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Letter to the Editors

Solution of Troesch's, and Other, Two Point Boundary Value Problems by Shooting Techniques

In the paper by Roberts and Shipman [1] much work seems to have been undertaken in solving a simple problem. If we define an order of difficulty in solving two point boundary value problems as

(a) one unknown such that the initial estimate allows integration to the end of the shooting range,

(b) more than one unknown such that the initial estimate allows integration to the end of the shooting range,

(c) such a poor initial estimate that integration to the end of the shooting range is not possible,

then Troesch's problem is in the easiest category (a).

In solving Troesch's problem by shooting, the cause of the difficulty is not in the fact per se that a pole can exist within the integration range but that the iteration technique must reject integrations which are divergent in $t < 1$. For example a Newton iteration with step δ can be rejected if the solution to the initial value problem is divergent, and a step $\frac{1}{2}\delta$ can be attempted instead.

In this letter such a technique is used to solve Troesch's problem and produces satisfactory results in a straightforward manner. Solutions to more difficult problems in categories (b) and (c) are also discussed.

(a) Consider Troesch's problem as an example. The problem is to solve

$$\dot{y}_1 = y_2$$
$$\dot{y}_2 = n \sinh ny,$$
$$y_1(0) = 0 \qquad y_1(1) = 1$$

To do this we estimate $y_2(0)$ and integrate to $t = 1$, where we find a calculated $y_1(1)$. We then improve $y_2(0)$ so that $y_1 \to 1$. Two items are important in carrying out this process. The first is to have an initial estimate of $y_2(0)$ such that integration can be made to $t = 1$; the most obvious choice is zero. Secondly, to ensure convergence we require $| y_1^{(m)}(1) - 1 |$ to grow smaller as the iteration number m increases. Thus, in applying Newton's method we halve, if necessary, the indicated change in $y_2(0)$, δ say, until $| y_1^{(m+1)}(1) - 1 | < | y_1^{(m)}(1) - 1 |$. During this process the change δ may give divergence of the initial value problem due to the pole in Troesch's problem. This divergence could for instance be determined by testing $| y_1(t)|$, but this was found impractical as noted later. Once divergence has been detected we reject the change δ and instead use $\frac{1}{2}\delta$ and repeat the process as many times as necessary.

An approximation to the gradient needed in Newton's method is found by making a small change to $y_1^{(m)}(0)$, say Δy (taken as $0.01.8e^{-n}$), and integrating to $t = 1$. The corresponding change in $(y_1^{(m)}(1) - 1)$, say ΔF, then gives

$$\delta = -\frac{y_1^{(m)}(1) - 1}{\Delta F/\Delta y}.$$

Newton's method with modifications as noted above is then applied, and iterations continued until $| y_1^{(m)}(1) - 1 | < 10^{-6}$.

The integration routine used in solving the initial value problem is Gear's [2] nonstiff integration method with accuracy 10^{-6}. The method has automatic step adjustment and, thus, takes care of the large gradients near $t = 1$ by taking smaller steps in the region of difficulty. This feature of taking smaller steps when necessary led to a problem in trying to decide when the initial value problem was divergent. In the first computer run the criterion of divergence was set as $| y_1(t)| > 100$. But with a particular choice of $y_2(0)$ which would have caused divergence it was found that a step length of less than 10^{-14} was required to achieve sufficient accuracy in $y_2(t)$ (which was $0(10^8)$) at $t \simeq 0.95$ thus preventing integration to a point at which $| y_1(t)| > 100$ ($y_1(0.95)$ was approximately 3). Because of this the criteria for divergence were set as $| y_1(t)| > 2$ and also $| y_2(t)| > 10^4$. The second computer run then produced solutions.

The solutions are almost identical to those of Roberts and Shipman except at $n = 5$ where the results of Roberts and Shipman have not converged to sufficient accuracy. The only discrepancy between the results with $n = 6$ or $n = 10$ was for $n = 10$, where this writer's results gave $y_2(1) = 148.4$ compared to 252.7 in [1]. The analytic solution [1, Eq. (8)], gives $y_2(1) = dy/dt(1) \simeq (2 \cosh 10 - 2)^{1/2} = 148.4$.

(b) Provided an initial estimate, that allows integration to the end of the shooting range, is available, application to larger systems follows in a manner similar to that above. However with larger systems a more sophisticated technique for iteration may be desirable. This writer usually uses Powell's technique [3] for minimizing a sum of squares. This technique applied to systems is illustrated in Refs. [4] and [5]. In these papers examples are given in which shooting methods are used to solve the two point boundary value problems resulting from the method of lines solutions to elliptic partial differential equations. It was not necessary to incorporate a divergence criterion in these examples, but it could have been included in the manner described later under (c). In order to integrate to the far end of the shooting range with the initial estimate a perturbation technique was used. The perturbations which were used changed a physical parameter such as Mach number from a small value at which a solution was easily obtained to larger values. For each calculation at a certain Mach number a reasonable estimate of the unknowns was available by extrapolation.

The use of such parameter perturbation is recommended since good initial estimates are clearly desirable in nonlinear problems.

The method of lines solutions mentioned above are a good example of the inherent instability which may be present when solving two point boundary value problems. This instability becomes more dominant as more lines are taken and multipoint methods [8] may eventually be necessary. However there are problems which are sensitive to initial estimates but which can be solved by an adaption of the continuation process. Such a technique for solution is described in (c) below. It will be seen that the method is similar to continuation but is automatic. We may perhaps refer to the method as "automatic continuation."

(c) Suppose that we cannot, with the initial estimate, integrate to the end of the shooting range. Let the unknowns at one end of the range by $y_1, y_2 \cdots y_m$, and let the boundary conditions at the other end ($t = t_f$ say) be $f_1 = f_2 = \cdots = f_m = 0$. Add to the unknowns (y_i) a new variable t_F, say, which represents the end of the shooting range on the current iteration. Add to the criteria $f_i = 0$ (applied at $t = t_F$ now) the extra condition $t_F - t_f = 0$. Thus, we have $m + 1$ equations to be satisfied by $m + 1$ unknowns and the problem is complete. t_F is chosen initially as a sufficiently small fraction of the total shooting range and the modified Newton method or Powell's method proceeds automatically.

To illustrate this technique the solutions to two problems are outlined below. The first is Troesch's problem with a poor initial estimate and the second is the problem due to Holt [6] which has been solved previously by continuation [7].

(i) Consider Troesch's problem with initial estimate $y_2(0) = 2(8e^{-n})$ (if $y_2(0) > 8e^{-n}$ then the pole lies within the integration range) and $t_F = 0.1$. Let the unknowns $y_2(0)$ and t_F be named x_1 and x_2, respectively, and suppose we apply Newton's method. In applying Newton's method changes δ_j are given by

$$\sum_{j=1}^{2} \frac{\partial f_i}{\partial x_j} \delta_j = -f_i \qquad (i = 1, 2),$$

and we approximate

$$\frac{\partial f_i}{\partial x_j} \quad \text{by} \quad \frac{f_i(x_j + \Delta x_j) - f_i(x_j)}{\Delta x_j},$$

where Δx_j is taken as $10^{-6}x_j$ or 10^{-6} if $x_j = 0$. In the above equation $f_1 = y_1(t_F) - 1$ and $f_2 = t_F - 1$. The new values x_j are then $x_j(\text{old}) + \alpha\delta_j$, where $\alpha = 1$ gives the full Newton step. α must be halved until the function $f_1^2 + f_2^2$ decreases. Provided the current point is not a minimum the function is almost guaranteed to decrease since Newton's 'direction' is most likely downhill. However, it may not be downhill for some cases since we approximate the derivatives $\partial f_i/\partial x_j$ by differences (Powell's method [3] is preferable). In Troesch's problem it was always downhill.

Note that in Newton's method the full step $\alpha = 1$ results in t_F being equal to t_f so that integration to the end of the shooting range is achieved. Once the first full step has been taken t_F will always remain equal to t_f. Note also that t_F is less than or equal to t_f for all iterations.

Newton's method modified as above and applied to Troesch's problem gave iterations as shown in Table I. With $n = 5$, 6, and 10 the number of iterations

TABLE I

Newton Iterations on Troesch's Problem

n	Iteration	$y_2(0)$	t_F	$y_1(t_F)$
5	0	0.1078	0.100	0.011
	2	0.3312	0.409	0.259
	4	0.1758	0.668	0.575
	6	0.0651	0.917	0.871
	8	0.0461	1.000	1.022
	10	0.0457	1.000	1.000
10	0	0.726, −3[a]	0.100	0.857, −4
	10	0.908, −1	0.442	0.706
	20	0.396, −1	0.523	0.656
	30	0.105, −1	0.653	0.594
	40	0.245, −2	0.799	0.608
	50	0.358, −3	1.000	1.106
	53	0.356, −3	1.000	1.000

[a] 0.726, −3 is equivalent to 0.726×10^{-3}.

required for convergence were 10, 11, and 53, respectively. It can be seen that when $n = 10$ convergence is slow (although in terms of computer time the method is still efficient), and it may be desirable to use a more efficient technique as described in example (ii) below.

(ii) The problem proposed by Holt [6] is a difficult two point boundary value problem since a slight deviation from the correct values at the beginning of the shooting range can cause divergence of the solution to the initial value problem. The equations to be solved are

$$\dot{y}_1 = y_2,$$
$$\dot{y}_2 = y_3,$$
$$\dot{y}_3 = -\left(\frac{3-n}{2}\right) y_1 y_3 - n y_2^2 + 1 - y_4^2 + s y_2,$$
$$\dot{y}_4 = y_5,$$
$$\dot{y}_5 = -\left(\frac{3-n}{2}\right) y_1 y_5 - (n-1) y_2 y_4 + s(y_4 - 1),$$

subject to

$$y_1(0) = 0 \qquad y_2(0) = 0 \qquad y_4(0) = 0$$

and

$$y_2(t_f) = 0 \qquad y_4(t_f) = 1,$$

where

$$n = -0.1, \qquad s = 0.2, \qquad t_f = 11.3.$$

Powell's method [3] is used to provide the iteration scheme for solving this two point boundary value problem. This method proceeds by minimizing

$$F = y_2^2(t_F) + (y_4(t_F) - 1)^2 + (t_F - 11.3)^2$$

with respect to $y_3(0)$, $y_5(0)$, and t_F. A divergence criterion has to be incorporated in the program so that an iteration in Powell's method will avoid a search in that region. A reasonable divergence criterion for this problem is $|y_2| > 10$. This is included in the program by setting $F = 10^{70}$ if $|y_2|$ becomes greater than 10 during the integration.

The initial estimates were chosen as $y_3(0) = -1$, $y_5(0) = 0.6$, and $t_F = 3.5$. The solution was found in 413 integrations requiring 21 secs on an IBM 360/85. The integration was carried out using Gears nonstiff DIFSUB package [2] with accuracy 10^{-4}. During the iteration procedure the divergence criterion mentioned above was encountered many times as would be expected in this sensitive problem.

In conclusion the combination of methods mentioned by Roberts and Shipman may be unnecessary in solving many two point boundary value problems and certainly it seems unnecessary for Troesch's problem.

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