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A CONNECTION BETWEEN QUARTIC SPLINE SOLUTION AND NUMEROV SOLUTION OF A BOUNDARY VALUE PROBLEM

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Abstract

This brief paper derives via quartic spline function a new consistency recurrence relation connecting the quartic spline function values at equidistant knots and the corresponding values of the second derivatives. It is shown how this consistency relation may be used in an algorithm for computing quartic spline approximations to the solution and its higher derivatives for a linear two-point boundary value problem. Some numerical evidence is also included to demonstrate the practical usefulness of the algorithm.

1. INTRODUCTION

We first introduce a sequence of grid points $\pi = \{x_n\}_{n=0}^{N+1}$ by dividing $[a, b]$ into $(N+1)$ equal parts so that

$$(1.1) \quad x_n = a + nh, \quad n=0(1)N+1,$$

with $h = (b-a)/(N+1)$. Many recurrence relations hold between the values of a spline and its derivatives at the equidistant knots x_n . A general result due to Swartz (1968) is given in the following theorem.

Theorem 1.1. For any spline function $s(x)$, of degree $m \geq 2$ and in $C^{m-1}[a, b]$; and for each ν , $0 \leq \nu \leq N+2-m$; and for each μ , $1 \leq \mu \leq m-1$; there is a linear relation between the m quantities $s_{j+\nu}$, and the m quantities, $s_{j+\nu}^{(\mu)}$, $0 \leq j \leq m-1$.

This relation is given by

$$(1.2) \quad \sum_{j=0}^{m-1} \alpha_j^{(m,\mu)} s_{j+\nu} = h^\mu \sum_{j=0}^{m-1} \beta_j^{(m)} s_{j+\nu}^{(\mu)}.$$

The general expressions for the coefficients $\alpha^{(m,\mu)}$ and $\beta^{(m)}$ are also given in Swartz paper.

In particular let $c(x)$ and $q(x)$ designate the cubic and quartic spline function respectively, then from Theorem 1.1 it follows that

$$(1.3) \quad \begin{cases} \text{(i)} & c_{i+1} - c_{i-1} = \frac{h}{3}(c'_{i-1} + 4c'_i + c'_{i+1}), \\ \text{(ii)} & c_{i-1} - 2c_i + c_{i+1} = \frac{h^2}{6}(c''_{i-1} + 4c''_i + c''_{i+1}), \end{cases}$$

$i=1(1)N$; and

$$(1.4) \quad \begin{cases} \text{(i)} & -q_i - 3q_{i+1} + 3q_{i+2} + q_{i+3} = \frac{h}{4}(q'_i + 11q'_{i+1} + 11q'_{i+2} + q'_{i+3}), \\ \text{(ii)} & q_i - q_{i+1} - q_{i+2} + q_{i+3} = \frac{h^2}{12}(q''_i + 11q''_{i+1} + 11q''_{i+2} + q''_{i+3}), \\ \text{(iii)} & -q_i + 3q_{i+1} - 3q_{i+2} + q_{i+3} = \frac{h^3}{24}(q'''_i + 11q'''_{i+1} + 11q'''_{i+2} + q'''_{i+3}), \end{cases}$$

$i=0(1)N-2$, and $c_i \equiv c(x_i)$, $q_i \equiv q(x_i)$ etc.

The use of cubic spline function $c(x)$ [Albasiny et al. (1969)]; Fyfe (1970)] in approximating continuously the solution of the following real two point boundary value problems

$$(1.5) \quad \begin{aligned} y''(x) &= f(x)y(x) + g(x), \quad f(x) \geq 0 \text{ on } [a, b] \\ y(a) - A &= y(b) - B = 0 \end{aligned}$$

leads to a three point recursion formula 1.3 (ii). The method of development, there, of 1.3 (ii) is altogether different from the one given by Swartz in Theorem 1.1. The relation 1.3 (ii) is used for the determination of the sequence $\{c_n\}$, $n=1(1)N$, $c_0=A$, $c_{n+1}=B$. Here c_n is assumed to approximate $y_n \equiv y(x_n)$ and $c''_n = f_n c_n + g_n$, $f_n \equiv f(x_n)$, $g_n \equiv g(x_n)$. The integer N is a suitable positive integer ≥ 1 , and we naturally assume that $y(x)$ is the unique solution of the differential system (1.5). The determination of the unknowns c_n , $n=1(1)N$ is effected by solving a system of linear equations whose associated matrix is a tridagonal matrix.

The relations (1.3) and (1.4) are reestablished by Meek (1973). Blue (1969) has obtained quintic spline solutions of the boundary value problem (1.5) But, more frequently [see Henrici (1962), Chap. 7], the problem (1.5) is solved by a well-known standard fourth order finite difference, namely, Numerov's method in which the sequence $\{z_n\}$ satisfies the recurrence relation

$$(1.6) \quad z_{n-1} - 2z_n + z_{n+1} = \frac{h^2}{12}(z''_{n-1} + 10z''_n + z''_{n+1}),$$

$n=1(1)N$, where now z_n is assumed to approximate y_n .

The main purpose of this note is to present a continuous approximation of the solution of (1.5) via quartic spline function $q(x)$ and to give an analysis in the sequel to establish a three point recurrence relation connecting the values of quartic spline and its second derivatives at the uniform knots x_n , namely,

$$(1.7) \quad q_{i-1} - 2q_i + q_{i+1} = \frac{h^2}{12}(q''_{i-1} + 10q''_i + q''_{i+1}),$$

$i=1(1)N$, in contrast to the four-point formula 1.4(ii) given by Swartz (1968). Note that (1.7) will mean that quartic spline values with uniform knots satisfy Numerov's formula (1.6).

Also, this fact that quartic spline values with uniform knots also satisfy (1.7), in addition to satisfying 1.4(ii), will have useful consequences as we shall see later on. We also remark that formula 1.4(ii) of Swartz is not unique, since, all linear combinations of (1.7) for two consecutive values of i will lead to a four-point relation between the quartic spline values and its second derivatives with uniform knots.

This approach of approximating $y(x)$ by $q(x)$ obviously has the extra advantage of continuous approximation of $y^{(m)}(x)$, $m \geq 1$. In the next section we develop the necessary formulae for quartic spline approximation of (1.5) and demonstrate that the Numerov's finite difference solution of (1.5) based on (1.6) is nothing but the discrete quartic spline solution of the corresponding boundary value problem.

2. QUARTIC SPLINE SOLUTION OF (1.5).

We recall that $q(x)$ is said to be a quartic spline over the set of grid points π if $q(x) \in [a, b]$ and $q(x)$ restricted to $[x_i, x_{i+1}]$ is a quartic polynomial for $i=0(1)N+1$. The space of all such polynomials is denoted by $s(\pi, 4)$. If in addition, we have the collocation conditions (using (1.5))

$$(2.1) \quad \begin{aligned} q''_i &= f_i q_i + g_i, \quad i=0(1)N+1, \\ q_0 &= A, \quad q_{n+1} = B, \end{aligned}$$

then $q(x)$ is said to be an $s(\pi, 4)$ -approximation of $y(x)$ at the grid points in π . This approximate function $q(x)$ is not uniquely determined by the data (2.1), since $\dim s(\pi, 4)$ is $N+5$. Roughly speaking there is still one degree of freedom left, calling for a suitable additional end condition linearly independent of those given by (2.1). In fact, as we shall see later on, this extra end condition is provided with by prescribing q'_i at $i=0$ or $N+1$.

We now proceed to develop the necessary consistency relation. Let $y(x) \simeq q(x) = P_i(x)$, $x \in [x_i, x_{i+1}]$, $i=0(1)N+1$

where we write

$$(2.2) \quad P_i(x) = a_i(x-x_i)^4 + b_i(x-x_i)^3 + c_i(x-x_i)^2 + d_i(x-x_i) + e_i,$$

and $q(x) \in C^3[a, b]$. We adopt the convention that

$$(2.3) \quad P_i(x_j) = q_j, \quad P'_i(x_j) = F_j, \quad P''_i(x_j) = M_j, \quad x_j \in [x_i, x_{i+1}],$$

and thus we determine the five coefficients in (2.2) in terms of q_i, q_{i+1}, F_i, M_i and M_{i+1} . An easy calculation shows that

$$(2.4) \quad \begin{cases} a_i = -(q_{i+1} - q_i)/h^4 + F_i/h^3 + (M_{i+1} + 2M_i)/(6h^2) \\ b_i = 2(q_{i+1} - q_i)h^3 - 2F_i/h^2 - (M_{i+1} + 5M_i)/(6h) \\ c_i = 0.5M_i, \quad d_i = F_i, \quad e_i = q_i, \quad i=0(1)N. \end{cases}$$

The continuity of the first derivative at $x=x_i$ [that is $P'_{i-1}(x_i) = P'_i(x_i)$] yields

$$(2.5) \quad 4h^3a_{i-1} + 3h^2b_{i-1} + 2hc_{i-1} + d_{i-1} = d_i,$$

which on using (2.4) reduces to

$$(2.6) \quad F_i + F_{i-1} = 2(q_i - q_{i-1})/h + h(M_i - M_{i-1})/6.$$

Similarly, the continuity of the third derivative at $x=x_i$ yields

$$(2.7) \quad 4ha_{i-1} + b_{i-1} = b_i,$$

which by (2.4) reduces to

$$(2.8) \quad F_i + F_{i-1} = (q_{i+1} - q_{i-1})/h - h(M_{i+1} + 8M_i + 3M_{i-1})/12.$$

The elimination of $(F_i + F_{i-1})$ from the relations (2.6) and (2.8) gives

$$(2.9) \quad \begin{aligned} 2(q_i - q_{i-1})/h + h(M_i - M_{i-1})/6 &= (q_{i+1} - q_{i-1})/h \\ &- h(M_{i+1} + 8M_i + 3M_{i-1})/12. \end{aligned}$$

On simplifying this preceding relation we get

$$(2.10) \quad q_{i-1} - 2q_i + q_{i+1} = \frac{h^2}{12}(M_{i-1} + 10M_i + M_{i+1}),$$

$i=1(1)N$, which is the same as the Numerov's formula. Here $M_i = f_i q_i + g_i$, $i=0(1)N+1$. The unknowns q_i are first determined by solving a tridiagonal system of linear equations based on (2.10). The formula (2.6) or (2.8) can then be used to evaluate F_i provided we know the starting value F_0 (or F_{N+1}). Approximate values of these are given by Usmani (1976) in the form

$$(2.11) \quad F_0 = [-q_0 + q_1 - h^2(5M_0 + M_1)/12 - h^3(f'_0 q_0 + g'_0)/12] / [h(1 + h^2 f_0/12)],$$

$$(2.12) \quad F_{N+1} = [-q_N + q_{N+1} + h^2(M_N + 5M_{N+1})/12 - h^3(f'_{N+1} q_{N+1} + g'_{N+1})/12] / [h(1 + h^2 f_{N+1})/12].$$

However, (2.6) is unsuitable for the computation of the sequence $\{F_i\}$ because it is unstable and its solution has the form

$$(2.13) \quad F_i = (-1)^i F_0 + \sum_{m=1}^i (-1)^{i-m} \phi_m, \quad i=1(1)N+1,$$

where $\phi_i = 2(q_i - q_{i-1})/h + h(M_i - M_{i-1})/6$. In practice we compute F_1 from (2.6) and then the sequence F_i , $i=2(1)N+1$ from the consistency relation

$$(2.14) \quad \begin{aligned} F_{i+1} &= F_{i-1} + h(M_{i-1} + 4M_i + M_{i+1})/3, \\ &i=1(1)N. \end{aligned}$$

This preceding consistency relation can be developed by obtaining the five coefficients in (2.2) in terms of $q_i, F_i, F_{i+1}, M_i, M_{i+1}$ and then employing the continuity of the third derivative $P''_{i-1}(x_i) = P''_i(x_i)$ at $x = x_i$. Note that the solution of (3.14) has the form

$$(2.15) \quad F_i = \begin{cases} (F_0 + F_2 + \dots + F_{i-2}) + (\phi_1 + \phi_3 + \dots + \phi_{i-1}), & i \text{ even} \\ (F_1 + F_3 + \dots + F_{i-2}) + (\phi_2 + \phi_4 + \dots + \phi_{i-1}), & i \text{ odd,} \end{cases}$$

$i = 2(1)N + 1$, where $\phi_i \equiv h(M_{i-1} + 4M_i + M_{i+1})/3$.

Thus, the knowledge of $q_i, F_i, M_i, i = 0(1)N + 1$, enables us to write down all the coefficients of the quartic spline in each subinterval as given by (2.4). A quartic spline approximation of the third derivative of $y(x)$ at the knots is then obtained by

$$(2.16) \quad y''_i \simeq q''_i = 6b_i, \quad i = 0(1)N$$

and

$$(2.17) \quad \begin{aligned} y''_N &\simeq 24ha_N + 6b_N \\ &= -12(q_{N+1} - q_N)/h^3 + 12F_N/h^2 + 3(M_{N+1} + M_N)/h. \end{aligned}$$

Finally, the approximation of $y(x)$ or its successive derivatives at points other than grid points in π will be carried out by evaluating or differentiating the appropriate quartic polynomial.

However, if we compute the derivatives of order ≥ 3 by the overdifferentiation of the differential equation in (1.5), [instead of using (2.16) and (2.17)], then an $O(h^4)$ accuracy is observed in the values of the third derivatives at the knots.

3. ERROR ANALYSIS

Let $y(x) \in C^6[a, b]$ and let the error in the quartic spline approximation to y_i be $e_i = y_i - q_i$. It is well-known [Henrici, 1962] that if $e = (e_i)$, then

$$(3.1) \quad |e_i| \leq \frac{1}{480}(x_i - a)(b - x_i)h^4 Y_6$$

where $Y_i = \max_x |y^{(i)}(x)|$. In particular

$$(3.2) \quad |e_1| \leq \frac{1}{480}h(b-h)h^4 Y_6 = O(h^5)$$

and

$$(3.3) \quad ||e|| = \max_i |e_i| \leq \frac{h^4}{1920}(b-a)^2 Y_6 = Kh^4 = O(h^4),$$

where K is a constant independent of h . For an error bound sharper than the one given by (3.3), the reader is referred to Fischer and Usmani (1969, p. 135).

Since $q''_i \equiv M_i = f_i q_i + g_i$, we have

$$(3.4) \quad \max_i |y''_i - q''_i| \leq FKh^4 = O(h^4), \quad i = 0(1)N + 1,$$

where $F = \max |f(x)|$,

The local truncation error T_i associated with the difference equation (2.6) is

$$(3.5) \quad T_i = -\frac{1}{360}h^4 y^{(5)}(\xi_i), \quad x_{i-1} < \xi_i < x_{i+1}.$$

Using (2.6) for $i=1$, (3.2), (3.4) and (3.5), we easily prove that

$$(3.6) \quad |y'_i - q'_i| = O(h^4).$$

The local truncation error τ_i associated with (2.14) is

$$(3.7) \quad \tau_i = -\frac{h^5}{90}y^{(6)}(\eta_i), \quad x_{i-1} < \eta_i < x_{i+1}.$$

If we set $\sigma_i = |y'_i - q'_i|$, then it follows from (2.14) and (3.7) that

$$(3.8) \quad \begin{cases} \sigma_{i+1} \leq \sigma_{i-1} + O(h^5) & i=1(1)N, \\ \sigma_0 = 0 & \text{(assuming } F_0 \text{ is given).} \end{cases}$$

We now prove from (3.8), using mathematical induction, that

$$(3.9) \quad \max_i |y'_i - q'_i| = O(h^4), \quad i=2(1)N+1.$$

On combining (3.6) and (3.9), we have

$$(3.10) \quad ||e'|| = \max_i |y'_i - q'_i| = O(h^4), \quad i=2(1)N+1.$$

In an analogous manner we prove that

$$(3.11) \quad \max_i |y_i''' - q_i'''| = O(h^2), \quad 0 \leq i \leq N+1,$$

see Appendix. We summarize the above results in the following theorem.

Theorem 3.1 Let $y(x) \in C^6[a, b]$ be the exact solution of the boundary value problem (1.5), and $g(x)$ be the quartic spline solution approximating $y(x)$. Then

$$\max_i |y_i^{(\mu)} - q_i^{(\mu)}| = O(h^{\Delta(\mu)}), \quad i=0(1)N+1,$$

and where $\Delta(\mu) = 4 - \frac{1}{3}(\mu-1)(\mu-2)$, $\mu=1, 2, 3$.

4. A NUMERICAL ILLUSTRATION

We obtain continuous quartic spline approximation of the boundary value problem

$$(4.1) \quad y''(x) = 2x^{-2}y(x) - x^{-1}, \quad y(2) = y(3) = 0,$$

with $y(x) = (19x - 5x^2 - 36x^{-1})/38$. All computations are carried out using double precision arithmetic in order to keep the rounding errors negligible as compared to the discretization errors.

We solve the boundary value problem using cubic and quartic spline functions. Note that the formula (2.10) is such that the truncation error associated with it can be expanded in power of h^2 and it satisfies the conditions of Theorem 7.4 [Henrici (1962)], Richardson h^2 -extrapolation method can be used to push the accuracy of quartic spline solution to $O(h^6)$. This means that

$$(4.2) \quad q_i = [q_{i, rh} - r^4 q_{i, h}] / (1 - rh^4) + O(h^6),$$

where $q_{i, h}$ denotes the quartic spline approximations to $y(x_i)$ with the step-size h , it being assumed that $(b - a)$ is an integral multiple of h . From (4.2), it follows that the extrapolated value

$$(4.3) \quad \tilde{q}_i = (a_{i, rh} - r^4 q_{i, h}) / (1 - rh^4)$$

approximates y_i with $O(h^6)$ -accuracy. We chose $r = 1/2$ in practice. These results will finally be compared with the author's sixth order finite difference method [Usmani (1973)]. All these experiments are briefly summarized in Tables I and II.

TABLE I
MAXIMUM OBSERVED ERRORS IN MODULUS ($h = 2^{-m}$, $m = 1(1)6$)

h	y_i	y'_i	y''_i	y'''_i
2^{-1}	0.389-4*	0.424-3	0.125-4	0.241-1
2^{-2}	0.265-5	0.335-4	0.986-6	0.927-2
2^{-3}	0.174-6	0.272-5	0.628-7	0.290-2
2^{-4}	0.110-7	0.193-6	0.400-8	0.814-3
2^{-5}	0.685-9	0.129-7	0.250-9	0.216-3
2^{-6}	0.429-10	0.832-9	0.157-10	0.556-4

* We write 0.389-4 for 0.389×10^{-4} .

TABLE II

N	maximum observed errors in modulus based on			
	$O(h^2)$ cubicspline	$O(h^4)$ quartic spline	$O(h^6)$ finite difference Usmani (1973)	$O(h^6)$ solution based on (3. 3)
1	0.693-3	0.389-4	0.209-5	0.176-6
3	0.165-3	0.260-5	0.377-7	0.323-8
7	0.417-4	0.174-6	0.647-9	0.556-10
15	0.104-4	0.110-7	0.102-10	0.879-12
31	0.261-5	0.685-9	0.159-12	

5. CONCLUSION

In conclusion we would like to mention two more observations in contrast to Theorem 1.1. Let $s(x)$ designate the sexic spline function. Then a long but simple analysis similar to the one given in Section 2 leads to the following five-point recurrence rela-

tions (instead of six-point relations)

$$(5.1) \quad s_{i-2} + 8s_{i-1} - 18s_i + 8s_{i+1} + s_{i+2} = \frac{h^2}{30} [s''_{i-2} + 56s''_{i-1} + 246s''_i + 56s''_{i+1} + s''_{i+2}],$$

and

$$(5.2) \quad s_{i-2} - 4s_{i-1} + 6s_i - 4s_{i+1} + s_{i+2} = \frac{h^4}{360} [s^{(4)}_{i-2} + 56s^{(4)}_{i-1} + 246s^{(4)}_i + 56s^{(4)}_{i+1} + s^{(4)}_{i+2}].$$

The use of (5.1) has been demonstrated in obtaining a sextic spline solution of (1.5) [Usmani (1978)].

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APPENDIX

Proof of (3.11)

Since

$$T_i = 6b_i$$

$$(A. 1) \quad = \frac{12}{h^3}(q_{i+1} - q_i) - \frac{12}{h^2}F_i - \frac{1}{h}(M_{i+1} + 5M_i), \quad \text{by (2. 5),}$$

hence

$$\begin{aligned} T_i + T_{i-1} &= \frac{12}{h^3}(q_{i+1} - q_{i-1}) - \frac{12}{h^2}(F_i + F_{i-1}) - \frac{1}{h}(M_{i+1} + 6M_i + 5M_{i-1}) \\ &= \frac{12}{h^3}(q_{i+1} - 2q_i + q_{i-1}) - \frac{1}{h}(M_{i+1} + 8M_i + 3M_{i-1}), \quad \text{by (2. 6)} \\ (A. 2) \quad &= \frac{2}{h}(M_i - M_{i-1}), \quad \text{by (2. 10).} \end{aligned}$$

From (A. 2), we also have

$$(A. 3) \quad T_{i+1} + T_i = \frac{2}{h}(M_{i+1} - M_i).$$

We now subtract (A. 2) from (A. 3) to get the consistency relation

$$(A. 4) \quad T_{i+1} - T_{i-1} = \frac{2}{h}(M_{i+1} - 2M_i + M_{i-1}), \quad i=1(1)N.$$

It is easy to verify that the local truncation error ρ_i associated with (A.4) is

$$(A. 5) \quad \rho_i = \frac{1}{6}h^3 y^{(6)}(\zeta_i), \quad i=1(1)N.$$

We now compute T_i , $i=1, 2$ from (A. 1). The local truncation error w_i associated with (A. 1) is

$$(A. 6) \quad w_i = \frac{1}{15}h^2 y^{(5)}(\bar{w}_i), \quad x_i < \bar{w}_i < x_{i+1}.$$

Note that, it follows from (3. 1) that

$$(A. 7) \quad |e_i| = O(h^5), \quad i=1, 2.$$

We set

$$(A. 8) \quad e_i'' = y_i''' - T_i, \quad i=0(1)N+1$$

Now it is easily proved that

$$(A. 9) \quad e_i''' = O(h^2), \quad i=1, 2$$

using (A. 1), (A. 6), (A.7) and (A. 9).

We next compute $\{T_i\}$, $i=2(1)N$, from the consistency relation (A.4). The error equation is written down in an usual manner in the form (from (A. 4) and (A. 5))

$$(A. 10) \quad \begin{cases} |e''_{i+1}| \leq |e''_{i-1}| + O(h^3), \text{ by (3. 4) and (A. 5)} \\ |e''_i| = O(h^2), i=1, 2, \text{ by (A. 9).} \end{cases}$$

From the preceding inequality we easily deduce, from mathematical induction, that

$$(A. 11) \quad |e''_i| = O(h^2), i=0(1)N.$$

In an analogous manner, we establish from (2.17) that

$$(A. 12) \quad |e''_{N+1}| = O(h^2).$$

On combining (A. 11) and (A. 12), we have desired result (3. 11).