

The numerical solution of multipoint boundary value problems

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ABSTRACT

Multipoint boundary value problems (MPBVP's) for ordinary differential equations arise naturally in technical applications. For a given dynamic system with n degrees of freedom, there may be available exactly n states observed at n different times. A mathematical description of such a system results in an n -point BVP. The discretization of certain BVP's for partial differential equations over irregular domains with the method of lines also forms MPBVP.

In this paper we are concerned with finding numerical solutions of MPBVP's by converting these to equivalent initial value problems.

1. INTRODUCTION

Generally for the boundary value problems the actual construction of a solution, even though it may be known to exist and to be unique (see, e.g., [10]-[18]) is a more difficult matter than constructing the solution of the equivalent initial value problems, for two point boundary value problems (TPBVP's) "shooting methods" (see [1]-[9]). For numerical solutions of MPBVP's only little work has been done, for example Urabe [19], [20] has used Chebyshev series method, Bellman etc. [21] have used quasilinearization, Meyer [11] has used invariant imbedding and several others have used finite difference methods. Since we will convert MPBVP's to its equivalent initial value problems we shall not only need the existence of the unique solution of the boundary value problem but also need the existence, uniqueness and stability of the initial value problems for the given differential equations.

In 1956 Goodman and Lance [7] developed a practical shooting method (method of adjoints) for TPBVP's. In section 2 it is realized that if the adjoint equations for linear ordinary differential equations are integrated with proper conditions this method can also be used for MPBVP's and we find the set of missing initial conditions in one pass through the process. In section 3 we present that this method can be used directly for the most general linear implicit MPBVP's also. Section 4 deals with another practical method for finding missing initial conditions method of complementary functions which was used previously by Miele [8] for TPBVP's. In section 5 we prove that the method of adjoints and the method of complementary functions are theoretically the same, where as in computational realization both are different and choosing one of them depends

on the particular problem, for TPBVP's see [6]. In section 6 we show how the method of adjoints for linear problems can be applied in an iterative fashion to solve nonlinear MPBVP's. In every iteration we obtain corrections to the trial values for the missing initial conditions. In section 7 we once again use the method of adjoints for most general implicit MPBVP's. In section 8 we prove that the method of adjoints for nonlinear MPBVP's used in an iterative fashion is actually a realization of Newton's method for solving a system of equations. In section 9 we give two linear examples, the first with known analytic solution; the second we have integrated numerically and shown that the results agree with the results obtained in [11] using invariant imbedding. Some nonlinear practical problems and their solutions using the methods of this paper will be published subsequently.

2. GENERAL METHOD OF ADJOINTS

Consider the set of n linear ordinary differential equations with variable coefficients

$$\dot{y} = A(t)y + f(t) \quad (2.1)$$

where

$A(t) = n \times n$ matrix with elements $a_{ij}(t)$, $i, j = 1, 2, \dots, n$

$y(t) = n \times 1$ vector with components $y_1(t), y_2(t), \dots, y_n(t)$

$\dot{y}(t) = n \times n$ vector, derivative of y with respect to t ,

with components, $\dot{y}_1, \dot{y}_2, \dots, \dot{y}_n$

$f(t) = n \times 1$ vector with components $f_1(t), f_2(t), \dots, f_n(t)$.

Our concern is about the solution of (2.1) satisfying the boundary conditions

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$$y_{i_{k_j}}(t_j) = c_{i_{k_j}} \quad (2.2)$$

where $j = 1, 2, \dots, N$ ($2 \leq N \leq n$); $t_1 < t_2 < \dots < t_N$; $k_1 = 1, 2, \dots, k_1$; $k_2 = 1, 2, \dots, k_2$; ...; $k_N = 1, 2, \dots, k_N$ such that

$$\sum_{j=1}^N k_j = n.$$

The subscripts on the specified boundary conditions are written i_{k_j} to allow for the possibility that the set of variables specified at the boundary conditions may not be disjoint. For example, let $n = 7$, $N = 4$, $y_1(t_1)$, $y_3(t_1)$, $y_2(t_2)$, $y_3(t_3)$, $y_1(t_4)$, $y_6(t_4)$, $y_7(t_4)$ so y_1 is fixed at t_1 and t_4 also y_3 is fixed at t_1 and t_3 , where no condition is prescribed at y_4 and y_5 . The indexing for the boundary conditions is

$$\begin{aligned} i_{11} &= 1, i_{21} = 3, i_{12} = 2, i_{13} = 3, i_{14} = 1, \\ i_{24} &= 6, i_{34} = 7. \end{aligned}$$

We shall further assume that k_1 is greater than all other k_j , $j = 2, 3, \dots, N$ otherwise the role of t_1 and the boundary point where the greatest k_j is defined can be interchanged.

The adjoint system for (2.1) is defined as

$$\dot{x} = -A^T(t)x \quad (2.3)$$

where

$x(t)$ = the adjoint variable vector, an $n \times 1$ vector with components $x_1(t), x_2(t), \dots, x_n(t)$

$A^T(t)$ = $n \times n$ matrix, the transpose of the matrix $A(t)$.

Now we multiply the i -th equation of (2.1) by $x_i(t)$, summing over all n equations, to obtain

$$\sum_{i=1}^n x_i(t) \dot{y}_i = \sum_{i=1}^n [x_i(t) \sum_{j=1}^n a_{ij}(t) y_j(t)] + \sum_{i=1}^n x_i(t) f_i(t). \quad (2.4)$$

Similarly we multiply the i -th equation of (2.3) by $y_i(t)$, summing over all n equations, to obtain

$$\sum_{i=1}^n \dot{x}_i y_i(t) = - \sum_{i=1}^n [y_i(t) \sum_{j=1}^n a_{ji}(t) x_j(t)]. \quad (2.5)$$

On adding (2.4) and (2.5), we find

$$\begin{aligned} \sum_{i=1}^n [x_i(t) \dot{y}_i + \dot{x}_i y_i(t)] &= \sum_{i=1}^n \frac{d}{dt} x_i(t) y_i(t) \\ &= \frac{d}{dt} \sum_{i=1}^n x_i(t) y_i(t) = \sum_{i=1}^n x_i(t) f_i(t). \end{aligned} \quad (2.6)$$

On integrating (2.6) over $[t_1, t]$, we have

$$\sum_{i=1}^n x_i(t) y_i(t) - \sum_{i=1}^n x_i(t_1) y_i(t_1) = \int_{t_1}^t \sum_{i=1}^n x_i(s) f_i(s) ds. \quad (2.7)$$

Equation (2.7) is called the fundamental identity for the method of adjoints.

To utilize this identity (2.7) we backward integrate the adjoint equations (2.3) k_j times from the point t_j , $j = 2, 3, \dots, N$ and hence the total $(n - k_1)$ times with the conditions

$$x_i^{m(k_j)}(t_j) = \begin{cases} 1 & i = i_{k_j} \\ 0 & i \neq i_{k_j} \end{cases} \quad j = 2, 3, \dots, N \quad (2.8)$$

where the superscript $m(k_j)$ refers to the m -th backward integration of the adjoint equations (2.3) from the point t_j and i_{k_j} refers to the subscripts of the boundary condition $y_{i_{k_j}}(t_j)$ in (2.2).

Using (2.8) in (2.7) and arranging the terms, we obtain

$$\begin{aligned} \sum_{\substack{i=1 \\ i \neq i_{k_1}}}^n x_i^{m(k_j)}(t_1) y_i(t_1) &= y_{i_{k_j}}(t_j) - \sum_{i=i_{k_1}}^{i_{k_1}} x_i^{m(k_j)}(t_1) y_i(t_1) \\ &\quad - \int_{t_1}^{t_j} \sum_{i=1}^n x_i^{m(k_j)}(s) f_i(s) ds \quad j = 2, 3, \dots, N. \end{aligned} \quad (2.9)$$

In (2.9), $y_{i_{k_j}}(t_j)$, $j = 1, 2, \dots$, are specified in (2.2).

The $x_i^{m(k_j)}(t)$ and $x_i^{m(k_j)}(t_1)$, $j = 2, 3, \dots, N$ are known from backward integration of the adjoint equations (2.3). The $f_i(t)$ are known functions of t . Hence the generation of (2.9) for the $(n - k_1)$ specified boundary conditions $y_{i_{k_j}}(t_j)$, $j = 2, 3, \dots, N$, yields a set of $(n - k_1)$ linear algebraic equations in the $(n - k_1)$ unknowns $y_i(t_1)$, where $i \neq i_{k_1}$, $i = 1, 2, \dots, n$.

3. LINEAR IMPLICIT BOUNDARY CONDITIONS

Consider the system of n linear ordinary differential equations (2.1), together with the most general implicit boundary conditions

$$\begin{aligned} \sum_{i=1}^n a_{1p,i} y_i(t_1) + \sum_{i=1}^n a_{2p,i} y_i(t_2) + \dots + \sum_{i=1}^n a_{Np,i} y_i(t_N) \\ = c_p \end{aligned} \quad (3.1)$$

where $a_{jp,i}$, c_p , $j = 1, 2, \dots, N$, $i, p = 1, 2, \dots, n$ are known constants.

Let us integrate the adjoint equations (2.3) backward once for each $y_i(t_j)$, $j = 2, 3, \dots, N$ appearing in (3.1), using the conditions

$$\begin{aligned} x_i^{m(jp)}(t_j) &= a_{jp,i} \\ j &= 2, 3, \dots, N \\ i, p &= 1, 2, \dots, n \end{aligned} \quad (3.2)$$

where $x_i^{m(p)}(t_j)$ = the i-th component at t_j for the m-th backward integration.

Substituting (3.2) in the equation (2.7), we obtain

$$\begin{aligned} & \sum_{i=1}^n a_{2,p,i} y_i(t_2) - \sum_{i=1}^n x_i^{m(2p)}(t_1) y_i(t_1) \\ &= \int_{t_1}^{t_2} \sum_{i=1}^n x_i^{m(2p)}(s) f_i(s) ds \\ & \sum_{i=1}^n a_{3,p,i} y_i(t_3) - \sum_{i=1}^n x_i^{m(3p)}(t_1) y_i(t_1) \\ &= \int_{t_1}^{t_3} \sum_{i=1}^n x_i^{m(3p)}(s) f_i(s) ds \\ & \dots \dots \\ & \sum_{i=1}^n a_{N,p,i} y_i(t_N) - \sum_{i=1}^n x_i^{m(Np)}(t_1) y_i(t_1) \\ &= \int_{t_1}^{t_N} \sum_{i=1}^n x_i^{m(Np)}(s) f_i(s) ds. \end{aligned} \quad (3.3)$$

Adding all the equations of (3.3) and using (3.1), we find

$$\begin{aligned} & \sum_{i=1}^n \{a_{1,p,i} + x_i^{m(2p)}(t_1) + x_i^{m(3p)}(t_1) \\ &+ \dots + x_i^{m(Np)}(t_1)\} y_i(t_1) \\ &= c_p - \left\{ \int_{t_1}^{t_2} \sum_{i=1}^n x_i^{m(2p)}(s) f_i(s) \right. \\ &+ \left. \int_{t_1}^{t_3} \sum_{i=1}^n x_i^{m(3p)}(s) f_i(s) \right. \\ &+ \left. \dots + \int_{t_1}^{t_N} \sum_{i=1}^n x_i^{m(Np)}(s) f_i(s) ds \right\} \\ & p = 1, 2, \dots, n. \end{aligned} \quad (3.4)$$

This is a set of n equations in the n unknowns $y_i(t_1)$, $i = 1, 2, \dots, n$. Thus the linearity of the differential equations, the linearity of the implicit boundary conditions, and the proper choice of the terminal conditions for the adjoint equations permit us to solve this problem directly as for the standard case of section 2.

4. METHOD OF COMPLEMENTARY FUNCTIONS

Here once again we shall consider boundary value problem (2.1), (2.2). We know from the variation of constants method that the general solution of (2.1) can be given as

$$y(t) = U(t) y(t_1) + \int_{t_1}^t U(t) U(s)^{-1} f(s) ds \quad (4.1)$$

where $U(t) = n \times n$ matrix solution of the homogeneous matrix - matrix equation

$$\dot{U} = A(t) U(t) \quad (4.2)$$

where $U(t_1) = I$, the identity $n \times n$ matrix.

The second term of (4.1) is the particular solution $w(t) = n \times 1$ vector with components $w_i(t)$, $i = 1, 2, \dots, n$ of (2.1) with initial conditions $w_i(t_1) = 0$, $i = 1, 2, \dots, n$. The general solution of (2.1) may be expressed in component form as

$$y_j(t) = \sum_{s=1}^n u_j^{(s)}(t) y_s(t_1) + w_j(t), \quad j = 1, 2, \dots, n \quad (4.3)$$

where $u^{(s)}(t)$ is the s-th column of $U(t)$. Rewriting (4.3) as

$$y_j(t) = \sum_{s \neq i_{k_1}}^n u_j^{(s)}(t) y_s(t_1) + \sum_{s=i_{k_1}}^{i_{k_1}} u_j^{(s)}(t) y_s(t_1) + w_j(t)$$

then the expression

$$v_j(t) = \sum_{s=i_{k_1}}^{i_{k_1}} u_j^{(s)}(t) y_s(t_1) + w_j(t)$$

is simply the j-th component of the solution $v(t)$ of the inhomogeneous system (2.1) with the initial conditions

$$\begin{aligned} v_j(t_1) &= y_j(t_1) & j = i_{k_1} \\ v_j(t_1) &= 0 & j \neq i_{k_1} \end{aligned} \quad (4.4)$$

Hence (4.3) may be written as

$$y_j(t) = \sum_{s \neq i_{k_1}}^n u_j^{(s)}(t) y_s(t_1) + v_j(t), \quad j = 1, 2, \dots, n. \quad (4.5)$$

Thus integrating $\dot{u} = A(t)u$ only $(n - k_1)$ times with the initial conditions

$$u_j^{(s)}(t_1) = \begin{cases} 1 & j = s \neq i_{k_1} \\ 0 & j \neq s \end{cases}$$

and a particular solution $v(t)$ is integrated once with the conditions (4.4) for a total of $(n - k_1 + 1)$ integrations.

Now from (4.5) choose only those j's on which the boundary conditions other than at t_1 are prescribed. We get on arranging the terms

$$\begin{aligned} & \sum_{s \neq i_{k_1}}^n u_{i_{k_1}}^{(s)}(t_j) y_s(t_1) = y_{i_{k_1}}(t_j) \\ & - \left[\begin{array}{c} i_{k_1} \\ \sum_{s=i_{k_1}}^{i_{k_1}} u_{i_{k_1}}^{(s)}(t_j) y_s(t_1) \end{array} \right] - w_{i_{k_1}}(t_j) \\ & j = 2, 3, \dots, N \end{aligned} \quad (4.6)$$

Which is a sum of $(n - k_1)$ algebraic equations in $(n - k_1)$ unknowns $y_s(t_1)$, $s \neq i_{k_1}$, $s = 1, 2, \dots, n$.

5. COMPARISON OF THE TWO METHODS

We shall show that the two methods, the method of adjoints and the method of complementary functions are theoretically the same.

First we shall show that the coefficients of $y_i(t_1)$ in both the equations (2.9) and (4.6) are the same.

The matrix - matrix equation (4.2) may be written as n matrix vector equations

$$\dot{u}_i^{(s)} = A(t) u_i^{(s)}, \quad s = 1, 2, \dots, n. \quad (5.1)$$

Consider the initial conditions for (5.1) as

$$u_i^{(s)}(t_1) = \begin{cases} 1 & i = s \\ 0 & i \neq s; i, s = 1, 2, \dots, n. \end{cases} \quad (5.2)$$

Corresponding to (5.1) for each s the adjoint equation is

$$\dot{x}^{(k)} = -A(t)^T x^{(k)}, \quad k = 1, 2, \dots, n. \quad (5.3)$$

Consider the conditions for (5.3) as (2.8).

For (5.1) and (5.3) the equation (2.7) takes the form

$$\sum_{i=1}^n x_i^{(k)}(t) u_i^{(s)}(t) = \sum_{i=1}^n x_i^{(k)}(t_1) u_i^{(s)}(t_1) \quad (5.4)$$

using (2.8) and (5.2) in (5.4) we obtain

$$\sum_{i=1}^m x_i^{m(k_j)}(t_j) u_i^{(s)}(t_j) = \sum_{i=1}^m x_i^{m(k_j)}(t_1) u_i^{(s)}(t_1)$$

or

$$u_{i_{k_j}}^{(s)}(t_j) = x_s^{m(k_j)}(t_1), \quad j = 2, 3, \dots, N \\ s = 1, 2, \dots, n. \quad (5.5)$$

Equation (5.5) demonstrates that the coefficients of $y_i(t_1)$, $i = 1, 2, \dots, n$ are identical.

We shall now show that

$$w_{i_{k_j}}(t_j) = \int_{t_1}^{t_j} \sum_{i=1}^n x_i^{m(k_j)}(s) f_i(s) ds \\ j = 2, 3, \dots, N. \quad (5.6)$$

Since $w(t)$ is a solution of (2.1) with the initial condition $w(t_1) = 0$, we can express $w(t)$ as from (4.1)

$$w(t) = \int_{t_1}^t U(t) U(s)^{-1} f(s) ds$$

which by premultiplying by $x(t)^T$ gives

$$x(t)^T w(t) = \int_{t_1}^t x(t)^T U(t) U(s)^{-1} f(s) ds. \quad (5.7)$$

Now, we know that if $U(t)$ is the solution of (4.2) then the solution of $\dot{x} = -A^T(t)x$ is $x(t) = U(t)^{-T} x(t_1)$ and hence $x(s) = U(s)^{-T} U(t)^T x(t)$. Substituting this in (5.7), to obtain

$$x(t)^T w(t) = \int_{t_1}^t x^T(s) f(s) ds$$

which is in component form

$$\sum_{i=1}^n x_i(t) w_i(t) = \int_{t_1}^t \sum_{i=1}^n x_i(s) f_i(s) ds. \quad (5.8)$$

Using the solutions of (5.3) with conditions (2.8) in (5.8), we obtain the required equation (5.6).

6. NONLINEAR PROBLEMS

Consider the set of n ordinary differential equations

$$\dot{y}_i = g_i(y_1, y_2, \dots, y_n, t), \quad i = 1, 2, \dots, n \quad (6.1)$$

together with the boundary conditions (2.2).

To solve nonlinear problems the method of adjoints for linear problems discussed in section 2 can be applied in an iterative fashion. Here we just give the method; estimates of the speed of convergence and error will be given in section 8.

Assume trial values $y_i(t_1)$, $i \neq i_{k_1}$, $i = 1, 2, \dots, n$ and integrate (6.1); let $y_i(t)$ be solutions corresponding to guessed values at the point t_1 . Let us consider a nearby solution $y_i(t) + \delta y_i(t)$, $i = 1, 2, \dots, n$ where $\delta y_i(t)$ is often called the variation, a first order correction to $y_i(t)$ to produce the actual solution of (6.1), (2.2).

The differential equations of the nearby solutions are

$$\dot{y}_i(t) + \delta \dot{y}_i(t) = g_i[y_1(t) + \delta y_1(t), y_2(t) + \delta y_2(t), \dots, y_n(t) \\ + \delta y_n(t), t] \quad i = 1, 2, \dots, n. \quad (6.2)$$

Expanding the right hand side of (6.2) in a Taylor's series up to and including first order terms, we obtain the variational equations

$$\delta \dot{y}_i(t) = \sum_{j=1}^n \frac{\partial g_i}{\partial y_j} \delta y_j(t), \quad i = 1, 2, \dots, n \quad (6.3)$$

where the partial derivatives $\frac{\partial g_i}{\partial y_j}$ are evaluated at (y_1, y_2, \dots, y_n) .

The adjoint equations to the variational equations are

$$\dot{x}_i = - \sum_{j=1}^n \frac{\partial g_i}{\partial y_j} x_j, \quad i = 1, 2, \dots, n. \quad (6.4)$$

The fundamental identity (2.7) for (6.3) and (6.4) reduces to

$$\sum_{i=1}^n x_i(t) \delta y_i(t) - \sum_{i=1}^n x_i(t_1) \delta y_i(t_1) = 0. \quad (6.5)$$

We have interpreted the variation $\delta y_i(t)$ to be the difference between the true but unknown and the calculated solution i.e.

$$\delta y_i(t) = y_{i(\text{true})}(t) - y_{i(\text{calc})}(t), \\ i = 1, 2, \dots, n \\ t_1 \leq t \leq t_N. \quad (6.6)$$

Since equations (6.3) for $\delta y_i(t)$ are only approximate systems, the process of finding the true solutions will be an iterative process which terminates when $\delta y_i(t)$, $i = 1, 2, \dots, n$; $t_1 \leq t \leq t_N$ are sufficiently small (preassigned tolerance). We always take $\delta y_{i_{k_1}}(t_1) = 0$,

$k_1 = 1, 2, \dots, k_1$ i.e. $y_{i_{k_1}(\text{calc})}(t_1)$ is equal to

the given conditions. The equation (6.6) is better written as

$$[\delta y_i(t)]^{(k)} = y_i(\text{true})(t) - [y_i(\text{calc})(t)]^{(k)} \quad (6.7)$$

where superscript k denote k -th iteration. With this equation (6.5) takes the form

$$\sum_{i=1}^n [x_i(t)]^{(k)} [\delta y_i(t)]^{(k)} - \sum_{\substack{i \neq i_{k_1} \\ i=1}} [x_i(t_1)]^{(k)} [\delta y_i(t_1)]^{(k)} = 0. \quad (6.8)$$

Now integrate adjoint equations (6.4) backward with the conditions (2.8), we finally obtain

$$\sum_{\substack{i \neq i_{k_1} \\ i=1}} [x_i^{m(k_j)}(t_1)]^{(k)} [\delta y_i(t_1)]^{(k)} = [\delta y_{i_{k_1}}(t_j)]^{(k)} \quad j = 2, 3, \dots, N \quad (6.9)$$

which is a sum of $(n - k_1)$ algebraic equations in $(n - k_1)$ unknowns $[\delta y_i(t_1)]^{(k)}$, $i \neq i_{k_1}$, $i = 1, 2, \dots, n$. For the next iteration through the process the new conditions are found from

$$[y_{i_{k_1}}(t_1)]^{(k+1)} = y_{i_{k_1}}(t_1), \quad k_1 = 1, 2, \dots, k_1 \quad (6.10)$$

$$[y_i(t_1)]^{(k+1)} = [y_i(t_1)]^{(k)} + [\delta y_i(t_1)]^{(k)},$$

$$i \neq i_{k_1}, \quad i = 1, 2, \dots, n,$$

and the calculations will terminate whenever

$$\max \{[\delta y_{i_{k_1}}(t_j)]^{(k)}, \quad j = 2, 3, \dots, N\}$$

is less than a preassigned tolerance.

Thus for the nonlinear differential equations the method of adjoints is an iterative process, which also computes only the corrections to the trial values for the missing conditions at t_1 .

7. IMPLICIT BOUNDARY CONDITIONS FOR NON-LINEAR PROBLEMS

The most general implicit boundary conditions for the nonlinear system (6.1) are given by n nonlinear relations which are functions of $y(t_1), y(t_2), \dots, y(t_N)$

$$q_i[y(t_1), y(t_2), \dots, y(t_N)] = 0 \quad (7.1)$$

$$i = 1, 2, \dots, n.$$

To solve (6.1) with the boundary conditions (7.1), first assume a set of trial conditions $y_i(t_1)$, $i = 1, 2, \dots, n$ and integrate (6.1) from t_1 to t_N .

Now we define the variation in q_i as

$$\delta q_i = q_i(\text{true}) - q_i(\text{calc}), \quad i = 1, 2, \dots, n$$

since $q_i(\text{true}) = 0$, it follows that

$$\delta q_i = -q_i(\text{calc}), \quad i = 1, 2, \dots, n. \quad (7.2)$$

We define the variation in q_i in another way as

$$\begin{aligned} \delta q_i &= \sum_{j=1}^n \frac{\partial q_i}{\partial y_j(t_1)} \delta y_j(t_1) + \sum_{j=1}^n \frac{\partial q_i}{\partial y_j(t_2)} \delta y_j(t_2) \\ &\quad + \dots + \sum_{j=1}^n \frac{\partial q_i}{\partial y_j(t_N)} \delta y_j(t_N) \end{aligned} \quad i = 1, 2, \dots, n \quad (7.3)$$

where $\frac{\partial q_i}{\partial y_j(t_s)}$; $i, j = 1, 2, \dots, n$; $s = 1, 2, \dots, N$ can

be found analytically from (7.1). Equations (7.3) are a set of n equations in Nn variables $\delta y_i(t_s)$, since δq_i is known from (7.2).

For every $y_j(t_s)$ which appears in the set of implicit boundary conditions (7.1), the adjoint equations (6.4) must be integrated backward with the conditions

$$x_{i,j}^{(s)}(t_s) = \begin{cases} 1 & i=j \quad i, j = 1, 2, \dots, n \\ 0 & i \neq j \quad s = 2, 3, \dots, N \end{cases}$$

By the identity (6.5), we obtain the set of $(N - 1)n$ equations

$$\sum_{i=1}^n x_{i,j}^{(s)}(t_1) \delta y_i(t_1) = \delta y_j(t_s). \quad (7.4)$$

If we substitute (7.4) in (7.3), we obtain

$$\begin{aligned} \delta q_i &= \sum_{j=1}^n \frac{\partial q_i}{\partial y_j(t_1)} \delta y_j(t_1) \\ &\quad + \sum_{j=1}^n \frac{\partial q_i}{\partial y_j(t_2)} \left[\sum_{p=1}^n x_{p,j}^{(2)}(t_1) \delta y_p(t_1) \right] \\ &\quad + \dots + \sum_{j=1}^n \frac{\partial q_i}{\partial y_j(t_N)} \left[\sum_{p=1}^n x_{p,j}^{(N)}(t_1) \delta y_p(t_1) \right] \end{aligned} \quad i = 1, 2, \dots, n$$

a set of n equations in the n unknowns $\delta y_j(t_1)$, $j = 1, 2, \dots, n$. Once $\delta y_j(t_1)$ are known, new trial values at the point t_1 are formed using $y_j(t_1) + \delta y_j(t_1)$, $j = 1, 2, \dots, n$.

8. CONVERGENCE AND ERROR ANALYSIS

For the problem (6.1), (2.2) the missing conditions at t_1 are obtained by the iterative process. We solve $(n - k_1)$ algebraic equations (6.9) to obtain

$[\delta y_i(t_1)]^{(k)}$, $i \neq i_{k_1}$, $i = 1, 2, \dots, n$ and the next $(k + 1)$ -th iteration is obtained by (6.10).

Denote the solution of (6.1) by

$$y_i[y_1(t_1), y_2(t_1), \dots, y_n(t_1), t], \quad i = 1, 2, \dots, n$$

which is continuously dependent on $y_{i_{k_1}}(t_1)$ and the assumed conditions $y_i(t_1)$, $i \neq i_{k_1}$, $i = 1, 2, \dots, n$. If we define

$$\Phi_{i_{k_1}}(t_j) = c_{i_{k_1}} - y_{i_{k_1}}[y_1(t_1), y_2(t_1), \dots, y_n(t_1), t_j] \quad (8.1)$$

$$j = 2, 3, \dots, N$$

then solving (6.1), (2.2) is equivalent to finding

$y_i(t_1)$, $i \neq i_{k_1}$, $i = 1, 2, \dots, n$ for which

$$\Phi_{i_{k_1}}(t_j) = 0, \quad j = 2, 3, \dots, N.$$

Assume that the k -th approximation to the vector of $(n - k_1)$ missing conditions $[y_i(t_1)]^{(k)}$, $i \neq i_{k_1}$, $i = 1, 2, \dots, n$ has been found.

Newton's method gives as the $(k + 1)$ -st approximation for all $i \neq i_{k_1}$, $i = 1, 2, \dots, n$ by the equations

$$[\Phi_{i_{k_1}}(t_j)]^{(k)} + \sum_{s=1}^n \left[\frac{\partial \Phi_{i_{k_1}}(t_j)}{\partial y_s(t_1)} \right]^{(k)} \cdot \{[y_s(t_1)]^{(k+1)} - [y_s(t_1)]^{(k)}\} = 0 \quad (8.2)$$

$$j = 2, 3, \dots, N.$$

Since $y_{i_{k_1}}[y_1(t_1), y_2(t_1), \dots, y_n(t_1), t_j]$ is a function of $y_s(t_1)$, $s = 1, 2, \dots, n$ the total variation can be expressed as

$$[\delta y_{i_{k_1}}(t_j)]^{(k)} = \sum_{s=1}^n \left[\frac{\partial y_{i_{k_1}}(t_j)}{\partial y_s(t_1)} \right]^{(k)} [\delta y_s(t_1)]^{(k)}$$

which is from (8.1)

$$[\delta y_{i_{k_1}}(t_j)]^{(k)} = - \sum_{s=1}^n \left[\frac{\partial \Phi_{i_{k_1}}(t_j)}{\partial y_s(t_1)} \right]^{(k)} [\delta y_s(t_1)]^{(k)} \quad (8.3)$$

Comparing (8.3) and (6.9), we find that

$$[x_s^{m(k_j)}(t_1)]^{(k)} = - \left[\frac{\partial \Phi_{i_{k_1}}(t_j)}{\partial y_s(t_1)} \right]^{(k)} \quad (8.4)$$

$$s \neq i_{k_1}, \quad s = 1, 2, \dots, n$$

$$j = 2, 3, \dots, N$$

and hence equations (6.9) can be written as

$$- \sum_{s=1}^n \left[\frac{\partial \Phi_{i_{k_1}}(t_j)}{\partial y_s(t_1)} \right]^{(k)} [\delta y_s(t_1)]^{(k)} = [\delta y_{i_{k_1}}(t_j)]^{(k)} \quad (8.5)$$

Equation (8.5) can be written using (8.1), (6.7) and (6.10)

$$[\Phi_{i_{k_1}}(t_j)]^{(k)} + \sum_{s=1}^n \left[\frac{\partial \Phi_{i_{k_1}}(t_j)}{\partial y_s(t_1)} \right]^{(k)} \{[y_s(t_1)]^{(k+1)} - [y_s(t_1)]^{(k)}\} = 0 \quad j = 2, 3, \dots, N$$

which is the same as (8.2). Hence the method used to find the missing conditions at t_1 is equivalent to Newton's method to solve the system of equations. Therefore the Kantorovich sufficiency theorem ([23] p. 367) can be applied which furnishes a theoretical basis for the convergence of the process and an estimate of the rate of convergence.

Equations (8.4) show that for k -th iteration the partial derivatives required by Newton's method to solve the problem (6.1), (2.2) were obtained by backward integration of the k -th system of adjoint equations (6.4) with the conditions (2.8). If we use the modified Newton method i.e.

$$[\Phi_{i_{k_1}}(t_j)]^{(k)} + \sum_{s=1}^n \left[\frac{\partial \Phi_{i_{k_1}}(t_j)}{\partial y_s(t_1)} \right]^{(0)} \{[y_s(t_1)]^{(k+1)} - [y_s(t_1)]^{(k)}\} = 0 \quad j = 2, 3, \dots, N \quad (8.6)$$

then we need to integrate only once the adjoint equations but the rate of convergence will be slower. The numerical experience for certain problems shows that the modified Newton method requires less computer time than the original Newton method, see [6]. The results of Urabe [22] give the component-wise convergence and the error estimates for the modified Newton method.

9. SOME EXAMPLES

Example 1.

Consider the boundary value problem

$$\begin{bmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & -1 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ t^2 + t \end{bmatrix} \quad (9.1)$$

$$y_1(0) = 0, y_2(\pi/4) = 1, y_3(\pi/2) = -2,$$

for which the unique solution is

$$y_1(t) = c_1 e^t + c_2 \cos t + c_3 \sin t - t^2 - 3t - 1$$

$$y_2(t) = c_1 e^t - c_2 \sin t + c_3 \cos t - 2t - 3$$

$$y_3(t) = c_1 e^t - c_2 \cos t - c_3 \sin t - 2 \quad (9.2)$$

where

$$A c_1 = \frac{\pi}{2} + 4 + \frac{1}{\sqrt{2}},$$

$$A c_2 = \exp(\pi/4) + \frac{1}{\sqrt{2}} \exp(\pi/2) - \pi/2 - 4,$$

$$c_3 = \exp(\pi/2) c_1, A = \exp(\pi/4) + \frac{1}{\sqrt{2}} \exp[(\pi/2)+1].$$

The adjoint equations are

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{bmatrix} = \begin{bmatrix} 0 & 0 & -1 \\ -1 & 0 & 1 \\ 0 & -1 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \quad (9.3)$$

$$\text{The solution of (9.3) satisfying } x_1^{(1)}(\pi/4) = 0,$$

$$x_2^{(1)}(\pi/4) = 1, x_3^{(1)}(\pi/4) = 0 \text{ is}$$

$$x_1^{(1)}(t) = \frac{1}{2} \exp(\pi/4 - t) - \frac{1}{\sqrt{2}} \cos t$$

$$x_2^{(1)}(t) = \frac{1}{\sqrt{2}} (\sin t + \cos t)$$

$$x_3^{(1)}(t) = \frac{1}{2} \exp(-\frac{\pi}{4} - t) - \frac{1}{\sqrt{2}} \sin t$$

and satisfying

$$x_1^{(2)}(\pi/2) = 0, x_2^{(2)}(\pi/2) = 0, x_3^{(2)}(\pi/2) = 1 \text{ is}$$

$$x_1^{(2)}(t) = \frac{1}{2} \exp(-\frac{\pi}{2} - t) + \frac{1}{2} (\cos t - \sin t)$$

$$x_2^{(2)}(t) = -\cos t$$

$$x_3^{(2)}(t) = \frac{1}{2} \exp(\pi/2 - t) + \frac{1}{2} (\cos t + \sin t).$$

Equations (2.9) for this problems are

$$x_2^{(1)}(0) y_2(0) + x_3^{(1)}(0) y_3(0) = y_2(\pi/4) - x_1^{(1)}(0) y_1(0) - \int_0^{\pi/4} (t^2 + t) x_3^{(1)}(t) dt$$

$$x_2^{(2)}(0) y_2(0) + x_3^{(2)}(0) y_3(0) = y_3(\pi/2) - x_1^{(2)}(0) y_1(0) - \int_0^{\pi/2} (t^2 + t) x_3^{(2)}(t) dt .$$

On substituting the values we obtain

$$\begin{aligned} \frac{1}{\sqrt{2}} y_2(0) + \frac{1}{2} \exp(\pi/4) y_3(0) &= 1 - \frac{3}{2} \exp(\pi/4) + 3 + \pi/2 - \sqrt{2} \\ &- y_2(0) + \frac{1}{2} [\exp(\pi/2) + 1] y_3(0) \\ &= -2 - \frac{3}{2} \exp(\pi/2) + \frac{7}{2}. \end{aligned} \quad (9.4)$$

Solving (9.4), we find

$$A y_2(0) = (4 + \pi/2 - \sqrt{2}) [\exp(\pi/2) + 1] - 3 \exp(\pi/4)$$

$$A y_3(0) = 8 + \pi - 3 \exp(\pi/4) - \frac{3}{2} \exp(\pi/2) - \frac{1}{2}$$

which agrees with the answer obtained from the solution (9.2), as it should be.

Example 2.

Consider the boundary value problem

$$\begin{bmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \\ \dot{y}_4 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & -\frac{1}{(2-t^2)} & 0 \\ 0 & 0 & 0 & 1 \\ -40 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 2-t^2 \end{bmatrix}$$

$$y_1(.2) = 0.0448156, \quad y_1(.4) = 0.0433224 \quad (9.5)$$

$$y_1(.6) = 0.0410152, \quad y_1(.8) = 0.0381534.$$

The adjoint equations for (9.5) are integrated with the initial conditions

$$x_1^{(i)}(t_i) = 1, \quad x_2^{(i)}(t_i) = 0, \quad x_3^{(i)}(t_i) = 0, \quad x_4^{(i)}(t_i) = 0 \quad i = 1, 2, 3$$

$$(t_1 = .2, t_2 = .4, t_3 = .6) \text{ from } t_i \text{ to } .8, \text{ using the}$$

Runge-Kutta method with step size $h = .01$. On substituting these values in the equations (2.9) we obtain the missing values $y_2(.8)$, $y_3(.8)$ and $y_4(.8)$.

The equation (9.5) was integrated with the given and obtained values of $y_i(.8)$ ($i = 1, 2, 3, 4$) using once again the Runge-Kutta method with step size $h = .01$. We obtain at $t = 1$, the following result

$$y_1(1) = 0.035063 \quad (.035058)$$

$$y_2(1) = -0.015708 \quad (-.015739)$$

$$y_3(1) = 0.000492 \quad (.000503)$$

$$y_4(1) = 0.007136 \quad (.007199)$$

where the values in parentheses are the numerical results given by Meyer [11] using the invariant imbedding method and solving the invariant equations using the Runge-Kutta method, with step size $h = .001$.

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