The Numerical Integration of Two-Point Boundary Value Problems

1. Introduction. A general system of linear, ordinary, differential equations may be written, in matrix notation

$$\dot{Y} = A(t)Y + F(t), \tag{1}$$

where the dot denotes differentiation with respect to the independent variable, t; Y is the column matrix of unknowns,

$$\begin{bmatrix} y_1 \\ \cdot \\ \cdot \\ y_n \end{bmatrix},$$

$A(t)$ is a square matrix, and $F(t)$, the forcing functions, is another column matrix,

$$\begin{bmatrix} f_1 \\ \cdot \\ \cdot \\ \cdot \\ f_n \end{bmatrix}.$$

Suppose that r values $y_1(0) \cdots y_r(0)$ are given and at $t = T, (n - r)$ of the y_i's are given, *viz.*: y_{i_k}, $k = 1, \cdots, (n - r)$. In order to solve (1) using high speed computing machinery, whether analogue or digital, it is essential to have n conditions at one end of the interval $0 - T$. One possibility is to carry the constants $y_{r+1}(0) \cdots y_n(0)$ along as unknowns during the integration, and then to determine them when the far end is reached. Another possibility consists of guessing $y_{r+1}(0) \cdots y_n(0)$ and then adjusting them. These techniques have been described by Tifford [1]. The first of these methods is awkward especially if a large number of unknowns must be carried; the second requires more integrations than the methods described below.

This paper is concerned with methods for converting a two-point boundary value problem into an initial value problem. For linear systems the conversion is accomplished with a finite number of integrations. In section 2, where nonlinear systems are considered, an iterative procedure is required.

2. Linear Systems—Method of Adjoint Equations. The adjoint system was developed by Bliss [2]; more recent developments are described by Wright [3]. The system adjoint to (1) is, by definition,

$$-\dot{X} = \bar{A}(t)X, \tag{2}$$

where the bar denotes the transposed matrix and X is a column matrix

$$\begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}.$$

The x_i's and y_i's are related by

$$\frac{d}{dt}(x_i y_i) = x_i f_i, \tag{3}$$

where the repeated suffix implies summation from 1 to n. A proof of (3) follows:
Consider

$$\frac{d}{dt}(x_i y_i) \equiv \frac{d}{dt}(\bar{X}Y) = \bar{X}\dot{Y} + \dot{\bar{X}}Y.$$

Substituting for the derivatives from (1) and (2) there is obtained

$$\begin{aligned} \frac{d}{dt}(x_i y_i) &= \bar{X}(AY + F) - (\overline{AX})Y \\ &= \bar{X}AY + \bar{X}F - (\bar{X}A)Y. \end{aligned}$$

The first and last terms cancel identically and the result (3) follows.

Integrating (3) over the interval $[0,T]$, it is found that

$$x_i(T)y_i(T) - x_i(0)y_i(0) = \int_0^T x_i(t)f_i(t)dt. \tag{4}$$

This fundamental result is the one-dimensional form of Green's theorem.

The aim is now to calculate $y_{r+1}(0) \cdots y_n(0)$ using the given conditions. The method described in this section will utilize the adjoint system (2), whereas in the next section the original equations (1), only, will be used.

The adjoint system (2) must be integrated $(n - r)$ times from T to 0 subject to certain starting values. These are chosen such that the $x_i(T)$'s are all zero except one. For the m^{th} integration this exception is the x_i which appears as the coefficient of $y_{i_m}(T)$ in (4), and which may be designated by $x_{i_m}(T)$. For simplicity $x_{i_m}(T)$ is chosen to be unity.

Let ${}_m x_i(t)$ be the value of x_i deduced from the m^{th} integration of the adjoint system. The fundamental result (4) holds for each integration of the adjoint system, and this is expressed by rewriting it

$${}_m x_i(T)y_i(T) - {}_m x_i(0)y_i(0) = \int_0^T {}_m x_i(t)f_i(t)dt. \tag{5}$$

But since all $x_i(T)$'s were chosen zero except $x_{i_m}(T)$, the first summation reduces to a single term and (5) becomes

$${}_m x_i(0)y_i(0) - y_{i_m}(T) = \int_T^0 {}_m x_i(t)f_i(t)dt. \tag{6}$$

This is a system of $(n - r)$ linear algebraic equations for the $(n - r)$ unknowns $y_i(0)$, $i = r + 1 \cdots n$.

With these values determined (1) can now be integrated from 0 to T, as an initial value problem. The total number of integrations consists of $(n - r)$ of the adjoint system plus one of the original given system.

3. Linear Systems—Method of Complementary Functions. In this case the homogeneous equation, derived from (1),

$$\dot{u} = A(t)u \tag{7}$$

is integrated from 0 to T $(n - r)$ times. The m^{th} time the initial conditions are

$$\begin{aligned} {}_m u_i(0) &= 0 \quad i \neq r + m \\ &= 1 \quad i = r + m, \end{aligned}$$

where ${}_m u_i(t)$ is the result of the m^{th} integration of $u_i(t)$.

Next the non-homogeneous equation

$$\dot{V} = A(t)V + F(t) \tag{8}$$

is integrated once, from 0 to T, subject to

$$\begin{aligned} v_i(0) &= y_i(0) \quad i = 1 \cdots r \\ &= 0 \qquad i = r + 1 \cdots n. \end{aligned}$$

The general solution of (1), subject to the given conditions can be written

$$y_i(t) = C_p \, {}_p u_i(t) + v_i(t), \tag{9}$$

where the C_p's are constants determined from the $(n - r)$ equations

$$y_{i_k}(T) = C_p \, {}_p u_{i_k}(T) + v_{i_k}(T) \quad k = 1 \cdots (n - r). \tag{10}$$

In this equation the left-hand side is given and the quantities $u_i(T)$ and $v_i(T)$ have been determined from the integrations of (7) and (8). By letting $t = 0$ in (9) it is seen that $C_p = y_{r+p}(0)$, $p = 1 \cdots n - r$.

The method of complementary functions takes less time than the method of adjoint equations for a single problem, but it is not so suitable when solutions are required for a large number of different forcing functions, F, or for a large number of different boundary conditions.

4. Nonlinear Systems. A general system of nonlinear, ordinary, differential equations may be written

$$\dot{y}_i(t) = g_i(y_1 \cdots y_n, t) \quad i = 1 \cdots n, \tag{11}$$

where it is assumed that the functions g_i are once differentiable with respect to all the y_i's. Once again the boundary conditions are specified as $y_1(0) \cdots y_r(0)$ and $y_{i_k}(T)$, $k = 1 \cdots (n - r)$. The procedure is to estimate $y_{r+1}(0) \cdots y_n(0)$ which estimates are denoted by $y^*_{r+1}(0) \cdots y_n^*(0)$. Equations (11) can now be integrated as an initial value problem, and the solutions are denoted by $y_i^*(t)$. In general, it will be found that the computed values of $y_{i_k}(T)$, $k = 1 \cdots (n - r)$ namely, $y^*_{i_k}(T)$, differ from the given values of $y_{i_k}(T)$. To obtain the correct solution of the system (11) the difference between $y^*_{i_k}(T)$ and the given $y_{i_k}(T)$ must be made as small as possible.

Define $\delta y_i(t)$ by

$$\delta y_i(t) = y_i(t) - y_i^*(t) \quad i = 1 \cdots n. \tag{12}$$

Substituting $y_i(t)$ in (11) there results, to a first approximation,

$$\delta \dot{y}_i(t) = \left(\frac{\partial g_i}{\partial y_j}\right) \delta y_j. \tag{13}$$

The equations adjoint to (13) are

$$-\dot{x}_i = \left(\frac{\partial g_j}{\partial y_i}\right) x_j. \tag{14}$$

Since non-homogeneous terms are absent from (13) the Green's theorem for (13) and (14) reduces to

$$x_i(T)\delta y_i(T) - x_i(0)\delta y_i(0) = 0. \tag{15}$$

The quantities required are $\delta y_i(0)$, $i = r + 1 \cdots n$. To obtain $(n - r)$ equations, for these $(n - r)$ unknowns, (14) is integrated from T to 0 $(n - r)$ times; the result of the m^{th} integration is denoted by ${}_m x_i(t)$. Equation (15) holds for each integration of the adjoint system, and this may be expressed by rewriting it

$${}_m x_i(T)\delta y_i(T) - {}_m x_i(0)\delta y_i(0) = 0 \quad m = 1 \cdots (n - r). \tag{16}$$

The m^{th} time the adjoint equations are integrated the starting values are that all $x_i(T)$'s are zero except the coefficient of $\delta y_{i_m}(T)$ which is chosen to be unity. The first summation in (16) now reduces to a single term; furthermore, $\delta y_i(0)$, $i = 1 \cdots r$ are identically zero. Hence (16) reduces to

$$\delta y_{i_m}(T) - {}_m x_{r+i}(0)\delta y_{r+i}(0) = 0 \quad m = 1 \cdots (n - r), \tag{17}$$

where the summation on i extends from 1 to $(n - r)$. Substituting these values into (12) the improved estimate of $y_i(0)$, $i = r + 1 \cdots n$ are obtained. In the case of nonlinear systems (11) is integrated again, using the improved estimates, and the process is repeated. In the special case where the g_i's are linear functions

of y_i (13) is exact and the new estimates of the initial values are precise after only one application of the method. This method, when applied to linear systems, is similar to the second method described by Tifford [1].

5. Remarks. The problem was posed such that the y_i's were given at either end of the interval $0 - T$. The methods are easily extended, if instead, $n - p$ linear relations are prescribed between the $y_i(0)$'s and p between the $y_i(T)$'s. The methods may also be generalized to convert three or more point boundary value problems into an initial value problem.

An alternative method, suitable for nonlinear systems, has been presented by Lance and Deland [4]. This method is also one of iteration but it involves numerical differentiation and for this reason is less accurate per iteration than the method presented in section 4.

If large scale computing machines are not available then relaxation methods can be used to solve systems of differential equations. Allen [5] states that if relaxation methods are to be used then an equal number of boundary conditions must be specified at each end of the interval, and for this reason the number of equations, n, must be even. Allen presents a method for converting problems which are not stated in this form into this form. The authors considered using the methods given above as an alternative to Allen's. Although, it is possible to do this, Reid [6] has shown that the conversion is unnecessary and that relaxation can be used directly regardless of how the boundary conditions are distributed. Reid also shows that the number of equations need not be even.

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The authors wish to thank Mr. A. H. Flax who suggested the basic idea of section 3.

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