bmatrix}.$$

Note that the boundary conditions $y(0) = 0$, $y(1) = 0$ have been used to obtain this formulation. We rewrite Equation (3) in the fixed point form

$$h^2 A^{-1} F(T, Y) = Y, \quad (4)$$

and then use iteration to obtain three solutions Y_1, Y_2, Y_3 of this problem that are viewed as crude approximations for y_1, y_2, y_3 at the mesh points.

Based on qualitative estimates in [Henderson and Thompson 2000], we expect Y_1 (the “small” solution) to have a maximum less than 1, Y_2 , to have a maximum greater than 1, but a value at $1/4$ less than 2, and Y_3 (the “large” solution) to have a value at $1/4$ greater than 2. So we seed the iteration with initial vectors which satisfy these requirements. It turns out that Y_1 and Y_3 are attractors for this discrete problem, but Y_2 is a repeller. So, we “back” into an approximation for Y_2 by using averages of approximations for Y_1 and Y_3 ; details can be found in [Ballard et al. 2006], where one can find numerical results of the full computation. The same method will be used below.

3. Solutions with infinite slopes at endpoints

Example 3.1. For $0 < t < 1$, we now let

$$f(t, y) = \begin{cases} \frac{3(1-t)^2 + 4t(1-t) + 4t^2}{16t^{3/2}(1-t)y}, & 0 < y \leq 1, \\ (2-y) \frac{3(1-t)^2 + 4t(1-t) + 4t^2}{16t^{3/2}(1-t)} + 40(y-1), & 1 < y < 2, \\ 40, & 2 \leq y. \end{cases}$$

The asymptotic formulas in [Taliaferro 1979] (see also [Baxley and Thompson 2000, Theorem 10], [Baxley and Martin 2000, Lemma 12]) suggest that solutions to Equation (1) and (2) should now have infinite slope at both endpoints. Also the behavior of $f(t, y)$ resembles that of the first example, so it seems likely that there will be three solutions.

If $y(t)$ is any solution of Equation (1) and (2), then $y(t)$ is near zero in a neighborhood of the endpoints. Thus to examine asymptotic behavior near the endpoints, we let

$$\phi(t) = \frac{3(1-t)^2 + 4t(1-t) + 4t^2}{16t^{3/2}(1-t)},$$

and we see that

$$\phi(t) \sim \frac{3}{16}t^{-3/2}, \quad \text{as } t \rightarrow 0^+; \quad \phi(t) \sim \frac{1}{4}(1-t)^{-1}, \quad \text{as } t \rightarrow 1^-.$$

Thus the asymptotic formulas in Taliaferro [1979], Baxley [1995], and Baxley and Thompson [2000] indicate that any solution $y(t)$ of Equation (1) and (2) will exhibit the asymptotic behavior

$$y(t) \sim Qt^{(\alpha+2)/(\lambda+1)} = Qt^{1/4}, \quad \text{as } t \rightarrow 0^+, \quad (5)$$

where $\alpha = -1.5$, $\lambda = 1.0$, and

$$Q = \left(\frac{3(\lambda+1)^2}{16(\alpha+2)(\lambda-\alpha-1)} \right)^{1/(\lambda+1)} = 1.$$

A similar analysis leads to

$$y(t) \sim (1-t)^{1/2}, \quad \text{as } t \rightarrow 1^-. \quad (6)$$

To compute approximations for these three solutions, the overall strategy is the same as before. We wish to use shooting, taking advantage of the asymptotic formulas (5) and (6) as we did in [Baxley 1995; Baxley and Thompson 2000], but as before we need a first step to find crude approximations for the three solutions.

In our first effort, we used the same iteration scheme as in Example 2.1, but found that it gave poor accuracy. After some confusion, we discovered that the

problem lay in the matrix A , and the correction comes from a careful analysis of our approximation for $y''(t_k)$.

Approximating $y'(t_k)$ with a backward difference quotient

$$y'(t_k) \approx \frac{y(t_k) - y(t_{k-1})}{h},$$

where $h = t_k - t_{k-1}$, we then approximate $y''(t_k)$ with a forward difference quotient

$$y''(t_k) = \frac{y'(t_{k+1}) - y'(t_k)}{h}.$$

We combine these to get the usual second order divided difference quotient. But if we focus on an endpoint, say t_1 , we are led, in the approximation for $y''(t_1)$, to replace $y'(t_1)$ with $y(t_1)/h$. This, it turns out, is a blunder. To see why, we apply Equation (5) to conclude

$$y'(t) \sim \frac{1}{4}t^{-3/4}, \quad \text{as } t \rightarrow 0^+, \quad \text{and} \quad \frac{y(t)}{t} \sim t^{-3/4}, \quad \text{as } t \rightarrow 0^+.$$

Thus

$$y'(t) \sim \frac{1}{4} \frac{y(t)}{t}, \quad \text{as } t \rightarrow 0^+.$$

Therefore, a better approximation for $y'(t_1)$ is $\frac{1}{4} \frac{y(t_1)}{h}$, which leads to the approximation

$$y''(t_1) \approx \frac{-\frac{5}{4}y(t_1) + y(t_2)}{h^2}.$$

A similar analysis shows that a better approximation for $y''(t_n)$ is

$$y''(t_n) \approx \frac{y(t_{n-1}) - \frac{3}{2}y(t_n)}{h^2}.$$

So we modify the earlier matrix A to obtain instead

$$A = \begin{bmatrix} -\frac{5}{4} & 1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -2 & 1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -\frac{3}{2} \end{bmatrix}.$$

4. Numerical calculations

We now discuss numerical calculations for Example 3.1, beginning with the approximation of the larger solution y_3 . For the results reported here, we began by dividing our interval $[0, 1]$ into 8 equal parts, seeking approximations of $y_3(t_k)$,

	$y_3(1/32)$	$y_3(1/4)$	$y_3(1/2)$	$y_3(31/32)$
unmodified A	0.5853	3.6660	4.8982	0.5347
modified A	2.2798	5.1757	6.1415	1.2206

Table 1. Results of discrete iteration for large solution.

where $t_k = k/8$, $k = 1, 2, \dots, 7$. We seeded the iteration with the vector $Y = (1.8, 2.4, 2.7, 3.0, 2.7, 2.4, 1.8)$. Of course, we do not expect the solution to be symmetric about $t = 0.5$, but otherwise this approximation has roughly the right shape, with the value at $t = 1/4$ greater than 2, and the value at $t = 1/2$ less than 6. We iterated the fixed point form Equation (4) (with the 7×7 matrix A) 7 times, then extended this approximation, dividing the interval into 16 equal parts, by linear interpolation (we approximated $y(1/16) = 0.6y(1/8)$ and $y(15/16) = 0.6y(7/8)$). We then iterated the fixed point form (with the 15×15 matrix A) 7 times. Finally, we doubled the number of subintervals again by the same procedure and iterated 7 times with the 31×31 matrix A . The final iterate is then our approximation for Y_3 , which in turn approximates y_3 . The first component of Y_3 is then our approximation for $y_3(1/32)$, the 15th component is our approximation for $y_3(1/2)$ and the last component is our approximation for $y_3(31/32)$. In Table 1, we report the numerical results, not only using the modified matrix A above but also, for comparison, of the unmodified matrix A used for Example 2.1. Note how significant is the effect of the modification of A . All calculations for this iterative procedure were done using MATLAB. The large solution Y_3 is an asymptotically stable attractor and we obtained the same result with a variety of initial seeds.

The value of our approximation for $y_3(1/2)$ using the modified A is disconcerting, since it exceeds 6.0. We would expect from the qualitative Henderson–Thompson type estimates that the maximum value of our solution would be less than 6.0. This is actually the case, but our initial approximation is too rough to confirm this expectation.

Using the asymptotic estimate $y(t) \sim t^{1/4}$, we expect that $(32)^{1/4}y(1/32) = Q \approx 1.0$. Computing this value from Table 1, we get the value $Q = 5.422$ (resp. $Q = 1.392$) for the modified (resp. unmodified) matrix A . The effect of the modification is clearly large. The asymptotic estimate $y(t) \sim (1-t)^{1/2}$ and the corresponding expectation $(32)^{1/2}y(31/32) = P \approx 1.0$ leads to the value $P = 6.905$ (resp. $P = 3.025$) for the modified (resp. unmodified) matrix A . The import of the difference is fully realized only in passing to step 2 of our procedure and solving Equation (1) and (2) by shooting.

The shooting procedure, using the computed values of Q and P (with the modified A) to seed the shooting, and essentially Newton's method to adjust values of

interval	Q	$y_3(1/4)$	$y_3(1/2)$	P
[.03, .97]	5.118	5.067	6.055	6.650
[.02, .98]	3.916	4.647	5.698	5.265
[.01, .99]	2.491	4.209	5.334	3.661
[.002, .998]	1.298	3.918	5.091	1.890

Table 2. Shooting results for large solution.

Q and P so that the solutions to the appropriate initial and terminal value problems meet at $t = 0.5$ with altitudes and slopes agreeing to two decimal places, led to the results reported in Table 2. Since $1/32 \approx 0.03$, we first solved the boundary value problem, replacing the interval $[0, 1]$ with $[\text{.03}, \text{.97}]$. Note that the values of $Q = 5.118$ and $P = 6.650$ reported in Table 2 are quite close to the seed values predicted by the modified A , but quite far from the seed values predicted by the unmodified A . (In fact, using the seed values from the unmodified A caused our computer program to terminate before completion.) We then enlarged this interval in steps of 0.004 by subtracting 0.002 from the left endpoint and adding 0.002 to the right endpoint and using the final values of Q and P from the previous step as seeds for Q and P on the current step. We report only a few of the results in Table 2, where it is seen that these values of Q and P are indeed moving (slowly) toward 1.0 and the value of the solution at $t = 0.5$ is falling significantly below $y = 6.0$ as expected from the Henderson–Thompson estimates. We also report the value of the solution at $t = 0.25$, where the Henderson–Thompson estimates would expect $y > 2.0$.

All computations involving shooting were done using the FORTRAN subroutine RKF45 [Forsythe et al. 1977] of Shampine and Watts. For these calculations, we only asked RKF45 for three decimal place accuracy and consequently that the altitude and slope of the solution agree to two decimal places at $t = 0.5$. Thus, the results of the shooting procedure should only be trusted to two decimal places. Of course, the difference in the computed solutions and the true solution depends also on replacing the interval $[1, 0]$ by a smaller interval and using the asymptotic formulas to generate initial and terminal conditions. The computation in [Baxley 1991; Baxley and Thompson 2000] suggests that good approximation demands using an interval as large as $[\text{.001}, \text{.999}]$.

We now discuss the smaller solution y_1 . (This solution $y_1(t) = t^{1/4}(1-t)^{1/2}$ is known in closed form [Baxley 1995]; it can be quickly verified by direct substitution.) The iterative procedure using Equation (4) now has interesting features. The iteration exhibits characteristics of a two cycle, but also the two cycle to which the sequence of iterates converges appears to depend on the initial seed, a characteristic

$y_1(1/32)$	$y_1(1/4)$	$y_1(1/2)$	$y_1(31/32)$
0.3903	0.5168	0.4913	0.1623

Table 3. Results of discrete iteration for small solution.

interval	Q	$y_1(1/4)$	$y_1(1/2)$	P
[.03, .97]	.951	.6045	.5898	.981
[.02, .98]	.967	.6079	.5918	.987
[.01, .99]	.983	.6105	.5933	.994
[.002, .998]	.997	.6121	.5942	.999

Table 4. Shooting results for small solution.

of chaotic behavior. This iteration is taking place in a space of dimension 7, then 15, and finally 31. We tried a variety of initial seeds for the iteration and in every case the smaller of the two cycle was a reasonable approximation for the solution y_1 . Some initial seeds provided very good approximations. These approximations were reasonable in the sense that the value of y at $1/32, 31/32$ provided values of Q, P close enough to give convergence of the Newton iterates in the shooting method. In Table 3, we provide results of this iteration, only for the modified matrix A . We seeded the discrete iteration with the vector $Y = (.3, .4, .45, .5, .45, .4, .3)$ and show the results for the smaller member of the resulting two cycle.

$y_2(1/32)$	$y_2(1/4)$	$y_2(1/2)$	$y_2(31/32)$
0.6006	1.1068	1.2415	0.2438

Table 5. Results of discrete iteration for middle solution.

interval	Q	$y_2(1/4)$	$y_2(1/2)$	P
[.03, .97]	1.270	1.122	1.306	1.312
[.02, .98]	1.195	1.116	1.322	1.249
[.01, .99]	1.107	1.110	1.338	1.161
[.002, .998]	1.025	1.107	1.348	1.053

Table 6. Shooting results for middle solution.

Using the values in Table 3 for $y_1(1/32)$ and $y_1(31/32)$, we compute the seed values $Q = 0.93$ and $P = 0.92$ for the shooting method. We report the results of shooting in Table 4. Note that the values of Q and P are now quite close to 1. Also note that the closed form solution gives $y_1(1/4) = 0.6124$ and $y_1(1/2) = 0.5946$, so that our final approximation for y_1 is actually correct to three decimal places.

Finally, we pass to the middle solution y_2 . As indicated earlier, the approximation Y_2 is a repeller for the discrete iteration. We proceed as we did in [Ballard et al. 2006]. We begin with Z_1 and Z_3 , the 31 dimensional vectors which emerge from the discrete iteration as approximations for the solutions Y_1 and Y_3 . We average these two vectors to get a vector Z_2 . We then iterate one time to see if this seed vector is moving toward Z_1 or Z_3 . If it is moving toward Z_1 , we replace Z_1 by Z_2 ; otherwise we replace Z_3 by Z_2 . We repeat this process until Z_1 and Z_3 differ by less than 0.001 in the 16th component. At this point, Z_1 and Z_3 are viewed as both close to the repeller Y_2 , but on opposite sides. However, they are formed from averages of the original Z_1 and Z_3 and as such do not have the appropriate shape for Y_2 . Thus we iterate once beginning with the final Z_1 and once beginning with the final Z_3 . This iteration reshapes Z_1 and Z_3 without serious movement. We then take the average of these reshaped versions as our approximation for Y_2 . In Table 5, we provide the result of this computation.

The values of $y_2(1/32)$ and $y_2(31/32)$ in Table 5 give us the seed values $Q = 1.43$ and $P = 1.38$ for shooting. These results are given in Table 6. Note again that the values of Q and P are moving towards 1.

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