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ABSTRACT

This article describes the application of cubic spline fitting to a set of points:

$$(t_i, x_i); i = 1, I \quad \text{with } I \geq 3$$

to obtain:

(1) a computational definition of a smooth curve, $x(t)$;

(2) an estimate of the first derivative, x', at each t_i;

(3) an estimate of the second derivative, x'', at each t_i;

(4) an interpolated value for x at any t, $t_1 \leq t \leq t_I$;

(5) an estimate of the integral,

$$\int_{t_1}^{t_I} x(t)\, dt \quad .$$

The t_i must be distinct and increasing with i, but need not be uniformly spaced.

INTRODUCTION

A t-dependent quantity, $x(t)$, frequently is known (from observation, from a table, etc) only in the discrete form as a set of points:

$$(t_i, x_i); i = 1, I.$$

with the t_i distinct and increasing with i. The cubic spline function $s(t)$

which fits the table, (t_i, x_i) has the following properties:

(1) over any subinterval $[t_{i-1}, t_i]$; $i = 2, I$ the function $s(t)$ is a cubic in t.

(2) $s(t_i) = x_i$; $i = 1, I$ (exact fit)

(3) over the whole interval $[t_1, t_I]$ s has continuous first and second derivatives, $s'(t)$ and $s''(t)$

(4) $\int_{t_1}^{t_I} [s''(t)]^2 dt$ in minimized.

By (1), we mean that for any i; $i = 2, I - 1$ with $s = s_-$ on $[t_{i-1}, t_i]$ and $s = s_+$ on $[t_i, t_{i+1}]$ that s_- and s_+ are cubics (not generally identical), however by (3), $s'_-(t_i) = s'_+(t_i)$ and $s''_-(t_i) = s''_+(t_i)$. By (4), we mean that for any function $g(t)$ satisfying (2) and (3),

$$\int_{x_1}^{x_I} [s''(t)]^2 dt \leq \int_{x_1}^{x_I} [g''(t)]^2 dt .$$

It is computationally convenient to assume that

$$x(t) \equiv s(t) \quad \text{on} \quad [t_1, t_I] .$$

since $s(t)$ is completely determined thereon by the known

$$(t_i, x_i); \; i = 1, I$$

and by the readily computable

$$s'_i \equiv s'(t_i); \; i = 1, I.$$

Recalling that $s_i = x_i$ and that s is a cubic on each subinterval, simple computational processes on the values

$$(t_i, s_i, s'_i); \; i = 1, I$$

provide for interpolation, second order differentiation, and integration.

CUBIC SPLINE FIT, FIRST DERIVATIVE

The problem of defining s is logically equivalent to finding s_i'; i = 1, I since for any i; i = 2, I, the cubic segment of s on the sub-interval $[t_{i-1}, t_i]$ is well defined by $(t_{i-1}, s_{i-1}, s_{i-1}')$ and (t_i, s_i, s_i'). We now describe the computation for the s_i'.

If x_1' and x_I' are known, we set $s_1' = x_1'$ and $s_I' = x_I'$ then solution of the linear system:

$$s_1' = x_1' \tag{1}$$

$$(t_{i+1} - t_i)\, s_{i-1}' + 2\,(t_{i+1} - t_{i-1})\, s_i' + (t_i - t_{i-1})\, s_{i-1}' = 3\{(t_{i+1} - t_i)(x_i - x_{i-1})/(t_i - t_{i-1}) + (t_i - t_{i-1})(x_{i+1} - x_i)/(t_{i+1} - t_i) \quad i = 2, I-1 \tag{2}$$

$$s_I' = x_I' \tag{3}$$

provides the values s_i'; i = 1, I.

In the (more common) case that the terminal derivatives x_1' and x_I' are not known, replacements must be found for Equations (1) and (3).

Reference 1 imposes the condition that s have no curvature at t_1 and t_I; i.e., $s''(t_1) = 0$ and $s''(t_I) = 0$ which gives

$$2\, s_1' + s_2' = 3\,(x_2 - x_1)/(t_2 - t_1) \tag{1$'$}$$

and

$$s_{I-1}' + 2\, s_I' = 3\,(x_I - x_{I-1})/(t_I - t_{I-1})\,. \tag{3$'$}$$

Solution of the linear system consisting of Equation (1´), Equations (2) and Equation (3´) gives the s_i' subject to this condition.

Reference 2 imposes the condition of constant curvature very near t_1 and t_I by requiring that s_1' be the slope of a circle passing through

(t_1, x_1) and (t_2, x_2) having the slope s'_2 at t_2 and that s'_I be the slope of a circle passing through (t_{I-1}, x_{I-1}) and (t_I, x_I) having the slope s'_{I-1} at t_{I-1} which gives:

$$s'_1 = \{2\,(x_2 - x_1)/(t_2 - t_1) + s'_2\,[\,(x_2 - x_1)^2/(t_2 - t_1)^2 - 1]\,\}/(1 + s'_2)^2 \qquad (4)$$

$$s'_I = \{2\,(x_I - x_{I-1})/(t_I - t_{I-1}) + s'_{I-1}\,[\,(x_I - x_{I-1})^2/(t_I - t_{I-1})^2 - 1]\,\}/(1 + s'_{I-1})^2 \qquad (5)$$

Unfortunately, Equations (4) and (5) are not linear in s'_2 and s'_{I-1}, respectively; hence, the system (4), (2), (5) cannot be solved as a linear system. The reference proposes an iterative process whereby first estimates is made for s'_2 and s'_{I-1}, Equations (4) and (5) are solved for s'_1 and s'_I. Equations (2) can then be solved as a linear system for s'_i; $i = 2, I - 1$. Then, the new values of s'_2 and s'_{I-1} can be used in Equations (4) and (5) and iteration continued until s'_2 and s'_{I-1} no longer change appreciably. The authors assure us that the process is rapidly convergent.

We propose the condition that s is a cubic at t_1 and t_I whose slope s'_1 is dependent on (t_1, x_1), (t_2, x_2), and (t_3, x_3) and whose slope s'_I is dependent on (t_I, x_I), (t_{I-1}, x_{I-1}) and (t_{I-2}, x_{I-2}) which gives:

$$s'_1 + a_1\, s'_2 = b_1\, s_1 + c_1\, s_2 + d_1\, s_3 \qquad (1'')$$

where

$$d_1 = (t_2 - t_1)^2/\{(t_3 - t_1)^3 - 2\,(t_2 - t_1)(t_3 - t_1)^2 + (t_2 - t_1)^2(t_3 - 1)\}$$

$$c_1 = d\,\{2\,(t_3 - t_1)^3 - 3\,(t_2 - t_1)(t_3 - t_1)^2\}/(t_2 - t_1)^3$$

$$b_1 = -c_1 - d_1$$

$$a_1 = d\,(t_3 - t_1) + c\,(t_2 - t_1) - 1$$

and

$$s'_I + a_I s'_{I-1} = b_I s_I + c_I s_{I-1} + d_I s_{I-2} \quad (3'')$$

a_I, b_I, c_I, d_I appropriately defined.

Equations (1'') and (3'') are linear; hence, Equation (1''), Equation (2), and Equation (3'') consitute a linear system which can be solved for s'_i; i = 1, I.

SECOND DERIVATIVE

The values of the second derivative

$$s''_i = s''(t_i)$$

can be readily computed from the set:

$$(t_i, s_i, s'_i); i = 1, I$$

by

$$s''_i = \{6 (s_k - s_i)/(t_k - t_i) + 2 s'_k + 4 s'_i\}/(t_k - t_i)$$

where t_k is adjacent to t_i. The formula is exact for a cubic between t_k and t_i. For i = 2, I - 1, the k may be either i - 1 or i + 1. The result will be the same for either choice since the cubic on $[t_{i-1}, t_i]$ has the same second derivative at t_i as the cubic on $[t_i, t_{i+1}]$.

INTERPOLATION

Interpolation for x(t*) with

$$t_1 < t^* < t_I$$

is accomplished by computing s(t*) by Hermite interpolation. For some i; i = 1, I - 1 we have

$$t_i \le t^* \le t_{i+1}.$$

Let

$$h = t^* - t_i \qquad H = t_{i+1} - t_i$$

then let

$$a = (3\,h^2 H - 2\,h^3)/H^3$$

$$b = 1 - a$$

$$c = (h^3 - h^2 H)/H^2$$

$$d = h - h^2/H + c$$

and finally,

$$s(t^*) = a\, s_{i+1} + b\, s_i + c\, s'_{i+1} + d\, s'_i\,.$$

This formula is exact for cubics; hence, the value s(t*) is exact for s and is an estimate for x(t*).

INTEGRATION

The integral

$$\int_{t_1}^{t_I} s\, dt = \sum_{i=1}^{I-1} \int_{t_i}^{t_{i+1}} s\, dt. \qquad (6)$$

On each of the subintervals $[\, t_i,\ t_{i+1}]$; $i = 1,\ I - 1$, the function s is a cubic and

$$\int_{t_i}^{t_{i+1}} s\, dt = (t_{i+1} - t_i)(s_{i+1} + s_i)/2 + (t_{i+1} - t_i)^2 (s'_i - s'_{i+1})/12$$

is exact for cubics. The sum of all such subintegrals gives

$$\int_{t_1}^{t_I} s\, dt$$

which can be used as an estimate for

$$\int_{t_1}^{t_I} x(t)\, dt.$$

CONCLUSION

The cubic spline s(t) is a computationally convenient fit for a table

$(t_i, x_i); i = 1, I; I \geq 3.$

It lends itself conveniently to numerical differentiation, interpolation and numerical integration.

The cubic spline fit having a continuous second derivative and piecewise constant third derivative is much smoother than polygonal (broken line) fitting which is continuous and has a piecewise constant first derivative and smoother than local cubic fitting which has a continuous first derivative and piecewise constant second derivatives.

Exact polynomial fitting of (t_i, x_i) may introduce many inflection points and extreme curvature over a short arc. The minimization property (4) of spline fitting tends to prevent such occurrences.

Cubic spline fitting is exact on (t_i, x_i) in contrast to least square fitting which admits residual errors. These residual errors, particularly if they alternate in sign from point-to-point, may introduce unreasonable variation in derivative values.

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