BOUNDARY VALUE PROBLEMS

The basic theory of boundary value problems for ODE is more subtle than for initial value problems, and we can give only a few highlights of it here. For notational simplicity, abbreviate *boundary value problem* by *BVP*.

We begin with the two-point BVP

$$y'' = f(x, y, y'), \quad a < x < b$$
$$A \begin{bmatrix} y(a) \\ y'(a) \end{bmatrix} + B \begin{bmatrix} y(b) \\ y'(b) \end{bmatrix} = \begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix}$$

with A and B square matrices of order 2. These matrices A and B are given, along with the right-hand boundary values γ_1 and γ_2. The problem may not be solvable (or uniquely solvable) in all cases, and we illustrate this with some examples (also given in the text).

EXAMPLE #1:

$$
\begin{gathered}
y'' = -\lambda y, \quad 0 < x < 1 \\
y(0) = y(1) = 0
\end{gathered}
\tag{1}
$$

The differential equation

$$y'' + \lambda y = 0$$

has the general solution

$$
Y(x) = \begin{cases}
c_1 e^{\mu x} + c_2 e^{-\mu x}, & \lambda < 0,\ \mu = (-\lambda)^{\frac{1}{2}} \\
c_1 + c_2 x, & \lambda = 0 \\
c_1 \cos(\mu x) + c_2 \sin(\mu x) & \lambda > 0,\ \mu = (\lambda)^{\frac{1}{2}}
\end{cases}
$$

In the first two cases, if we apply the boundary conditions, we find they imply $c_1, c_2 = 0$. For the third case, we obtain the conditions

$$c_1 = 0, \quad c_2 \sin(\mu) = 0$$

The condition $\sin(\mu) = 0$ is equivalent to

$$
\begin{aligned}
\mu &= \pm\pi, \pm 2\pi, \pm 3\pi, \cdots \\
\lambda &= \pi^2, 4\pi^2, 9\pi^2, \cdots
\end{aligned}
\tag{2}
$$

This yields a nonzero solution for (1) of

$$Y(x) = c \sin(\mu x)$$

for any real number $c \neq 0$. If λ is not from the list in (2), then the only possible solution of (1) is $Y(x) \equiv 0$.

EXAMPLE #2:

$$\begin{gathered} y'' = -\lambda y + g(x), \quad 0 < x < 1 \\ y(0) = y(1) = 0 \end{gathered} \tag{3}$$

If λ is not chosen from (2), then we can solve this boundary value problem as an integral formula known as *Green's formula:*

$$Y(x) = \int_0^1 G(x,t) g(t)\, dt, \quad 0 \leq x \leq 1 \tag{4}$$

$$G(x,t) = \begin{cases} G_0 \equiv -\dfrac{\sin(\mu t) \sin \mu (1-x)}{\mu \sin \mu}, & x \geq t \\ G_1 \equiv -\dfrac{\sin(\mu x) \sin \mu (1-t)}{\mu \sin \mu}, & x \leq t \end{cases}$$

With these,

$$G(0, t) = G(1, t) \equiv 0$$

$$G_0(x, x) = G_1(x, x)$$

$$\frac{\partial G_0(x, x)}{\partial x} - \frac{\partial G_1(x, x)}{\partial x} = 1$$

and with these properties, we can show formula (4) satisfies (3). To show this is the only solution, suppose there is a second solution $Z(x)$. Then subtract the two equations

$$\begin{aligned} Y'' &= -\lambda Y + g(x) \\ Z'' &= -\lambda Z + g(x) \end{aligned}$$

to get

$$E'' = -\lambda E, \quad E(0) = E(1) = 0$$

with $E = Y - Z$. Then example #1 implies $E(x) \equiv 0$.

If λ is chosen from (2), however, then (3) will not, in general, have a solution. To illustrate the possibilities, let $\lambda = \pi^2$. Then (3) has a solution if and only if

$$\int_0^1 g(x) \sin(\pi x)\, dx = 0$$

In this case, the general solution of (3) is given by

$$Y(x) = c \sin(\pi x) + \frac{1}{\pi} \int_0^1 g(t) \sin(\pi(x - t))\, dt$$

where c is arbitrary.

THEOREM

Consider the two-point BVP

$$
\begin{aligned}
y'' = p(x)y' + q(x)y + g(x), \quad a < x < b \\
A \begin{bmatrix} y(a) \\ y'(a) \end{bmatrix} + B \begin{bmatrix} y(b) \\ y'(b) \end{bmatrix} = \begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix}
\end{aligned}
\qquad (5)
$$

The *homogeneous form* of this problem is given by

$$
\begin{aligned}
y'' = p(x)y' + q(x)y, \quad a < x < b \\
A \begin{bmatrix} y(a) \\ y'(a) \end{bmatrix} + B \begin{bmatrix} y(b) \\ y'(b) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}
\end{aligned}
\qquad (6)
$$

Theorem The nonhomogeneous problem (5) has a unique solution $Y(x)$ on $[a, b]$, for each set of given data $\{g(x), \gamma_1, \gamma_2\}$, if and only if the homogeneous problem (6) has only the trivial solution $Y(x) \equiv 0$.

The proof uses the theory of integral equations of Fredholm type; and of necessity, it is omitted here.

For the general BVP

$$y'' = f(x, y, y'), \quad a < x < b$$

$$A \begin{bmatrix} y(a) \\ y'(a) \end{bmatrix} + B \begin{bmatrix} y(b) \\ y'(b) \end{bmatrix} = \begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix}$$

an existence and uniqueness theorem is given in the book, on page 436. Generally when dealing with the numerical solution, we assume the BVP has a unique solution.

The more general form of BVP is to write it in the form

$$\begin{array}{c} \mathbf{y}' = \mathbf{f}(x, \mathbf{y}), \quad a < x < b \\ A\mathbf{y}(a) + B\mathbf{y}(b) = \gamma \end{array} \tag{7}$$

with $\mathbf{y} \in \mathbb{R}^n$, A and B square matrices of order n, and $\gamma \in \mathbb{R}^n$ given data. There is a theory for these problems that is analogous to that for the two-point BVP, but we omit it here and in the text. We will examine numerical methods for the two-point problem, although most schemes generalize to (7).

SHOOTING METHODS

The central idea is to reduce solving the BVP to that of solving a sequence of inital value problems (IVP). To simplify the presentation, we consider a BVP with *separated boundary conditions*:

$$\begin{gathered} y'' = f(x, y, y'), \quad a < x < b \\ a_0 y(a) - a_1 y'(a) = \gamma_1 \\ b_0 y(b) + b_1 y'(b) = \gamma_2 \end{gathered} \tag{8}$$

Solve the initial value problem

$$\begin{gathered} y'' = f(x, y, y'), \quad a < x < b \\ y(a) = a_1 s - c_1 \gamma_1, \quad y'(a) = a_0 s - c_0 \gamma_1 \end{gathered} \tag{9}$$

The constants c_0, c_1 are arbitrary satisfying

$$a_1 c_0 - a_0 c_1 = 1$$

of which there are many possible choices. The parameter s is the *shooting parameter*, and it is to be chosen to find a solution satisfying the boundary conditions at $x = b$.

Let $Y(x;s)$ be a solution of (9). Then for any choice of the unspecified parameter s, the function $Y(x;s)$ satisfies the boundary condition

$$a_0 Y(a;s) - a_1 Y'(a;s) = \gamma_1$$

To see this,

$$\begin{aligned} a_0 Y(a;s) - a_1 Y'(a;s) &= a_0 \left(a_1 s - c_1 \gamma_1\right) \\ &\qquad - a_1 \left(a_0 s - c_0 \gamma_1\right) \\ &= \left(a_1 c_0 - a_0 c_1\right) \gamma_1 = \gamma_1 \end{aligned}$$

We want to choose s so as to have $Y(x;s)$ also satisfy the boundary condition

$$b_0 Y(b;s) + b_1 Y'(b;s) = \gamma_2$$

Introduce

$$\varphi(s) = b_0 Y(b;s) + b_1 Y'(b;s) - \gamma_2$$

We want to find $s = s^*$ for which $\varphi(s^*) = 0$.

Look at Newton's method for solving this problem:

$$s_{m+1} = s_m - \frac{\varphi(s_m)}{\varphi'(s_m)}, \quad m = 0, 1, ... \tag{10}$$

Differentiate the definition

$$\varphi(s) = b_0 Y(b; s) + b_1 Y'(b; s) - \gamma_2$$

to obtain

$$\varphi'(s) = b_0 \xi_s(b) + b_1 \xi_s'(b)$$

$$\xi_s(x) = \frac{\partial Y(x; s)}{\partial s}$$

Since $Y(x; s)$ satisfies

$$\begin{gathered} Y''(x; s) = f(x, Y(x; s), Y'(x; s)), \quad a < x < b \\ Y(a; s) = a_1 s - c_1 \gamma_1, \quad Y'(a; s) = a_0 s - c_0 \gamma_1 \end{gathered} \tag{11}$$

differentiate it with respect to s to obtain

$$\begin{aligned} \xi_s''(x) = f_2 &\left(x, Y(x; s), Y'(x; s)\right) \xi_s(x) \\ &+ f_3 \left(x, Y(x; s), Y'(x; s)\right) \xi_s'(x) \\ \xi_s(a) = a_1, &\quad \xi_s'(a) = a_0 \end{aligned} \tag{12}$$

We combine (11) and (12) and rewrite them as a system of four first order equations, for the knowns $Y(x;s), Y'(x;s), \xi_s(x), \xi_s'(x)$, and we solve for their values at b. Then we proceed with the iteration (10), to find a new value of s_{m+1} from the value s_m.

It can be shown that if a method of order p is used, then of course, all errors at $x = b$ are of order $O(h^p)$ where h is the stepsize. Then it can also be proven that

$$s_h^* = s^* + O(h^p)$$

where s_h^* is the limit of $\{s_m\}$ obtained when using the numerical method of order p. Moreover,

$$E_h \equiv \max_{a \le x \le b} |Y(x) - y_h(x; s_h^*)| = O(h^p)$$

with $y_h(x; s_h^*)$ the numerical solution.

EXAMPLE

Solve

$$y'' = -y + \frac{2\,(y')^2}{y}, \quad -1 < x < 1$$

$$y(-1) = y(1) = \frac{1}{e + e^{-1}} \doteq .324027137$$

The true solution is

$$Y(x) = \frac{1}{e^x + e^{-x}}$$

The initial value problem for the shooting method is

$$y'' = -y + \frac{2\,(y')^2}{y}, \quad x \geq -1$$

$$y(-1) = \frac{1}{e + e^{-1}}, \quad y'(-1) = s$$

The function $\varphi(s)$ is

$$\varphi(s) = Y(1; s) - \frac{1}{e + e^{-1}}, \quad \varphi'(s) = \xi_s(1)$$

The associated problem for ξ_s is

$$\xi_s''(x) = \left[-1 - 2\left(\frac{y'}{y}\right)^2\right]\xi_s + 4\frac{y'}{y}\xi_s'$$

$$\xi_s(-1) = 0, \quad \xi_s'(-1) = 1$$

We use a second order Runge-Kutta method, which has an error $O(h^2)$. In this instance, the true s^* is known:

$$s^* = \frac{e - e^{-1}}{\left(e + e^{-1}\right)^2}$$

A table of the errors $s - s_h^*$ and E_h are given in Table 6.29 on page 440 of the text. They agree with the theoretical rates of $O(h^2)$.

FINITE DIFFERENCE METHODS

Finite difference methods can be applied to both the two-point 2^{nd} order BVP

$$y'' = f(x, y, y'), \quad a < x < b$$
$$A \begin{bmatrix} y(a) \\ y'(a) \end{bmatrix} + B \begin{bmatrix} y(b) \\ y'(b) \end{bmatrix} = \begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix}$$

and to the BVP set as a first order system,

$$\mathbf{y}' = \mathbf{f}(x, \mathbf{y}), \quad a < x < b$$
$$A\mathbf{y}(a) + B\mathbf{y}(b) = \gamma$$

To simplify the presentation here and in the text, I consider only the special case

$$\begin{aligned} y'' &= f(x, y, y'), \quad a < x < b \\ y(a) &= \gamma_1, \quad y(b) = \gamma_2 \end{aligned} \tag{13}$$

Later I consider some generalizations.

Recall the numerical differentiation formulas

$$g''(x) = \frac{g(x+h) - 2g(x) + g(x-h)}{h^2} - \frac{h^2}{12} g^{(4)}(\xi)$$

with $x - h \le \xi \le x + h$, and

$$g'(x) = \frac{g(x+h) - g(x-h)}{2h} - \frac{h^2}{6} g^{(3)}(\eta)$$

with $x - h \le \eta \le x + h$. These are from (5.7.18) and (5.7.11) of the text, respectively. Apply these to approximate

$$y'' = f(x, y, y'), \quad a < x < b$$
$$y(a) = \gamma_1, \quad y(b) = \gamma_2$$

We introduce a stepsize h and node points $\{x_i\}$ by

$$h = \frac{b-a}{n}, \quad x_i = a + ih, \quad i = 0, 1, ..., n$$

We approximate the BVP at each interior node point x_i, $i = 1, ..., n-1$. Let $Y(x)$ denote the true solution of the BVP.

Using the numerical derivative relations in

$$Y''(x_i) = f\left(x_i, Y(x_i), Y'(x_i)\right), \quad i = 1, ..., n-1$$

$$\begin{aligned} &\frac{Y(x_{i+1}) - 2Y(x_i) + Y(x_{i-1})}{h^2} - \frac{h^2}{12} Y^{(4)}(\xi_i) \\ &\quad = f\left(x_i, Y(x_i), \frac{Y(x_{i+1}) - Y(x_{i-1})}{2h} - \frac{h^2}{6} Y'''(\eta_i)\right) \end{aligned} \tag{14}$$

for $i = 1, ..., n-1$, with $x_{i-1} \le \xi_i, \eta_i \le x_{i+1}$. Note that at $i = 1$ in (14), the value $Y(x_0) = \gamma_1$ is needed; and at $i = n-1$, the value $Y(x_n) = \gamma_2$ is needed.

Dropping the error terms, we obtain the approximating system

$$\begin{aligned} &\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} \\ &\qquad = f\left(x_i, y_i, \frac{y_{i+1} - y_{i-1}}{2h}\right), \quad i = 1, ..., n-1 \\ &y_0 = \gamma_1, \quad y_n = \gamma_2 \end{aligned} \tag{15}$$

We can write this in matrix-vector form. Introduce

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_{n-1} \end{bmatrix}, \quad \widehat{\mathbf{f}}(\mathbf{y}) = \begin{bmatrix} f\left(x_1, y_1, \dfrac{y_2 - y_0}{2h}\right) \\ \vdots \\ f\left(x_{n-1}, y_{n-1}, \dfrac{y_n - y_{n-2}}{2h}\right) \end{bmatrix}$$

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

$$\mathbf{g} = \left[-\frac{\gamma_1}{h^2}, 0, ..., 0, -\frac{\gamma_2}{h^2}\right]^T$$

Then our discretization can be written

$$\frac{1}{h^2} A\mathbf{y} = \widehat{\mathbf{f}}(\mathbf{y}) + \mathbf{g} \tag{16}$$

This is a system of $n-1$ nonlinear equations in $n-1$ unknowns.

ERROR

Let the numerical solution also be denoted by $\mathbf{y}_h$. Then it can be shown under various assumptions on f and the BVP (13) that

$$\max_i |Y(x_i) - y_i| \leq c\, h^2$$

for all suitably small values of h. The theory for this is extended and fairly sophisticated, and we omit it here. References are given in the text.

This theory can also be extended to show that

$$Y(x_i) - y_i = G(x_i)h^2 + O\left(h^4\right), \quad i = 1, ..., n-1$$

with $G(x)$ independent of h, provided both the solution $Y(x)$ and the function $f(x, u, v)$ are sufficiently smooth. With this, one can then carry out Richardson extrapolation on the solution, as well as using Richardson's error estimation formulas.

NEWTON'S METHOD

There are a number of methods for solving nonlinear systems

$$\mathbf{g}(\mathbf{y}) = \mathbf{0}$$

with $\mathbf{g} : \mathbb{R}^N \to \mathbb{R}^N$. Here we consider Newton's method:

$$\mathbf{y}^{(m+1)} = \mathbf{y}^{(m)} - \left[\mathbf{G}(\mathbf{y}^{(m)})\right]^{-1} \mathbf{g}(\mathbf{y}^{(m)}), \quad m = 0, 1, ...$$

In this, $\mathbf{G}(\mathbf{y})$ denotes the Jacobian matrix for $\mathbf{g}(\mathbf{y})$:

$$[\mathbf{G}(\mathbf{y})]_{i,j} = \frac{\partial g_i(y_1, ..., y_N)}{\partial y_j}$$

From earlier in §2.11 of Chapter 2, this method converges quadratically to a root α if $\mathbf{G}(\alpha)$ is nonsingular and $\mathbf{y}^{(0)}$ is chosen sufficiently close to α:

$$\left\|\alpha - \mathbf{y}^{(m+1)}\right\|_\infty \le c \left\|\alpha - \mathbf{y}^{(m)}\right\|_\infty^2, \quad m \ge 0$$

for some $c > 0$.

SOLVING THE BVP SYSTEM

Recall the system (16) and write it as

$$\mathbf{g}(\mathbf{y}) \equiv \frac{1}{h^2}A\mathbf{y} - \widehat{\mathbf{f}}(\mathbf{y}) - \mathbf{g} = \mathbf{0} \tag{17}$$

with $N = n - 1$. Then

$$\mathbf{G}(\mathbf{y}) = \frac{1}{h^2}A - \widehat{\mathbf{F}}(\mathbf{y}) \tag{18}$$

with $\widehat{\mathbf{F}}(\mathbf{y})$ the Jacobian matrix for $\widehat{\mathbf{f}}(\mathbf{y})$. Since

$$\left[\widehat{\mathbf{f}}(\mathbf{y})\right]_i = f\left(x_i, y_i, \frac{y_{i+1} - y_{i-1}}{2h}\right)$$

$\widehat{\mathbf{F}}(\mathbf{y})$ is tridiagonal, with the formulas given on page 442 of the text. For example,

$$\left[\widehat{\mathbf{F}}(\mathbf{y})\right]_{i,i} = f_2\left(x_i, y_i, \frac{y_{i+1} - y_{i-1}}{2h}\right)$$

with

$$f_2(x, u, v) = \frac{\partial f(x, u, v)}{\partial u}$$

Another way of looking at the computation of the Jacobian $\mathbf{G}(\mathbf{y})$ for a function $\mathbf{g} : \mathbb{R}^N \rightarrow \mathbb{R}^N$ is as follows. The matrix function $\mathbf{G}(\mathbf{y})$ has the property that for any increment $\delta \in \mathbb{R}^N$,

$$\mathbf{g}(\mathbf{y}+\delta) - \mathbf{g}(\mathbf{y}) = \mathbf{G}(\mathbf{y})\delta + O\left(\|\delta\|^2\right) \qquad (19)$$

Thus if $\mathbf{g}(\mathbf{y})$ is a linear function,

$$\mathbf{g}(\mathbf{y}) = B\mathbf{y} \qquad (20)$$

with B a matrix of order $N \times N$, then

$$\mathbf{g}(\mathbf{y}+\delta) - \mathbf{g}(\mathbf{y}) = B\left(\mathbf{y}+\delta\right) - B\mathbf{y} = B\delta$$

with no $O\left(\|\delta\|^2\right)$ term. Therefore the Jacobian matrix of (20) is $\mathbf{G}(\mathbf{y}) = B$.

When dealing with nonlinear functions $\mathbf{g}(\mathbf{y})$ on vector spaces, especially infinite dimensional function spaces, the quantity $\mathbf{G}(\mathbf{y})$ is called the *Frechet derivative* of $\mathbf{g}(\mathbf{y})$.

Return to Newton's method

$$\mathbf{y}^{(m+1)} = \mathbf{y}^{(m)} - \left[\mathbf{G}(\mathbf{y}^{(m)})\right]^{-1} \mathbf{g}(\mathbf{y}^{(m)}), \quad m = 0, 1, ...$$

applied to the solution of

$$\mathbf{g}(\mathbf{y}) \equiv \frac{1}{h^2} A\mathbf{y} - \widehat{\mathbf{f}}(\mathbf{y}) + \mathbf{g} = \mathbf{0}$$

with

$$\mathbf{G}(\mathbf{y}) = \frac{1}{h^2} A - \widehat{\mathbf{F}}(\mathbf{y})$$

Rewrite the iteration as

$$\begin{aligned} \mathbf{y}^{(m+1)} &= \mathbf{y}^{(m)} - \delta^{(m)} \\ \mathbf{G}(\mathbf{y}^{(m)})\delta^{(m)} &= \mathbf{g}(\mathbf{y}^{(m)}), \quad m = 0, 1, ... \end{aligned}$$

This last system is tridiagonal, and thus it can be solved very rapidly. Often, the matrix $\mathbf{G}(\mathbf{y}^{(m)})$ may be kept constant over several iterations, to save further on the solution process; but this will change the quadratic convergence of the iterates to fast linear convergence.

EXAMPLE

Solve the BVP

$$y'' = -y + \frac{2\,(y')^2}{y}, \quad -1 < x < 1$$

$$y(-1) = y(1) = \frac{1}{e + e^{-1}} \doteq .324027137$$

The true solution is

$$Y(x) = \frac{1}{e^x + e^{-x}}$$

Newton's method was used to solve the nonlinear system, and the iteration was stopped when

$$\left\| \mathbf{y}^{(m)} - \mathbf{y}^{(m-1)} \right\|_\infty \le 10^{-10}$$

was satisfied. Also let

$$E_h = \max_{0 \le i \le h} |Y(x_i) - \mathbf{y}_h(x_i)|$$

n	E_h	*Ratio*
4	2.63E−2	
8	5.87E−3	4.48
16	1.43E−3	4.11
32	3.55E−4	4.03
64	8.86E−5	4.01

MODIFICATIONS

If our boundary conditions in involve derivatives, then these must also be approximated. For example,

$$Y(a) = Y'(a)$$

might be approximated by

$$y_0 = \frac{y_1 - y_0}{h}$$

although this is not a very accurate approximation. This new equation would be added to the approximations at the inner node points $x_1, ..., x_{n-1}$.