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GENERALIZATION OF SEGMENTED SPLINE FITTING OF THIRD ORDER

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By Jonathan D. Young

Abstract. The formulation for cubic spline fitting is presented in a generalized form so as to include as particular cases, the trigonometric, hyperbolic and damped-cubic splines. The formulation may provide for the investigation of other spline fits of third order.

1. Introduction: We consider the problem of constructing a fitting function $f(x)$, defined on an interval, $[x_1, x_n]$, with $f(x)$ to be used to estimate the behaviour of a function, $y(x)$, for which values

$$y_i \equiv y(x_i);\ i = 1, n \quad n \geq 3$$

are known and for which

either $$y_1' \equiv y_1'(x_1) \text{ and } y_n' \equiv y'(x_n)$$

or $$y_1'' \equiv y''(x_1) \text{ and } y_n'' \equiv y''(x_n)$$

are known or can be stipulated.

The function, $f(x)$, is to have the following properties:

1.1 Exact fitting of data

$$f(x_i) = y_i \quad i = 1, n$$

$$f'(x_1) = y_1' \text{ and } f'(x_n) = y_n'$$

or $$f''(x_1) = y_1'' \text{ and } f''(x_n) = y_n''$$

1.2 Continuity of f' and f''

$$f \in C_2 \text{ on } [x_1, x_n]$$

1.3 Convenient application.

Differentiation (first and second order), interpolation and integration of $f(x)$ provide estimates for their counter-processes on $y(x)$.

2. The Segment Function. On each subinterval, $[x_i, x_{i+1}]$; $i = 1, n - 1$, we construct a segment function, $g_i(u)$, as follows:

Let $\quad d_i = x_{i+1} - x_i \qquad i = 1, n - 1$

$$u = (x - x_i)/d_i \qquad 0 \le u \le 1$$

and let $\quad h(\xi)$ be a function having the following properties:

$$h(0) = 0 \qquad h(1) = 0$$
$$h'(0) = -1 \qquad h'(1) = \alpha$$
$$h''(0) = 0 \qquad h''(1) = \beta$$

where α and β are positive numbers. (ξ is notational, $0 \le \xi \le 1$)

Define

$$g_i(u) = y_i + (y_{i+1} - y_i)u + a_i h(u) + b_i h(1 - u); \; i = 1, n - 1 \quad (2.1)$$

(We note that h is the same function for all i, the coefficients a_i and b_i change with i).

For $x_i \le x \le x_{i+1}$ we define

$$f(x) \equiv g_i(u)$$

noting

$$f(x_i) = g_i(0) = y_i$$

and $$f(x_{i+1}) = g_i(1) = y_{i+1} \text{ as required.}$$

Differentiating g with respect to u we have

$$g_i'(u) = y_{i+1} - y_i + a_i h'(u) - b_i h'(1 - u) \tag{2.2}$$

$$g_i''(u) = a_i h''(u) + b_i h''(1 - u) \tag{2.3}$$

Evaluating at $u = 0$ and $u = 1$ we have:

$$g_i'(0) = y_{i+1} - y_i + a_i h'(0) - b_i h'(1) \tag{2.4}$$

$$= y_{i+1} - y_i - a_i - \alpha b_i$$

$$g_i'(1) = y_{i+1} - y_i + a_i h'(1) - b_i h'(0) \tag{2.5}$$

$$= y_{i+1} - y_i + \alpha a_i + b_i$$

$$g_i''(0) = a_i h''(0) + b_i h''(1) = \beta b_i \tag{2.6}$$

$$g_i''(1) = a_i h''(1) + b_i h''(0) = \beta a_i \tag{2.7}$$

whence

$$a_i = g_i''(1)/\beta \qquad b_i = g_i''(0)/\beta \tag{2.8}$$

Relating derivatives of g_i with respect to u to those of f with respect to x we have

$$g_i' = f' \frac{dx}{du} = d_i f' \qquad x_i \le x \le x_{i+1} \tag{2.9}$$

$$g_i'' = d_i f'' \frac{dx}{du} = d_i^2 f'' \qquad x_i \le x \le x_{i+1} \tag{2.10}$$

consequently,

$$a_i = d_i^2 f''(x_{i+1})/\beta \qquad b_i = d_i^2 f''(x_i)/\beta \tag{2.11}$$

3. Derivatives at Mesh Points. We have from Equation (2.9)

$$d_i f'(x_i) = g_i'(0) \qquad d_i f'(x_{i+1}) = g_i'(1)$$

and from Equations (2.4) and (2.5) with (2.11):

$$d_i f_i' = y_{i+1} - y_i - d_i^2 f_{i+1}''/\beta - \alpha d_i^2 f_i''/\beta \tag{3.1}$$

$$d_i f_{i+1}' = y_{i+1} - y_i + \alpha d_i^2 f_{i+1}''/\beta + d_i^2 f_i''/\beta \tag{3.2}$$

where f_i', f_{i+1}', f_i'' and f_{i+1}'' denote respectively $f'(x_i)$, $f'(x_{i+1})$, $f''(x_i)$ and $f''(x_{i+1})$.

Then from (3.1) and (3.2)

$$d_i[f_i' + \alpha f_{i+1}'] = (1+\alpha)(y_{i+1}-y_i) + (\alpha^2-1)f_{i+1}''d_i^2/\beta\,;\ i = 1, n-1 \tag{3.3}$$

or $$d_i[\alpha f_i' + f_{i+1}'] = (1+\alpha)(y_{i+1}-y_i) - (\alpha^2-1)f_i''d_i^2/\beta\,;\ i = 1, n-1 \tag{3.4}$$

We apply Equation (3.3) at i - 1 to obtain

$$d_{i-1}[f_{i-1}' + \alpha f_i'] = (1+\alpha)(y_i-y_{i-1}) + (\alpha^2-1)f_i''d_{i-1}^2/\beta\,;\ i = 2, n \tag{3.5}$$

From Equations (3.4) and (3.5) we obtain respectively

$$d_{i-1}[\alpha f_i' + f_{i+1}'] = d_{i-1}(1+\alpha)(y_{i+1}-y_i)/d_i - (\alpha^2-1)f_i''d_{i-1}d_i/\beta \tag{3.6}$$

$$d_i\left[f_{i-1}' + \alpha f_i'\right] = d_i(1+\alpha)(y_i-y_{i-1})/d_{i-1} + (\alpha^2-1)f_i''d_{i-1}d_i/\beta \tag{3.7}$$

and adding

$$d_i f_{i-1}' + \alpha(d_{i-1}+d_i)f_i' + d_{i-1}f_{i+1}' = (1+\alpha)\left[d_{i-1}(y_{i+1}-y_i)/d_i + d_i(y_i-y_{i-1})/d_{i-1}\right]$$
$$i = 2, n-1 \tag{3.8}$$

Equation (3.8) is a system of n-2 equations in n unknowns, f_i'. If y_1' and y_n' are given we set

$$f_1' = y_1' \quad \text{and} \quad f_n' = y_n'$$

and then have a determinate system (tridiagonal with diagonal dominance) to solve for the f_i'.

If y_1'' and y_n'' are specified we have from Equations 3.4 and 3.5

$$d_1[f_1' + \alpha f_2'] = (1 + \alpha)(y_2 - y_1) - (\alpha^2 - 1)y_1'' d_1^2/\beta$$

and

$$d_{n-1}[f_{n-1}' + \alpha f_n'] = (1 + \alpha)(y_n - y_{n-1}) + (\alpha^2 - 1)\, y_n'' d_{n-1}^2/\beta$$

to complete the system (which is again tridiagonal with dominance).

Having computed the first derivative values f_i'; i = 1, I, the second derivative values, f_i'', i = 1, I may be readily determined.

If f_i'' and f_n'' are not specified

$$f_1'' = \beta\left[(1 + \alpha)(y_2 - y_1)/d_1^2 - (\alpha f_1' + f_2')/d_1\right]/(\alpha^2 - 1)$$

$$f_n'' = \beta\left[(1 + \alpha)(y_n - y_{n-1})/d_{n-1}^2 - (\alpha f_n' + f_{n-1}')/d_{n-1}\right]/(1 - \alpha^2)$$

In any case

$$f_i'' = \beta\left[(1 + \alpha)(y_{i+1} - y_i)d_i^2 - (\alpha f_i' + f_{i+1}')/d_i\right]/(\alpha^2 - 1$$

provides the f_i'', i = 2, n - 1.

4. Interpolation. After values, f_i''; i = 1, n are determined interpolation for f(x), $f'(x)$ and $f''(x)$ for any x in x_1, x_n can be readily accomplished by the following:

a) If $x = x_i$ any $i = 1, n$

then $f(x) = y_i$, $f'(x) = f'_i$, $f''(x) = f''_i$

otherwise find i such that

$$x_i < x < x_{i+1}$$

With $d_i = x_{i+1} - x_i$ and $u = (x - x_i)/d_i$

$$f(x) = y_i + (y_{i+1} - y_i)u + d_i^2\left[f''_{i+1}h(u) + f''_i h(1-u)\right]/\beta$$

$$f'(x) = (y_{i+1} - y_i)/d_i + d_i\left[f''_{i+1}h'(u) = f''_i h'(1-u)\right]/\beta$$

$$f''(x) = \left[f''_{i+1}h''(u) + f''_i h''(1-u)\right]/\beta$$

5. Particular Functions, $h(u)$. The above development completes the general formulation for segmented spline fitting of third order. We turn now to specific applications.

5.1 Cubic spline

Let $h(\xi) = \xi^3 - \xi$

then $h(0) = 0$ and $h(1) = 0$

as required

and $h'(\xi) = 3\xi^2 - 1$

$h'(0) = -1$ as required

$h'(1) = 2 \equiv \alpha$

$h''(\xi) = 6\xi$

$h''(0) = 0$ as required

$h''(1) = 6 \equiv \beta$

Equation (3.7) becomes the well-known (See [1])

$$d_i f'_{i-1} + 2(d_{i-1} + d_i) f'_i + d_{i-1} f'_{i+1} = 3[d_{i-1}(y_{i+1} - y_i) d_i + d_i (y_i - y_{i-1})/d_{i-1}]$$

Similarly the remaining formulas can be particularized.

The cubic spline s(x) has the desirable property that among all functions f(x) having properties 1.1 and 1.2 we have

$$\int_{x_1}^{x_n} [s''(x)]^2 dx \leq \int_{x_1}^{x_n} [f''(x)]^2 dx$$

5.2 Hyperbolic Spline [2]

Let $h(\xi) = \dfrac{\sinh p\xi - \xi \sinh p}{\sinh p - p}$ $\quad p > 0$

Then for any p

$$h(0) = 0 \qquad h(1) = 0 \quad \text{as required}$$

$$h'(\xi) = \frac{p\cosh p\xi - \sinh p}{\sinh p - p}$$

$$h'(0) = -1 \quad \text{as required}$$

$$h'(1) = \frac{p\cosh p - \sinh p}{\sinh p - p} \equiv \alpha$$

$$h''(\xi) = \frac{p^2 \sinh p\xi}{\sinh p - p}$$

$$h''(0) = 0 \quad \text{as required}$$

$$h''(1) = \frac{p^2 \sinh p}{\sinh p - p} \equiv \beta$$

As before the general formulas can be used with the above definition of h. It should be noted that the limit case (p = 0)

of the hyperbolic spline is the cubic spline. When the cubic spline fitting curve contains inflection points which do not seem to be consonant with the data, the hyperbolic spline fit (with sufficiently large p) will not have these extraneous inflection points. (See [2]). In computation successive integer values of p (starting with 3) can be used. The values of α will be greater than 2.

5.3 Trigonometric Spline

Let $$h(\xi) = \frac{\sin p\xi - \xi \sin p}{\sin p - p} \qquad p > 0$$

Then for any p

$$h(0) = 0 \qquad h(1) = 0$$

$$h'(\xi) = \frac{p\cos p\xi - \sin p}{\sin p - p}$$

$$h'(0) = -1 \qquad h'(1) = \frac{p\cos p - \sin p}{\sin p - p} \equiv \alpha$$

$$h''(\xi) = \frac{-p^2 \sin p\xi}{\sin p - p}$$

$$h''(0) = 0 \qquad h''(1) = \frac{-p^2 \sinh p}{\sinh - p} \equiv \beta$$

Again the above can be used in the general formulas. The merit of the trigonometric spline fit is that it is sensitive is small oscillations in data and will in general have more pronounced inflection than the cubic spline fit. In computation only values of p such that $\alpha > 0$ should be used. In general the value of α is less than 2. Note also in the limit case (p = 0) the trigonometric spline becomes the cubic spline.

5.4 Damped Cubic Spline

Let $h(\xi) = \ell^{-p(1-\xi)}\xi^3 - \xi \qquad p > 0$

$h(0) = 0 \qquad h(1) = 0 \quad$ as required

$h'(\xi) = \ell^{-p(1-\xi)}(p\xi^3+3\xi^2) - 1$

$h'(0) = -1 \qquad$ as required

$h'(1) = 2+p \equiv \alpha$

$h''(\xi) = \ell^{-p(1-\xi)}(p^2\xi^3+6p\xi^2+6\xi)$

$h''(0) = 0 \qquad$ as required

$h''(1) = 6+6p+p^2 \equiv \beta$

The generalized formulas can be particularized for the damped cubic spline. The effect of the damping is similar to that of hyperbolic spline fitting in that it eliminates extraneous inflection points. In computation any values of $p > 0$ will show pronounced effect on the fit. The chief advantage of the damped spline over the hyperbolic spline is in its relative simplicity for computational purposes.

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1. G. Birkoff and C. R. deBoor, "Piecewise Polynomial Approximation", Approximation of Functions, H. L. Garabedian, Ed., (Elsevier Publishing Co., Amsterdam, 1965), 164-168

2. D. G. Schweichert, "An Interpolation Curve Using a Spline in Tension," J. of Math. Physics 45, (1966) pp. 312-217

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