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FUNCTION AND FIRST DERIVATIVE FITTING BY MODIFIED QUINTIC SPLINE

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November 1969

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ABSTRACT

An interpolation function is constructed when function and first derivative values are known for discrete values of the argument. It is assumed that terminal second derivatives are specified. The fitting curve consists of quintic arcs and is a modification of the quintic spline curve.

I. INTRODUCTION

We consider estimating the behaviour of a function, $f(t)$, given only, $f_i \equiv f(t_i)$, $f_i' \equiv f'(t_i)$ and $f_1'' \equiv f''(t_1)$ and $f_n'' \equiv f''(t_n)$ for $i = 1, n$ with $n \geq 5$. A similar but simpler problem is that of estimating f when only f_i and f_1' and f_n' or f_1'' and f_n'' are known and with $n \geq 3$. In this problem cubic spline fitting can be used [1]. If the f_i ; $i = 1, n$ and f_1' and f_n' and f_1'' and f_n'' are known, again with $n \geq 3$, quintic spline fitting which is discussed in the next section may be used. However neither of these fits utilizes the known values, f_i' ; $i = 2, n-1$. In section 3, we describe a modification of the quintic spline which does use all the available information. However the modification results in some sacrifice of the higher derivative continuity possessed by the quintic spline.

II. QUINTIC SPLINE FIT

The (unique) quintic spline function, $q(t)$, for data:

$$(t_i, f_i) \quad ; \quad i = 1, n \qquad n \geq 3$$

$$f_1', \; f_n'$$

$$f_1'', \; f_n''$$

has the following properties:

1. Exact fit of data

$$q_i = f_i \qquad i = 1, n$$

$$q_1' = f_1' \qquad q_n' = f_n'$$

$$q_1'' = f_1'' \qquad q_n'' = f_n''$$

2. Quintic segmentation

On each subinterval (t_i, t_{i+1}) ; $i = 1, n-1$ q is a quintic in t

3. Continuity of fourth derivative

$$q \in C_4 [t_1, t_n]$$

The following may be deduced:

4. Segmentwise constant fifth derivative

The fifth derivative exists and is constant on any subinterval, (t_i, t_{i+1}) ; $i = 1, n-1$ and these constants define a right fifth derivative at t_1, a left fifth derivative at t_n and left and right fifth derivatives (which are not in general equal) at the interior values, t_i ; $i = 2, n-1$

5. Segmentwise monotonic fourth derivative

On any subinterval, $[t_i, t_{i+1}]$ $i = 1, n-1$ either q^{iv} is constant or strictly increasing or strictly decreasing

6. Measure of discrepancy of fit

The differences between the left and right fifth derivatives may be used to construct a measure, μ, of fit discrepancy. We may define:

$$\mu = \sum_{i=2}^{n-1} (q_i^{vr} - q_i^{vl})^2$$

or

$$\mu = \max_{i=2,n-1} |q_i^{vr} - q^{vl}|$$

7. Minimization of L_4 norm

For all functions, h, satisfying properties (1) and (3)

$$\int_{t_1}^{t_n} (q^{iv})^2 \, dt \le \int_{t_1}^{t_n} (h^{iv})^2 \, dt$$

The construction of the quintic spline is well posed. Since each quintic segment is determined by six parameters (the coefficients of the quintic) we must have imposed six independent conditions for each subinterval $[t_i, t_{i+1}]$. Now at t_1 and t_n we have three conditions, namely the values of f, f' and f''. At each interior value of t, we have one condition in the value of f and two others induced by the "matching" of q', q'', q''' and q^{iv}. In fact, the equations relating q'_{i-1}, q'_i, q'_{i+1} q''_{i-1}, q''_i and q''_{i+1} may be expressed in a linear system for which the coefficient matrix has diagonal band (width six) form by means of which the system can be shown to be determinate.

III. MODIFIED QUINTIC SPLINE

We propose the construction of the (unique) modified quintic spline function, p(t), for the (complete) data:

$$(t_i, f_i, f'_i) \quad ; \quad i = 1, n \qquad n \ge 5$$

$$f''_1 \text{ and } f''_n$$

with the following properties:

1. Exact fit of data

$$p_i = f_i \qquad i = 1, n$$

$$p'_i = f'_i \qquad i = 1, n$$

$$p''_1 = f''_1 \text{ and } p''_n = f''_n$$

2. Quintic segmentation

on each subinterval, (t_i, t_{i+1}) ; $i = 1, n-1$ p is a quintic in t.

3. Continuity of <u>third</u> derivative

$$p \in C_3 [t_1, t_n]$$

4. Segmentwise constant fifth derivative (as in property 4. of quintic spline

5. Segmentwise monotonic fourth derivative

On any subinterval (t_i, t_{i+1}) either p^{iv} is constant or strictly increasing or strictly decreasing a right fourth derivative is defined at t_1, a left fourth derivative is defined, at t_n and at t_i ; $i = 2, n-1$, left and right fourth derivatives are defined.

6. Measure of discrepancy

Differences between left and right fourth and fifth derivatives may be used to construct a measure, μ, of fit discrepancy. We propose

$$\mu = \sum_{i=2}^{n-1} [(t_{i+1} - t_{i-1})(p_i^{vr} - p_i^{vl})/2.]^2 + [p_i^{ivr} - p_i^{ivl}]^2$$

or

$$\mu = \max_{i=2,n-1} [(t_{i+1} - t_{i-1}) \, |p_i^{vr} - p_i^{vl}|/2. + |p_i^{ivr} - p_i^{ivl}|$$

The construction of this modified quintic spline is well-posed at t_1 and t_n we have (as before) three conditions in the values of f, f' and f". At each interior value, t_i ; $i = 2, n-1$ we have two conditions in the

values of f and f' and a third induced by the "matching" of p'' and p'''. Thus for each interval $[t_i, t_{i+1}]$ we have the required six conditions.

The computation of p''_i ; $i = 2, n-1$ is sufficient to define the function, p, since then we shall have for each interval, $[t_i, t_{i+1}]$; $i = 1, n-1$ the values of p_i, p'_i, p''_i, p_{i+1}, p'_{i+1} and p''_{i+1}, which are sufficient to determine the quintic segment on that interval.

From the outlined properties we can expand p, p', p'', p''', p^{ivl} and p^{ivr} as Taylor series in $h = t - t_i$ whose highest non-zero term in p^{vl} or p^{vr}. Terms of order higher than p''_i can be eliminated from the relationships and setting $h_i = t_{i+1} - t_i$ we obtain

$$h_i^3 h_{i-1}^2 p''_{i-1} - 3(h_i^3 h_{i-1}^2 + h_i^2 h_{i-1}^3) p''_i + h_i^2 h_{i-1}^3 p''_{i+1}$$

$$= h_i^3 [20p_i - 20p_{i-1} - h_{i-1} (12p'_i + 8p'_{i-1})] \qquad i = 2, n-1$$

$$+ h_{i-1}^3 [20p_i - 20p_{i+1} + h_i(12p'_i + 8p'_{i+1})]$$

Using the exact fit property, we have

$$-3(h_2^3 h_1^2 + h_2^2 h_1^3) p''_2 + h_2^2 h_1^3 p''_3$$

$$= h_2^3 [20f_2 - 20f_1 - h_1(12f'_2 + 8f'_1)]$$

$$+ h_1^3 [20f_2 - 20f_3 + h_2(12f'_2 + 8f'_2)] \qquad - h_2^3 h_1^2 f''_1$$

$$h_i^3 h_{i-1}^2 p_{i-1}'' - 3(h_i^3 h_{i-1}^2 + h_i^2 h_{i-1}^3) p_i'' + h_i^2 h_{i-1}^3 p_{i+1}''$$

$$= h_i^3 [20f_i - 20f_{i-1} - h_{i-1} (12f_i' + 8f_{i-1}')]$$

$$+ h_{i-1}^3 [20f_i - 20f_{i+1} + h_i(12f_i' + 8f_{i+1}')] \qquad i = 3, n-2$$

and

$$h_{n-1}^3 h_{n-2}^2 p_{n-2}'' - 3(h_{n-1}^3 h_{n-2}^2 + h_{n-1}^2 h_{n-2}^3) p_{n-1}''$$

$$= h_{n-1}^3 [20f_{n-1} - 20f_{n-2} - h_{n-2}(12f_{n-1}' + 8f_{n-2}')]$$

$$+ h_{n-2}^3 [20f_{n-1} - 20f_n + h_{n-1}(12f_{n-1}' + 8f_n')] \qquad -h_{n-1}^2 h_{n-2}^3 f_n''$$

The above linear system is determinate to solve for p_i'' ; $i = 2, n-1$ since it is tridiagonal with diagonal dominance.

IV. COMPUTER ROUTINE, QUYNSP

A computer subroutine has been written in FORTRAN for the CDC 6600 which for input, (t_i, f_i, f_i'), f_1'' and f_n'' will construct the matrix for the linear system for p_i'', $i = 2, n-2$. This routine then calls the existing subroutine, SOLVYR, which solves the (tridiagonal, diagonally dominant) system for the values of the p_i''. Descriptions and listings for these subroutines may be obtained from the author.

V. Conclusion

Modified quintic splines provide convenient and usually satisfactory interpolating functions when function and first derivative values are known at five or more points.

VI. ACKNOWLEDGEMENT

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REFERENCE

[1] J. D. Young, UCLRL Report 17659, 1967

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