Cubic spline solutions to two-point boundary value problems

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The cubic spline approximation to a two-point boundary value problem for the differential equation $y'' + f(x)y' + g(x)y = r(x)$ is shown to reduce to the solution of a three-term recurrence relationship. For the special case when $f(x)$ is a constant, the approximation is shown to be simply related to a finite-difference representation and to have a local truncation error of order $\frac{1}{12}\delta^4 y$.

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In a recent paper Bickley (1968) has considered the use of the cubic spline for solving linear two-point boundary value problems. The essential feature of his analysis is that it leads to the solution of a set of linear equations whose matrix of coefficients is of upper Hessenberg form. The purpose of the present note is to show that the spline solution can be obtained by solving a set of equations with a tri-diagonal matrix of coefficients. The analysis is particularly straightforward when the first derivative is absent from the differential equation and this case is considered first in the paper, a simple connection being established between the spline solution and a finite-difference representation. The more general case when the first derivative term is present is considered subsequently and explicit formulae for the recurrence relation coefficients derived. In a simple special case the spline fit is again shown to be related to a finite-difference representation.

Description of procedure

It is shown by Ahlberg *et al.* (1967) that the cubic spline $S(x)$ interpolating to the function $y(x)$ at the knots $x_j = x_0 + jh$ $(j = 0, 1, \ldots, n)$ is given in the interval $x_{j-1} \leqslant x \leqslant x_j$ by the equation

$$S(x) = M_{j-1}\frac{(x_j - x)^3}{6h} + M_j\frac{(x - x_{j-1})^3}{6h} + \left(y_{j-1} - \frac{h^2}{6}M_{j-1}\right)\frac{(x_j - x)}{h} + \left(y_j - \frac{h^2}{6}M_j\right)\frac{(x - x_{j-1})}{h} \quad (1)$$

where $M_j = S''(x_j)$ and $y_j = y(x_j)$. Hence

$$S'(x_j+) = -\frac{h}{3}M_j - \frac{h}{6}M_{j+1} + \frac{y_{j+1} - y_j}{h} \quad (j = 0, 1, \ldots, n-1) \quad (2)$$

and

$$S'(x_j-) = \frac{h}{3}M_j + \frac{h}{6}M_{j-1} + \frac{y_j - y_{j-1}}{h} \quad (j = 1, 2, \ldots, n), \quad (3)$$

so that continuity of first derivatives implies

$$\frac{h}{6}M_{j-1} + \frac{2h}{3}M_j + \frac{h}{6}M_{j+1} = \frac{y_{j+1} - 2y_j + y_{j-1}}{h} \quad (j = 1, 2, \ldots, n-1). \quad (4)$$

If we are given the differential equation

$$y'' + f(x)y' + g(x)y = r(x) \quad (5)$$

with associated boundary conditions*

$$y(x_0) = a, \; y(x_n) = b \quad (6)$$

then the requirement that the spline approximation should satisfy the differential equation (5) at the knots $x_j (j = 0, 1, \ldots, n)$ leads, on using equations (2) and (3), to a set of relationships from which we can eliminate the unknowns $M_0, M_1, \ldots, M_n$. The result, in conjunction with the boundary conditions (6), is a set of tri-diagonal equations for the determination of $y_0, y_1, \ldots, y_n$.

Case (a)—first derivative absent

For the special case of

$$y'' + g(x)y = r(x) \quad (7)$$

the analysis is extremely simple. We obtain immediately from equation (7) that

$$M_j = r_j - g_j y_j \quad (j = 0, 1, \ldots, n) \quad (8)$$

where $g_j = g(x_j)$, $r_j = r(x_j)$, and substitution into equation (4) yields

$$y_{j+1}\left(1 + \frac{h^2}{6}g_{j+1}\right) - y_j\left(2 - \frac{2h^2}{3}g_j\right) + y_{j-1}\left(1 + \frac{h^2}{6}g_{j-1}\right) = \frac{h^2}{6}(r_{j+1} + 4r_j + r_{j-1}) \quad (j = 1, 2, \ldots, n-1). \quad (9)$$

This clearly corresponds to the finite-difference representation

$$\delta^2 y_j + h^2(1 + \tfrac{1}{6}\delta^2)g_j y_j = h^2(1 + \tfrac{1}{6}\delta^2)r_j \quad (10)$$

which has a local truncation error of order $\frac{1}{12}\delta^4 y$. We note that equation (10) is similar in appearance to the well-known Numerov formula (National Physical Laboratory (1961), p. 86) with $\frac{1}{6}\delta^2$ replacing $\frac{1}{12}\delta^2$. The latter formula has of course a smaller truncation error but does not produce such a smooth solution. Equation (10) has been used previously by Albasiny and Cooper (1963) for the solution of a problem in

* These conditions are taken for simplicity. More general boundary conditions of the form $\alpha y' + \beta y = \gamma$ are readily incorporated in the analysis.

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theoretical physics in which $y'''(x)$ was known to be discontinuous at the point $x = x_j$.

Equations (9) in conjunction with the boundary conditions (6) represent a tri-diagonal set of equations which are readily solved for the unknowns $y_0, y_1, \ldots, y_n$. The complete cubic spline solution is then given immediately by equations (8) and (1).

Example We consider the example discussed by Bickley (1968), namely

$$y'' + y + 1 = 0, \quad y(0) = y(1) = 0.$$

If we divide the interval [0, 1] into two equal sub-intervals, then from equation (9)

$$y(0\cdot 5) = 3/22$$

and from equation (8)

$$M_0 = M_2 = -1, \quad M_1 = -\frac{25}{22}.$$

Hence from equations (2) and (3)

$$S'(0) = \frac{47}{88}, \quad S'(0\cdot 5) = 0, \quad s'(1) = -\frac{47}{88}$$

and the spline solution is

$$S(x) = \frac{47}{88}x - \frac{1}{2}x^2 - \frac{1}{22}x^3 + \frac{1}{11}a\left(x - \frac{1}{2}\right)^3$$

where $a = 0$ for $x < 0\cdot 5$ and $a = 1$ for $x \geqslant 0\cdot 5$. This solution is, of course, identical with that obtained using Bickley's analysis.

Case (b)—first derivative present

More generally we are interested in spline approximations to equation (5), in which case the differential equation gives on using equations (2) and (3)

$$\left(1 - \frac{h}{3}f_j\right) M_j - \frac{h}{6}f_j M_{j+1} = r_j - g_j y_j - \frac{f_j}{h}(y_{j+1} - y_j) \qquad (j = 0, 1, \ldots, n-1) \qquad (11)$$

and

$$\frac{h}{6}f_j M_{j-1} + \left(1 + \frac{h}{3}f_j\right) M_j = r_j - g_j y_j - \frac{f_j}{h}(y_j - y_{j-1}) \qquad (j = 1, 2, \ldots, n). \qquad (12)$$

Equations (11) and (12) constitute $2n$ equations in the $2n + 2$ unknowns $M_0, M_1, \ldots, M_n$ and $y_0, y_1, \ldots, y_n$. Elimination of the M_j leads directly to $n - 1$ equations for the unknowns y_0 to y_n which, together with the two boundary conditions, are sufficient for their determination. We note that equations (11) and (12) imply the relations (4).

Addition of equations (11) and (12) gives the relationship

$$\frac{h}{6}f_j M_{j-1} + 2M_j + \frac{h}{6}f_j M_{j+1} = 2(r_j - g_j y_j) - \frac{f_j}{h}(y_{j+1} - y_{j-1}) \quad (j = 1, 2, \ldots, n-1) \quad (13)$$

and elimination of M_j between this equation and equation (4) yields

$$\left(1 + \frac{h}{3}f_j\right) y_{j+1} - 2\left(1 - \frac{h^2}{3}g_j\right) y_j + \left(1 - \frac{h}{3}f_j\right) y_{j-1} = \frac{2h^2}{3}r_j + \frac{h^2}{6}\left(1 - \frac{h}{3}f_j\right) M_{j-1} + \frac{h^2}{6}\left(1 + \frac{h}{3}f_j\right) M_{j+1} \qquad (j = 1, 2, \ldots, n-1). \qquad (14)$$

But an explicit expression can be obtained for M_{j-1} in terms of y_{j-1} and y_j by eliminating M_j between equation (11) (with j replaced by $j - 1$) and equation (12), namely

$$A_j M_{j-1} = \left(1 + \frac{h}{3}f_j\right)\left[r_{j-1} - g_{j-1}y_{j-1} - \frac{f_{j-1}}{h}(y_j - y_{j-1})\right] + \frac{h}{6}f_{j-1}\left[r_j - g_j y_j - \frac{f_j}{h}(y_j - y_{j-1})\right] \qquad (j = 1, 2, \ldots, n) \quad (15)$$

where

$$A_j = \left(1 - \frac{h}{3}f_{j-1}\right)\left(1 + \frac{h}{3}f_j\right) + \frac{h^2}{36}f_{j-1}f_j. \qquad (16)$$

Similarly M_{j+1} can be obtained in terms of y_{j+1} and y_j from equation (11) and equation (12) (with j replaced by $j + 1$), the resulting expression being

$$B_j M_{j+1} = \left(1 - \frac{h}{3}f_j\right)\left[r_{j+1} - g_{j+1}y_{j+1} - \frac{f_{j+1}}{h}(y_{j+1} - y_j)\right] - \frac{h}{6}f_{j+1}\left[r_j - g_j y_j - \frac{f_j}{h}(y_{j+1} - y_j)\right] \qquad (j = 0, 1, \ldots, n-1) \quad (17)$$

where

$$B_j = A_{j+1} = \left(1 - \frac{h}{3}f_j\right)\left(1 + \frac{h}{3}f_{j+1}\right) + \frac{h^2}{36}f_j f_{j+1}. \qquad (18)$$

Substitution of the expressions for M_{j-1} and M_{j+1} given by equations (15) and (17) into equation (14) leads after straightforward but tedious manipulation to the final three-term recurrence relationship for the spline approximation, namely

$$y_{j+1}\left(1 + \frac{h}{2}f_{j+1} + \frac{h^2}{6}g_{j+1}\right) A_j - y_j\left[\left(1 + \frac{h}{2}f_{j+1}\right) A_j + \left(1 - \frac{h}{2}f_{j-1}\right) B_j - \frac{2h^2}{3}g_j C_j\right] + y_{j-1}\left(1 - \frac{h}{2}f_{j-1} + \frac{h^2}{6}g_{j-1}\right) B_j = \frac{h^2}{6}(A_j r_{j+1} + 4C_j r_j + B_j r_{j-1}) \quad (j = 1, 2, \ldots, n-1) \qquad (19)$$

where A_j and B_j are given by equations (16) and (18) and

$$C_j = 1 + \frac{7h}{24}(f_{j+1} - f_{j-1}) - \frac{h^2}{12}f_{j-1}f_{j+1}. \qquad (20)$$

Formula (19) is the counterpart of formula (9) when the first derivative term is present and clearly reduces to the latter when $f(x) \equiv 0$. It also simplifies considerably when $f(x) =$ constant, say c. For then a factor $1 - \frac{h^2}{12}c^2$ cancels throughout and equation (19) reduces to

$$\delta^2 y_j + \frac{h}{2}c(y_{j+1} - y_{j-1}) + h^2\left(1 + \frac{1}{6}\delta^2\right)g_j y_j = h^2\left(1 + \frac{1}{6}\delta^2\right)r_j \quad (21)$$

which again has a local truncation error of order $\frac{1}{12}\delta^4 y$ (as in case (a)) and is the best three-point approximation to

$$y'' + cy' + g(x)y = r(x). \quad (22)$$

On solving equations (19) in conjunction with the boundary conditions (6) for the y_j, the full spline solution is obtained by direct substitution into equation (15) or (17) and (1). Derivatives at the nodal points may be calculated from equations (2) or (3).

We observe that a boundary condition of the form $\alpha y' + \beta y = \gamma$ at say $x = x_0$ may be approximated, on using equations (15), (17) and (2) by a two-term relationship connecting y_0 and y_1, so that the tri-diagonal structure of the equations for determining y_0 to y_n is retained.

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References

AHLBERG, J. H., NILSON, E. N., and WALSH, J. L. (1967). *The theory of splines and their applications*, Academic Press.

ALBASINY, E. L., and COOPER, J. R. A. (1963). The calculation of electronic properties of BH_4^-, CH_4 and NH_4^+ using one-centre self-consistent field wave functions, *Proc. Phys. Soc.*, Vol. 82, Part 2, p. 289.

BICKLEY, W. G. (1968). Piecewise cubic interpolation and two-point boundary problems, *Computer Journal*, Vol. 11, p. 206.

NATIONAL PHYSICAL LABORATORY (1961). *Modern computing methods*, Second edition. Her Majesty's Stationery Office, London.

Book Review

Stochastic Approximation and Nonlinear Regression, by A. E. Albert and L. A. Gardner; 204 pages. (*MIT Press*, 154s.)

Statistical inference may be defined as the art of drawing sensible conclusions from variable data, and the history of statistical theory is to some extent a development of ways of describing the variability of data and of assessing the relative merits of various possible conclusions. The problem, in anything like complete generality, is vast. Under certain strong restrictions substantial progress has been made, particularly in the 'stationary parametric' case, when the data may be regarded as realisations of mutually independent random variables with a common probability distribution of known functional form which involves one or more unknown parameters. Here the 'sensible conclusion' that is sought is a useful approximation for the unknown parameters, usually expressed as a fallible statement (or 'estimate') of what their actual values seem to be, together with some information about the degree of reliability of this statement.

The theory of this approach was brought to its full flowering by the late Sir Ronald Fisher. Crippling though the imposed restrictions appear to be, the theory nevertheless had (and has) a wide field of strictly practical applicability. Where the functional form of the underlying probability distributions is not known, or cannot reasonably be guessed, a closely related procedure is available in which the experimental data are expressed as random deviations from their average values, these average values being known (or postulated) functions—often linear—of given experimental conditions and unknown parameters. This so-called regression approach is widely used, particularly when the data are thought to be influenced by several experimental factors. The parameters to be estimated (usually by 'least squares') are then measures of the sensitivity of the system to changes in the experimental conditions. In this type of situation a body of experimental data may be likened to a parcel of gold-bearing ore: the quantity of golden information potentially available is finite, and the most efficient mathematical processes must be used to extract it, however protracted the computations. In the last couple of decades, however, increasing attention has been paid to the more complex situation where, instead of being concerned with the analysis of a completed experiment, the inferences we are interested in are related to an evolving system in which data becomes available sequentially, and analyses have to be made repeatedly—and rapidly—as fresh data comes in. Here an inference leads to the immediate action of modifying the system: indeed the whole purpose of making a fresh observation is to decide how next to modify the system—the 'system' being, for example, the progress of a chemical industrial reaction. In this type of situation the older static concept of efficiency of estimation may well have to be abandoned since the speed with which the estimate can be computed may be an overriding factor.

As a result of research and development in this area the subject is beginning to define itself and books are now beginning to appear with titles such as *Optimization and Control in Stochastic Systems*. It is to this class that the work under review belongs. Given data $\{Y_n\}$ from a time-series whose mean-value function $\{F_n(\theta)\}$ is of known form but involves an unknown parameter-vector θ, the problem of estimating θ in this regression-type problem by an efficient and rapid method is tackled by a 'differential correction' recursive approach in which the estimate t_{n+1} of θ at the $(n+1)$-th stage is defined in terms of t_n by an equation of the form

$$t_{n+1} = t_n + a_n\{Y_n - F_n(t_n)\}$$

where $\{a_n\}$ is a suitably chosen sequence of 'smoothing' vectors. The main aim of the monograph is to consider the effect of various choices of smoothing vectors on the estimates obtained.

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