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NUMERICAL APPLICATIONS OF CUBIC SPLINE FUNCTIONS

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August 1967

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ABSTRACT

This report discusses the application of cubic spline fitting to estimation of second derivatives for interpolation, and integration of a function $y(x)$ known only in discrete form as a table (x_i, y_i), $i = 1, I$.

INTRODUCTION

Let $y(x)$ be a function known only in the discrete form as a table of values,

$$x_i,\ y_i;\ i = 1,\ I;\ I \geq 3,$$

with the x_i distinct and monotonically increasing. Reference 1 describes the cubic spline fit, $f(x)$ for the set $(x_i,\ y_i)$, and outlines the computation whereby $f'_i \equiv f'(x_i)$, $i = 1$, I may be obtained. The values f'_i, together with $f_i \equiv f(x_i) = y_i$, uniquely determine $f(x)$ on the whole interval, $[x_1,\ x_I]$. The values $f'(x_i)$ may be used as estimates for $y'(x_i)$. The purpose of this report is to describe how the cubic spline fit $(x_i,\ y_i,\ f'_i)$, $i = 1$, I may be used in the common numerical processes of

(a) estimating $y''(x_i)$; $i = 1$, I,
(b) interpolating for $y(x)$; $x_1 < x < x_I$,
(c) integrating $y\,dx$ over $\left[x_{i-1},\ x_i\right]$; $i = 2$, I.

The processes applied to f are all exact, i.e., they give respectively f''_i, $f(x)$, and $\int f\,dx$. Each of these in f is an estimate of its counterpart in y.

ESTIMATE OF SECOND DERIVATIVE

With $f_i = y_i$, and f'_i as an estimate of y'_i at all the points x_i, $i = 1$, I, we may use f''_j as an estimate for y''_j at any $j = 1$, I. The value of f''_j may be readily computed from

$$f''_j = 6(f_k - f_j)/h^2 + (2f'_k + 4f'_j)/h,$$

where

$$h = x_j - x_k,$$

with x_k adjacent to x_j, i.e., $k = j - 1$ or $k = j + 1$. The formula is exact for cubics. It will be noted that for x_j interior--i.e., $j = 2$, $I - 1$--there is a choice of k. The result will be the same whether $k = j - 1$ or $k = j + 1$ is used, since the cubic on $\left[x_j,\ x_{j+1}\right]$ has the same second derivative of x_j as the cubic on $\left[x_{j-1},\ x_j\right]$.

INTERPOLATION

For x, with $x_j \leq x \leq x_{j+1}$; $j = 1$, $I - 1$, we wish to estimate $y(x)$. We can use f_j, f'_j, f_{j+1} and f'_{j+1} to obtain $f(x)$ by Hermite interpolation.

Let $h = x - x_j$, $\qquad s = x_{j+1} - x_j$;

then

$$f(x) = ay_{j+1} + by_j + cy'_{j+1} + dy'_j,$$

where

$$a = (3h^2 s - 2h^3)/s^3,$$
$$b = 1 - a,$$
$$c = (h^3 - h^2 s)/s^2,$$
$$d = h - h^2/s + c.$$

The formula is exact for cubics, hence the exact value of f(x) is obtained by interpolation. This value is an estimate for y(x).

INTEGRATION

In order to obtain an estimate of

$$\int_{x_{i-1}}^{x_i} y\,dx \qquad \text{for some } i;\ 2 < i < I,$$

we first integrate

$$\int_{x_{i-1}}^{x_i} f\,dx.$$

Let $s = x_i - x_{i-1}$; the formula

$$\int_{x_{i-1}}^{x_i} f\,dx = s(f_{i-1} + f_i)2 + s^2(f'_{i-1} - f'_i)/12$$

is exact for cubics, consequently exact for f. The result is an estimate for

$$\int_{x_{i-1}}^{x_i} y\,dx.$$

REFERENCE

1. J. D. Young, Approximate Differentiation by Cubic Spline Fitting, UCRL-17659, June 1967.

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