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Cubic spline solutions of boundary value problems over infinite intervals

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Abstract: A cubic spline method for the numerical solution of a two-point boundary value problem posed on an infinite interval involving a second order linear differential equation is described. By reducing the infinite interval to a finite interval which is large and imposing appropriate asymptotic boundary condition at the far end, the resulting boundary value problem is treated by using the cubic spline approximation. The tridiagonal system resulting from the spline approximation is efficiently solved by the method of sweeps. The stability of the method is analysed and the theory is illustrated by solving test examples.

Keywords: Boundary value problem, asymptotic boundary condition, cubic spline, methods of sweeps.

Introduction

The development of improved methods for solving two-point boundary value problems of practical significance is of great importance in Science and Engineering. In many cases, the domain of the governing equations of these problems is infinite or semi-infinite so that the special treatment is required for these so-called infinite interval problems. These problems occur very frequently and are of great importance in areas such as fluid dynamics, aerodynamics, quantum mechanics and electronics, etc. A few notable examples for these problems are Von Karman flows [11, 12], a combined forced and free convection flow over a horizontal plate [14], an eigen value problem for the Schrödinger equation [10] and several others. Often in most cases, the analytical solutions for these problems are not readily attainable and thus the problem is brought to the problem of finding efficient computational algorithms for obtaining numerical

Ever since the pioneering work by Ahlberg et al. [1], there has been a great deal of development in the theory of spline functions and their applications to several practical problems. Of these, the cubic splines have attained a prime place and have attracted the attention of many to solve, in particular, boundary value problems. This is possibly because these cubic splines are efficient and simple to use and possess important properties that are required of a good approximation. To cite a few, Bickley [5] has considered the use of cubic splines for solving linear two-point boundary value problems, which leads to the solution of a set of linear equations whose coefficient matrix is of upper Hessenberg form. The cubic spline method suggested by Bickley has also been examined by Fyfe [8] in combination with deferred correction to solve two-point boundary problems. Albasiny and Hoskins [2] have obtained spline solutions by solving a set of equations with a tri-diagonal matrix of coefficients. In another paper by the same authors [3], the cubic spline approximation has been applied to an integral equation reformulation of the original differential equation, which has been shown to have smaller truncation error than would be obtained by direct use of the cubic spline on the differential equation itself. Daniel [6] has proposed the use of acceleration with collocation for various types of spline approximation appropriate for two-point boundary value problems for both second order equations or first order systems. There are several other papers on this topic which we are unable to quote here due to lack of space, but little seems to have been done in using cubic splines to solve boundary value problems over infinite intervals.

The purpose of the present paper is to report the cubic spline procedure for numerically solving two-point boundary value problems over infinite intervals. We restrict our analysis here to the solution of linear two-point boundary value problems. Unlike the familiar three point finite difference discretization, second order accuracy is maintained even with a nonuniform mesh and relatively large changes in the grid spacing. Also spline approximation described here leads to tridiagonal systems. In the next section, the asymptotic boundary condition for the infinite interval problem is derived. In Section 3, the cubic spline formulation and the procedure is discussed with derivative boundary condition. In Section 4, the method of sweeps is given to improve upon the efficiency and computer time, to solve the tridiagonal system. The stability of the method is discussed in Section 5. Numerical examples and results are shown in Section 6 and discussion is drawn in Section 7.

2. Asymptotic boundary condition

We consider the linear two point boundary value problems of the form

$$Ly(x) \equiv y'' + p(x)y' + q(x)y = f(x),$$
 (2.1)

$$y(a) = \alpha, \tag{2.2}$$

$$y(\infty) = \beta$$
, or (2.3)

$$\operatorname{Lt}_{x\to\infty}y(x)=\beta$$

where the functions p(x), q(x) and f(x) are continuous and q(x) < 0.

In order to find the appropriate asymptotic boundary condition for the equation (2.1), rewrite (2.1) as a first order system in the form: Let y(x) = u(x), y'(x) = u'(x) = v(x), we have

$$u'(x) = v(x), \tag{2.4}$$

$$v'(x) + p(x)v(x) + q(x)u(x) = f(x), (2.5)$$

and correspondingly (2.2) and (2.3) become

$$u(a) = \alpha, \tag{2.6}$$

$$\operatorname{Lt}_{x \to \infty} u(x) = u_{\infty} = \beta.$$
(2.7)

Letting $U = (u,v)^{t}$, (t denotes transpose), we can write the first order system (2.4)-(2.5) in the matrix vector form

$$U' = A(x)U + b(x) = F(x, u)$$
(2.8)

where

$$A(x) = \begin{bmatrix} 0 & 1 \\ -q(x) & -p(x) \end{bmatrix}, \qquad b(x) = \begin{bmatrix} 0 \\ f(x) \end{bmatrix}.$$

A general theory for linear and nonlinear systems of the form (2.8) on semi infinite interval has been developed by Lentini and Keller [10]. We assume that

- (i) $\lim_{x \to \infty} A(x) = A$, a constant matrix.
- (ii) $\lim_{x\to\infty} dA(x)/dx = 0$,
- (iii) A(x) is piecewise continuously differentiable on (a, ∞) , and
- (iv) u_{∞} is required to be the root of $\lim_{x\to\infty} F(x, u) = 0$.

We also assume that A is in the canonical form such that $A = EJE^{-1} \neq 0$ (a zero matrix) and J has the block diagonal form $J = \operatorname{diag}(J^+, J^0, J^-)$ where J^+ contains eigenvalues of A with positive real part, J^0 the eigenvalues of A with zero real part and J^- the eigenvalues of A with a negative real part. The main idea is to find all bounded solutions and to eliminate the contribution from the unbounded solution of the equation (2.8). The behaviour at infinity of the solution of the system (2.8) is essentially given by the eigenvalues of the matrix.

$$A_{\infty} = \operatorname{Lt}_{X \to \infty} A(X) = \begin{bmatrix} 0 & 1 \\ K & L \end{bmatrix}$$

where $K = Lt_{x \to \infty} - q(x)$ and $L = Lt_{x \to \infty} - p(x)$.

Suppose the matrix A_{∞} has the eigen value λ_1 and λ_2 , then depending upon Re λ_1 , Re $\lambda_2 \ge 0$, we find the linearly independent solution which decay exponentially at infinity and the linearly independent solutions which are unbounded as $x \to \infty$. Since we need only one condition at the far end we expect only one eigen value with a positive real part and say, this eigen value is λ_1 . We introduce the projection matrix P_m of the form $P_m = [1, 0]$. (If the eigenvalue λ_2 is with a positive real part, we have $P_m = [0, 1]$).

Let E be a matrix of eigen vectors of A_{∞} ,

$$E = \begin{bmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{bmatrix}.$$

By calculating E^{-1} for which $E^{-1}A_{\infty}E = \text{diag}(\lambda_1, \lambda_2)$ we write the asymptotic boundary condition as

$$\lim_{x \to \infty} P_m E^{-1} F(x, u) = 0. \tag{2.9}$$

Equation (2.9) yields the condition at x = N where N is chosen by taking different values of X for which the computed solution approximates the actual solution.

3. Cubic spline formulation

In order to solve the finite interval problem obtained above, we give cubic spline procedure combined with the method of sweeps. For the sake of brevity, we assume that the asymptotic boundary condition (2.9) is of the form

$$\alpha_0 y(x_\infty) + \beta_0 y'(x_\infty) = K \tag{3.1}$$

for $x_{\infty} = N$, N large but finite, where α_0 , β_0 and K are known constants such that $\alpha_0 \beta_0 \ge 0$ and $|\alpha_0| = |\beta_0| \ne 0$. This guarantees the unique solution of the two-point boundary value problem given by (2.1), (2.2) and (3.1) (cf. Keller [9]).

We consider a mesh with grid points $a = x_0 < x_1 \cdots x_n = N$ with $h = x_i - x_{i-1} > 0$. The cubic spline S(x) interpolating to the function y(x) at the grid points is given in general by the equation

$$S(x) = M_{i-1}(x_i - x)^3 / 6h + M_i(x - x_{i-1})^3 / 6h + (y_{i-1} - \frac{1}{6}h^2 M_{i-1})(x_i - x) / h + (y_i - \frac{1}{6}h^2 M_i)(x - x_{i-1}) / h$$
(3.2)

where $M_i = S''(x_i)$ and $y_i = y(x_i)$.

Ahlberg et al. [1] have shown that if the function $y(x) \in C^4[a, N]$, then the spline function S(x) approximates y(x) at all points in [a, N] to fourth order in h. The unknown derivatives M_i are related by enforcing the continuity condition on S'(x).

Differentiating (3.2), we get

$$S'(x) = M_{i-1} \left[-\frac{1}{2} (x_i - x)^2 / h + \frac{1}{6} h \right] + M_i \left[\frac{1}{2} (x - x_{i-1})^2 / h - \frac{1}{6} h \right] + (y_i - y_{i-1}) / h.$$
(3.3)

From (3.3) we have the one sided limits of the derivative as

$$S'(x_i^+) = -\frac{1}{3}hM_i - \frac{1}{6}hM_{i+1} + (y_{i+1} - y_i)/h, \quad i = 0, 1, 2, ..., n - 1,$$
(3.4)

and

$$S'(x_i^-) = \frac{1}{3}hM_i + \frac{1}{6}hM_{i-1} + (y_i - y_{i-1})/h, \quad i = 1, 2, ..., n.$$
(3.5)

The continuity condition $S'(x_i^+) = S'(x_i^-)$ yields the relation

$$\frac{1}{6}hM_{i-1} + \frac{2}{3}hM_i + \frac{1}{6}hM_{i+1} = (y_{i+1} - 2y_i + y_{i-1})/h, \quad i = 1, 2, \dots, n-1.$$
 (3.6)

We now consider collocation of equation (2.1) at the equispaced grid points $x_j = x_0 + jh$ (j = 0, 1, ..., n) with $x_0 = a$, $x_n = N$ using as approximating function the cubic spline S(x) which interpolates to the function y(x) at these points. Using an approach similar to one in [2], the following tridiagonal system of equations is obtained:

$$B_i y_{i+1} - C_i y_i + D_i y_{i-1} = E_i, \quad i = 1, 2, ..., n-1$$
 (3.7)

where

$$B_i = a_i \left(1 + \frac{1}{2} h p_{i+1} + \frac{1}{6} h^2 q_{i+1} \right), \tag{3.8}$$

$$C_i = a_i \left(1 + \frac{1}{2} h p_{i+1} \right) + b_i \left(1 - \frac{1}{2} h p_{i-1} \right) - \frac{2}{3} h^2 q_i d_i, \tag{3.9}$$

$$D_{i} = b_{i} \left(1 - \frac{1}{2} h p_{i-1} + \frac{1}{6} h^{2} q_{i-1} \right), \tag{3.10}$$

$$E_i = \frac{1}{6}h^2(b_i f_{i-1} + 4d_i f_i + a_i f_{i+1}), \tag{3.11}$$

$$a_{i} = 1 - \frac{1}{3}hp_{i-1} + \frac{1}{3}hp_{i} - \frac{1}{12}h^{2}p_{i}p_{i-1}, \tag{3.12}$$

$$b_i = 1 - \frac{1}{3}hp_i + \frac{1}{3}hp_{i+1} - \frac{1}{12}h^2p_ip_{i+1}, \tag{3.13}$$

$$d_{i} = 1 - \frac{1}{12}h^{2}p_{i-1}p_{i+1} + \frac{7}{24}h(p_{i+1} - p_{i-1}). \tag{3.14}$$

4. Methos of sweeps

To solve the tridiagonal system given by (3.7), we make use of the method of sweeps. We seek a difference relation of the form

$$y_{i+1} = W_i Y_i + T_i, \quad i = 0, 1, 2, ..., n-1$$
 (4.1)

where W_i and T_i correspond to $W(x_i)$ and $T(x_i)$ and are to be determined.

By using (4.1) in (3.7), we have

$$Y_{i} = \frac{D_{i}}{(C_{i} - B_{i}W_{i})} Y_{i-1} + \frac{(B_{i}T_{i} - E_{i})}{(C_{i} - B_{i}W_{i})}.$$
(4.2)

But from (4.1) we have

$$Y_i = W_{i-1}Y_{i-1} + T_{i-1}. (4.3)$$

From (4.2) and (4.3) we get

$$W_{i-1} = D_i / (C_i - B_i W_i), (4.4)$$

$$T_{i-1} = (B_i T_i - E_i) / (C_i - B_i W_i). \tag{4.5}$$

To solve these recurrence relations for W_i and T_i (i = n - 2, ..., 0) we need to know the values of W_{n-1} and T_{n-1} .

From (3.1) for x = nh, we have

$$\alpha_0 y_n + \beta_0 y_n' = K. \tag{4.6}$$

Equation (4.6) can be approximated at $x = x_n$ by using the result

$$S'(x_n^-) = \frac{1}{3}hM_n + \frac{1}{6}hM_{n-1} + (y_n - y_{n-1})/h \tag{4.7}$$

where from [2], we have

$$M_{n} = (1/b_{n-1}) \left[\left(f_{n} - \frac{1}{3}hp_{n-1}f_{n} - \frac{1}{6}hp_{n}f_{n-1} \right) - y_{n} \left(q_{n} - \frac{1}{3}hp_{n-1}q_{n} + p_{n}/h - \frac{1}{2} \left(p_{n}p_{n-1} \right) \right) + y_{n-1} \left(p_{n}/h - \frac{1}{2} \left(p_{n-1}p_{n} \right) + \frac{1}{6}hp_{n}q_{n-1} \right) \right]$$

$$(4.8)$$

and

$$M_{n-1} = (1/a_n) \left[\left(f_{n-1} + \frac{1}{3} h p_n f_{n-1} + \frac{1}{6} h p_{n-1} f_n \right) - y_{n-1} \left(q_{n-1} + \frac{1}{3} h p_n q_{n-1} - p_{n-1} / h \right) \right]$$

$$- \frac{1}{2} p_n p_{n-1} - y_n \left(p_{n-1} / h + \frac{1}{6} h p_{n-1} q_n + \frac{1}{2} p_n p_{n-1} \right)$$

$$(4.9)$$

With b_{n-1} and a_n defined by (3.13) and (3.12) for i = n - 1 and n respectively.

Thus the discrete form of the asymptotic boundary condition (3.1) is given by

$$\alpha_1 y_n - \beta_1 y_{n-1} = \gamma_1 \tag{4.10}$$

where

$$\alpha_1 = \alpha_0 + \frac{1}{3} (h/a_n) \beta_0 \left(-q_n - p_n/h - \frac{1}{2} p_{n-1}/h + \frac{1}{4} h p_{n-1} q_n + \frac{1}{4} p_n p_{n-1} + 3 a_n/h^2 \right), \quad (4.11)$$

$$\beta_1 = \frac{1}{3} (h/a_n) \beta_0 \left(-p_n/h - \frac{1}{2} p_{n-1}/h + \frac{1}{2} q_{n-1} + \frac{1}{4} p_n p_{n-1} + 3a_n/h^2 \right), \tag{4.12}$$

$$\gamma_1 = K + \frac{1}{3} (h/a_n) \beta_0 \left(-f_n - \frac{1}{2} f_{n-1} + \frac{1}{4} h p_{n-1} f_n \right). \tag{4.13}$$

From (4.3) for i = n we have

$$y_n = W_{n-1}Y_{n-1} + T_{n-1}. (4.14)$$

Comparing (4.10) and (4.14), we have

$$W_{n-1} = \beta_1 / \alpha_1, \tag{4.15}$$

$$T_{n-1} = \gamma_1 / \alpha_1, \tag{4.16}$$

Then W_i 's and T_i 's (i = n - 2, n - 3, ..., 0) are obtained recursively in the backward sweep by using (4.15)–(4.16) as the initial values for W's and T's. Using the values of W_i 's and knowing the value of y_0 solution y_i 's (i = 0, ..., n) can be obtained by forward process by using (4.1).

5. Stability

We will now show that the method is computationally stable. By stability, we mean the effect of an error made in one stage of calculation is not propagated into larger errors at latter stages of computation. In other words, local errors are not magnified by further computation.

Let us now examine the recurrence relation given by (4.4). Suppose a small error E_i has been introduced in the calculation of W_i then we have

$$\tilde{W}_i = W_i + E_i, \tag{5.1}$$

and we are actually solving

$$\tilde{W}_{i-1} = D_i / (C_i - B_i \tilde{W}_i). \tag{5.2}$$

From (4.4) and (5.2), we have

$$E_{i-1} = D_i / (C_i - B_i (W_i + E_i)) - D_i / (C_i - B_i W_i)$$

$$= D_i B_i E_i \Big[C_i - B_i (W_i + E_i)^{-1} \Big] \Big[C_i - B_i W_i \Big]^{-1} = W_{i-1} (B_i / D_i) E_i W_{i-1}$$
(5.3)

under the assumption that initially the error is small.

Let us assume that $B_i > 0$ and $D_i > 0$ for $1 \le i \le n - 1$. Then from the definition of B_i , C_i and D_i and since q(x) < 0, it can easily be verified that $C_i > B_i + D_i$ for $1 \le i \le n - 1$. From (4.15), we have

$$W_{n-1} = \beta_1/\alpha_1$$

and $|W_{n-1}| < 1$, if M > 0 and $\beta_1 > -\frac{1}{2}M$, where

$$M = \alpha_0 + \frac{1}{3} (h/a_n) \beta_0 \left(-q_n - \frac{1}{2} q_{n-1} + \frac{1}{4} h p_{n-1} q_n \right). \tag{5.4}$$

Under this condition and making use of the assumptions on B_i , C_i and D_i , it follows very easily from (4.4) that

$$|W_i| < 1$$
 for $i = n - 2, n - 3, ..., 0,$ (5.5)

and thus

$$|W_i| < 1, \quad i = 0, 1, \dots, n - 1.$$
 (5.6)

From (5.3), it then follows that

$$|E_{i-1}| = |W_{i-1}|^2 \left| \frac{B_i}{D_i} \right| |E_i| < |E_i|, \text{ provided } |B_i| \le |D_i|$$
 (5.7)

making the recurrence relation (4.4) stable. Similar arguments will show that the recurrence relation (4.5) is also stable.

6. Test examples and numerical results

Example 1. To illustrate our method we solve:

$$LY(x) \equiv -y'' - 2y' + 2y = e^{-2x}, \tag{6.1}$$

$$y(0) = 1.0, (6.2)$$

$$y(\infty) = 0.0. \tag{6.3}$$

This problem has earlier been solved by Robertson [13] and its exact solution is given by

$$y(x) = \frac{1}{2} e^{-(1+\sqrt{3})x} + \frac{1}{2} e^{-2x}.$$
 (6.4)

The asymptotic boundary condition for this example can be written as

$$\frac{1}{3}\sqrt{3}y(x_m) + \frac{1}{6}\sqrt{3}(-1+\sqrt{3})y'(x_m) = 0. \tag{6.5}$$

The boundary value problem given by (6.1), (6.2) and (6.5) has been solved using cubic spline with method of sweeps and the numerical results are presented in Table 1.

Example 2. As a second example, we solve:

$$LY(x) \equiv -y'' + (1+1/x)y = 1/x^2,$$
 (6.6)

$$y(1) = 0.0, (6.7)$$

$$y(\infty) = 0.0. \tag{6.8}$$

Table 1 Numerical solution for Example 1

$x_{\infty} = N$	x	$h=\frac{1}{32}$	$h=\frac{1}{64}$	$h=\frac{1}{128}$	Exact solution
10	3.0	0.13759746 E - 02	0.137691756 E-02	0.13771534 E - 02	0.13772321 E-02
	6.0	0.31078798 E - 05	0.31095814 E-05	0.31100070 E - 05	0.31101148 E - 05
	8.0	0.56548516 E-07	0.56572160 E - 07	0.56576829 E-07	0.56428597 E - 07
	10.0	0.171415437 E - 08	0.16931479 E - 08	0.16824897 E-08	0.10312569 E-08
11	3.0	0.13759746 E-02	0.13769176 E-02	0.13771534 E - 02	0.13772321 E-02
	6.0	0.31078456 E - 05	0.31095483 E - 05	0.31099744 E - 05	0.31101148 E - 05
	8.0	0.56400702 E - 07	0.56428997 E-07	0.56435997 E-07	0.56428597 E-07
	10.0	0.10750475 E - 08	0.10741567 E - 08	0.10735823 E - 08	0.10312569 E - 08
	11.0	0.23189027 E-09	0.22904771 E-09	0.22760567 E-09	0.13951780 E-09
12	3.0	0.13759546 E - 02	0.13769176 E - 02	0.13771535 E-02	0.13772321 E-02
	6.0	0.31078433 E - 05	0.31095461 E-05	0.31099723 E - 05	0.31101148 E-05
	8.0	0.56391087 E - 07	0.56419684 E - 07	0.56426836 E-07	0.56428597 E-07
	10.0	0.10334734 E - 08	0.10338912 E - 08	0.10339729 E - 08	0.10312569 E-08
	12.0	0.31376740 E - 10	0.30992060 E-10	0.30796922 E-10	0.18878562 E-10

Table 2					
Numerical	results	for	the	Example	2

X	h = 1	$h=\frac{1}{2}$	$h=\frac{1}{4}$	$h=\frac{1}{8}$	$h=\frac{1}{16}$
1.0	0.00000000 E0				
5.0	0.40360315 E-1	0.39381625 E-1	0.39157992 E-1	0.39104661 E-1	0.39091525 E - 1
7.0	0.20131629 E-1	0.20066824 E - 1	0.20049654 E-1	0.2004548 E - 1	0.20044453 E - 1
9.0	0.11950688 E-1	0.11955937 E-1	0.119568133 E-1	0.119570277 E-1	0.119570816 E-1
15.0	0.42725024 E-2	0.42732625 E-2	0.42734530 E-2	0.42735006 E-2	0.42734978 E-2
25.0	0.15525067 E - 2	0.15525367 E - 2	0.15525442 E - 2	0.15507248 E - 2	_
30.0	0.10821151 E-2	0.108212507 E-2	0.10821275 E - 2	-	_
31.0	0.10140307 E - 2	0.10140887 E - 2	0.101409079 E-2	_	-
15.0	0.48447366 E-3	0.48447452 E - 3	0.46808327 E - 3	_	_
55.0	0.32530015 E - 3	0.32530616 E - 3	_	-	_
55.0	0.23342259 E - 3	_	_	_	_
75.0	0.17396594 E-3	_	_	_	_
77.0	0.153022182 E-3	_		_	_

This problem has earlier been considered by Fox [7] and later by Robertson [13]. The asymptotic boundary conditions in this case is given by

$$\frac{1}{2}y(x_m) + \frac{1}{2}y'(x_m) = 0. ag{6.9}$$

The resulting boundary value problem (6.6), (6.7) and (6.9) has been solved by the method described earlier and the numerical results are presented in Table 2.

7. Discussion

A cubic spline technique in combination with the method of sweeps has been presented for the approximate solution of two-point boundary value problems over infinite intervals. The method has been analysed for stability. Test examples, tackled earlier by Fox [7] and Robertson [13] have been solved to demonstrate the efficiency of the proposed method. For these examples, the asymptotic boundary condition at $x_{\infty} = N$ was first derived and the value $x_{\infty} = N$ was then varied until no significant change in the solutions was noticed. The computation was done on a DEC-1090 computer system in double precision arithmetic to ensure minimum round-off errors.

Table 1 represents the numerical solutions for Example 1 at some selected points by taking different mesh sizes (h) and different values of $x_{\infty} = N$. The values of N taken for computation are N = 10, 11 and 12 for different values of h. The exact solution of the problem is also presented and it is observed that the computed solutions compare favourably well with the exact solution. It is known for this example that the solution decays exponentially and this fact is reflected in the computer solutions for different values of N. It can be seen that the computed solutions for N = 12 show six to eleven place accuracy and thus N = 12 can be taken to represent the point at infinity for the problem.

The numerical solutions for Example 2 for different values of h are given in Table 2. It is evident from this table that the solutions decay relatively slowly which agrees with the observation made by Fox [7]. The computed solutions also compare very well with that obtained by

Robertson [13] and at $X_{\infty} = N = 9$, the solutions compare upto five places of decimal. The advantage in using cubic spline is that it not only gives an approximation to the solution y(x) but also an approximation to the derivative y'(x) at every point of the interval. Secondly, the cubic spline approximation approximates the given problem with a local truncation error of $O(h^4)$ especially when the function $f(x) \equiv 0$ or is equal to a constant, and leads to the solution of a tridiagonal system of equation the property, which is not normally shared by usual finite difference methods.

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