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CUBIC SPLINE FUNCTIONS

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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,

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

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) $\int_{t_1}^{t_I} [s''(t)]^2 dt$ is 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

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

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:

$$s'_1 = x'_1 \tag{1}$$

$$(t_{i+1} - t_i) s'_{i-1} + 2 (t_{i+1} - t_{i-1}) s'_i + (t_i - t_{i-1}) s'_{i-1} = 3 \left\{ \frac{(t_{i+1} - t_i)(x_i - x_{i-1})}{(t_i - t_{i-1})} + \frac{(t_i - t_{i-1})(x_{i+1} - x_i)}{(t_{i+1} - t_i)} \right\} \tag{2}$$

$(t_{i+1} - t_i) \quad i = 2, I - 1$

$$s'_I = x'_I \tag{3}$$

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 $s'_{I-1} + 2 s'_I = 3 (x_I - x_{I-1}) / (t_I - t_{I-1})$. (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_1' 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:

$$s_1' = \{2(x_2 - x_1)/(t_2 - t_1) + s_2' [(x_2 - x_1)^2/(t_2 - t_1)^2 - 1]\} / (1 + s_2'^2) \quad (4)$$

$$s_I' = \{2(x_I - x_{I-1})/(t_I - t_{I-1}) + s_{I-1}' [(x_I - x_{I-1})^2/(t_I - t_{I-1})^2 - 1]\} / (1 + s_{I-1}'^2) \quad (5)$$

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:

$$s_1' + a_1 s_2' = b_1 s_1 + c_1 s_2 + d_1 s_3 \quad (1'')$$

where

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

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

$$b_1 = -c_1 - d_1$$

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

and

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

a_I, b_I, c_I, d_I appropriately defined.

Equations (1'') and (3'') are linear; hence, Equation (1''), Equation (2), and Equation (3'') constitute a linear system which can be solved for $\hat{s}'_i; i = 1, I$.

SECOND DERIVATIVE

The values of the second derivative

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

can be readily computed from the set:

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

by

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

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

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

Let

$$h = t^* - t_i$$

$$H = t_{i+1} - t_i$$

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

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

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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