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NUMERICAL APPLICATIONS OF CUBIC SPLINE FUNCTIONS

Jonathan D. Young

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OF
CUBIC SPLINE FUNCTIONS

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ABSTRACT

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

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

to obtain:

(1) a computational definition of a smooth curve, \( x(t) \);
(2) an estimate of the first derivative, \( x'(t) \), at each \( t_i \);
(3) an estimate of the second derivative, \( x''(t) \), 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 \([t_l, t_I]\) \(s\) has continuous first and second derivatives, \(s'(t)\) and \(s''(t)\)

4. \(\int_{t_l}^{t_I} [s''(t)]^2 \, dt\) is minimized.

By (1), we mean that for any \(i; \ i = 2, I - 1\) with \(s = s_\cdot \) on \([t_{i-1}, t_i]\) and \(s = s_+ \) on \([t_i, t_{i+1}]\) that \(s_\cdot\) and \(s_+\) are cubics (not generally identical), however by (3), \(s'_\cdot(t_i) = s'_+(t_i)\) 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 \(x(t) \equiv s(t)\) on \([t_l, t_I]\).

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:

$$s'_1 = x'_1$$ (1)

$$(t_{i+1} - t_i) s'_{i-1} + 2 (t_{i+1} - t_{i-1}) s'_i + (t_i - t_{i-1}) s''_{i-1} = 3 \{(t_{i+1} - t_i)(x_i - x_{i-1})/(t_i - t_{i-1}) + (t_i - t_{i-1})(x_{i+1} - x_i)\}/(t_{i+1} - t_i) i = 2, I - 1$$ (2)

$$s'_I = x'_I$$ (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

$$2 s'_1 + s'_2 = 3 (x_2 - x_1)/(t_2 - t_1)$$ (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
(t₁, x₁) and (t₂, x₂) having the slope s₂ at t₂ and that s₁ be the slope of a circle passing through (t₁₋₁, x₁₋₁) and (t₁, x₁) having the slope s₁₋₁ at t₁₋₁ which gives:

\[ s₁ = \frac{2(x₂ - x₁)/(t₂ - t₁) + s₂^2 \left[ (x₂ - x₁)^2/(t₂ - t₁)^2 - 1 \right]}{(1 + s₂^2)^2} \]  

\[ (4) \]

\[ s₁' = \frac{2(x₁ - x₁₋₁)/(t₁ - t₁₋₁) + s₁₋₁^2 \left[ (x₁ - x₁₋₁)^2/(t₁ - t₁₋₁)^2 - 1 \right]}{(1 + s₁₋₁^2)^2} \]  

\[ (5) \]

Unfortunately, Equations (4) and (5) are not linear in s₂ and s₁₋₁, 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 s₂ and s₁₋₁, Equations (4) and (5) are solved for s₁ and s₁₋₁. Equations (2) can then be solved as a linear system for sᵢ, i = 2, I - 1. Then, the new values of s₂ and s₁₋₁ can be used in Equations (4) and (5) and iteration continued until s₂ and s₁₋₁ no longer change appreciably.

The authors assure us that the process is rapidly convergent.

We propose the condition that s is a cubic at t₁ and tᵢ whose slope sᵢ is dependent on (t₁, x₁), (t₂, x₂), and (tᵢ₊₁, xᵢ₊₁) and whose slope sᵢ₋₁ is dependent on (tᵢ₋₁, xᵢ₋₁), (tᵢ₋₁₋₁, xᵢ₋₁₋₁) and (tᵢ₋₂, xᵢ₋₂) which gives:

\[ sᵢ' + a₁ s₂' = b₁ s₁ + c₁ s₂ + d₁ s₃ \]  

where

\[ d₁ = (t₂ - t₁)^2/\{(t₃ - t₁)^3 - 2(t₂ - t₁)(t₃ - t₁)^2 + (t₂ - t₁)^2(t₃ - 1) \} \]

\[ c₁ = d \{ 2(t₃ - t₁)^3 - 3(t₂ - t₁)(t₃ - t₁)^2 \}/(t₂ - t₁)^3 \]

\[ b₁ = -c₁ - d₁ \]

\[ a₁ = d(t₃ - t₁) + c(t₂ - t₁) - 1 \]

and
Equations (1") and (3") are linear; hence, Equation (1"),
Equation (2), and Equation (3") constitute 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

\[ s''_i = \left\{ 6 \left( s_k - s_i \right) / (t_k - t_i) + 2 s_k' + 4 s_i' \right\} / (t_k - t_i) \]

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

\[ h = t^* - t_i \quad \quad H = t_{i+1} - t_i \]
then let

\[ a = \frac{(3 h^2 H - 2 h^3)}{H^3} \]

\[ b = 1 - a \]

\[ c = \frac{(h^3 - h^2 H)}{H^2} \]

\[ d = h - h^2 / H + c \]

and finally,

\[ s(t^*) = a s_i + b s_i + c s_i + d s_i \]

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.

REFERENCES


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