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On Spline-on-Spline Numerical Integration Formula

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1. INTRODUCTION AND DESCRIPTION OF METHOD

The spline-on-spline technique is of much use for calculating the second derivative of a function from its values on a uniform mesh. There is computational evidence that this gives better results than the traditional process using a single spline [1, 3]. For any integer $n \geqslant 1$, let Δ_n: $0 = x_0 < x_1 < \cdots < x_n = 1$ with knots $x_j = jh$. Given a sufficiently smooth function f defined on [0, 1], let s be an interpolatory cubic spline of f and p be a cubic spline-on-spline interpolant of s' defined by

$$\begin{aligned} &\text{(i)} \quad s_j = f_j \ (= f(x_j)) \qquad (0 \leqslant j \leqslant n) \\ &\text{(ii)} \quad p_j = s'_j \ (= s'(x_j)) \qquad (0 \leqslant j \leqslant n). \end{aligned} \tag{1}$$

Then we have the following asymptotic error estimate under approximate end conditions [2, 3]:

$$f''_j - p'_j = \frac{h^4}{90} f^{(6)}_j + O(h^6) \qquad (h \to 0) \tag{2}$$

while

$$f''_j - s''_j = \frac{h^2}{12} f^{(4)}_j + O(h^4) \qquad (h \to 0).$$

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In the present paper we shall consider an application of the spline-on-spline interpolation to a numerical integration of the form

$$\int_{x_j}^{x_{j+1}} f(x)\,dx \qquad \text{or} \qquad \int_{x_j}^{x_{j+1}} f(x)\,dx \Big/ \int_0^1 f(x)\,dx \ (0 \leqslant j \leqslant n-1). \tag{3}$$

Here we hope that the formula on $[x_j, x_{j+1}]$ has only evaluation knots x_i $(0 \leqslant i \leqslant n)$, i.e., $\int_{x_j}^{x_{j+1}} f(x)\,dx \sim$ "a linear combination of $f_0, f_1, ..., f_n$."

First we show that an integral of the spline-on-spline interpolant p of s' gives better results than the spline s itself i.e.,

$$\frac{1}{2}\left\{\int_{x_h}^{x} p(x)\,dx - \int_{x}^{x_{j+1}} p(x)\,dx + f_j + f_{j+1}\right\}$$
$$= f(x) - \frac{h^5}{6!}\left(t - \frac{1}{2}\right)(6t^4 - 12t^3 + 4t^2 + 2t + 5) f_j^{(5)}$$
$$+ O(h^6) \qquad (x_j \leqslant x \leqslant x_{j+1},\ t = (x - x_j)/h). \tag{4}$$

For the calculation of the above integral, we have the following identity that can be easily checked since p is cubic on $[x_j, x_{j+1}]$:

$$\int_{x_j}^{x} p(x)\,dx - \int_{x}^{x_{j+1}} p(x)\,dx$$
$$= h\{p_j \phi(1-t) - p_{j+1}\phi(t)\}$$
$$+ h^2\{p_j' \psi(1-t) + p_{j+1}' \psi(t)\} \qquad (t = (x - x_j)/h), \tag{5}$$

where

$$\phi(t) = \tfrac{1}{2} - 2t^3 + t^4$$
$$\psi(t) = \tfrac{1}{12} - \tfrac{2}{3}t^2 + \tfrac{1}{2}t^4.$$

On the other hand,

$$s(x) = f(x) - \frac{h^4}{4!} t^2(1-t)^2 f_j^{(4)}$$
$$+ O(h^5) \qquad (x_j \leqslant x \leqslant x_{j+1},\ t = (x - x_j)/h). \tag{6}$$

Next, integration of (4) gives the formula

$$\int_{x_j}^{x_{j+1}} f(x)\,dx \sim I_j(h) = \frac{h}{2}(f_j + f_{j+1}) + \frac{h^2}{10}(p_j - p_{j+1})$$
$$+ \frac{h^3}{120}(p_j' + p_{j+1}') \qquad (0 \leqslant j \leqslant n-1). \tag{7}$$

For the error

$$\int_{x_j}^{x_{j+1}} f(x)\,dx - I_j(h) = -\left(\frac{1}{7!}\cdot\frac{23}{12}\right) h^7 f_j^{(6)} + O(h^8). \tag{8}$$

Similarly, integration of the spline s gives the numerical quadrature [1]

$$\int_{x_j}^{x_{j+1}} f(x)\,dx \sim K_j(h) = \frac{h}{2}(f_j + f_{j+1}) - \frac{h^2}{12}(s'_j - s'_{j+1}) \qquad (0 \leqslant j \leqslant n-1). \tag{9}$$

For the error,

$$\int_{x_j}^{x_{j+1}} f(x)\,dx - K_j(h) = \frac{h^5}{720} f_{j+1/2}^{(4)} - \frac{h^7}{2016} f_{j+1/2}^{(6)} + O(h^8), \tag{10}$$

where $g_{j+1/2} = g((x_j + x_{j+1})/2)$. By means of the asymptotic expansion (10), Richardson extrapolation gives an $O(h^7)$ approximation without having to calculate the spline-on-spline interpolant, i.e.,

$$\int_{x_j}^{x_{j+1}} f(x)\,dx - \frac{1}{15}\{16K_j(h) - K_j(2h)\} = \frac{8}{7!} h^7 f_{j+1/2}^{(7)} + O(h^8). \tag{11}$$

Since the ratio of the asymptotic error estimates (8) and (11) is approximately 23/96 ($\doteqdot$ 1/4), our spline-on-spline integration formula gives better results than the Richardson extrapolation of a single spline one. As for computational effort, we have to solve two linear systems of order $(n/2+1)$ and $(n+1)$ to determine s_{2h} and s_h in the extrapolation. In the spline-on-spline technique, the coefficient matrices for determining s_h and p_h are exactly the same and so p_h is determined with a little additional effort. For an efficient algorithm for solving the systems, see [1, p. 14]. Hence we are justified using the spline-on-spline integration formula instead of the extrapolation of the single spline one.

2. Asymptotic Error Estimates

Since s (or p) depends upon $n+3$ parameters, there are two additional conditions to (1)(i) (or (1)(ii)) required for a unique determination of the spline s (or p). Here we take these two end ones:

$$\begin{aligned} &\text{(i)} \quad \Delta^r s_0' = \nabla^r s_n' = 0 \\ &\text{(ii)} \quad \Delta^r p_0' = \nabla^r p_n' = 0, \end{aligned} \tag{12}$$

where r is a nonnegative integer and Δ (∇) is the forward (backward) difference operator. By repeated use of the consistency relation for the cubic spline s,

$$\frac{1}{6}(s_{j-1}' + 4s_j' + s_{j-1}') = \frac{1}{2h}(s_{j+1} - s_{j-1}), \tag{13}$$

$\Delta^r s_0' = 0$ can be equivalently rewritten as

$$s_0' + a_r s_1' = L_r(s_0, s_1, ..., s_r) \qquad (r \neq 2), \tag{14}$$

where a_r is a rational number and $L_r(s_0, s_1, ..., s_r)$ is a linear combination of $s_0, s_1, ..., s_r$ (for these, see [3]). For example,

$$a_6 = 15/4$$

$$L_6(s_0, s_1, ..., s_6) = (865d_1 - 226d_2 + 53d_3 - 10d_4 + d_5)/144,$$

where d_i means the right-hand side of (13).

In order to prove (4) and (8), we shall require

Lemma 3. *Under the end conditions* (12), *we have*

$$\begin{aligned} &\text{(i)} \quad f_j' - p_j \,(= f_j' - s_j') = \frac{h^4}{180} f_j^{(5)} - \frac{h^6}{1512} f_j^{(7)} \\ &\qquad\qquad + O(h^{\min(8,r)}) \qquad (0 \leqslant j \leqslant n) \\ &\text{(ii)} \quad f_j'' - p_j' = \frac{h^4}{90} f_j^{(6)} - \frac{h^6}{756} f_j^{(8)} \\ &\qquad\qquad + O(h^{\min(7,r-1)}) \qquad (0 \leqslant j \leqslant n). \end{aligned} \tag{15}$$

This proves the following

THEOREM. *For $r \geqslant 6$, under (12) we have*

(i) $\frac{1}{2}[h\{p_j \phi(1-t) - p_{j+1}\phi(t)\} + h^2\{p_j'\psi(1-t) + p_{j+1}'\psi(t)\} + f_j + f_{j+1}] = f(x) + O(h^5)$ $(x_j \leqslant x \leqslant x_{j+1},\ t = (x-x_j)/h,\ 0 \leqslant j \leqslant n-1)$,

where $O(h^5)$ is to be replaced with $O(h^6)$ at $x = (x_j + x_{j+1})/2$;

(ii) $$\int_{x_j}^{x_{j+1}} f(x)\,dx = \frac{h}{2}(f_j + f_{j+1}) + \frac{h^2}{10}(p_j - p_{j+1}) + \frac{h^3}{120}(p_j' + p_{j+1}') - \left(\frac{1}{7!}\cdot\frac{23}{12}\right) h^7 f_j^{(6)} + O(h^8) \qquad (0 \leqslant j \leqslant n-1).$$

COROLLARY. *For $r \geqslant 6$,*

$$\int_0^1 f(x)\,dx - \sum_{j=0}^{n-1} I_j(h) = -\left(\frac{1}{7!}\cdot\frac{23}{12}\right) h^6\{f^{(5)}(1) - f^{(5)}(0)\} + O(h^7), \tag{16}$$

where, by use of the consistency relation for cubic spline p,

$$\sum_{j=0}^{n-1} I_j(h) = \frac{h}{2}(f_0 + 2f_1 + \cdots + 2f_{n-1} + f_n) + \frac{h^2}{120}(11p_0 - p_1 + p_{n-1} - 11p_n) + \frac{h^3}{360}(2p_0' + p_1' + p_{n-1}' + 2p_n'). \tag{17}$$

Finally, we note that the extrapolate of the trapezoidal rule also gives

$$\int_0^1 f(x)\,dx - T_2(h) = -\tfrac{2}{945} h^6\{f^{(5)}(1) - f^{(5)}(0)\} + O(h^8), \tag{18}$$

where $T_0(h) = h(f_0 + 2f_1 + \cdots + 2f_{n-1} + f_n)$, $T_1(h) = \{4T_0(h) - T_0(2h)\}/3$, and $T_2(h) = \{16T_1(h) - T_1(2h)\}/15$. By (16) and (18), we see that the rate of the errors of our method and the extrapolation of the trapezoidal rule is about 23/128 ($\doteqdot$ 1/5.5).

TABLE I

	e^x		e^{5x}	
n	κ	ε	κ	ε
16	1.11	4.31–11[a]	2.70	2.82–5
32	1.04	6.30–13	1.69	2.77–7
64	1.02	9.69–15	1.22	3.11–9
128			1.06	4.23–11
256			1.02	6.35–13

[a] We denote 4.31×10^{-11} by 4.31–11.

3. Numerical Illustration

The results of some numerical experiments are given in Table I for the functions e^x and e^{5x}. Here we choose $r = 6$.

$$\kappa(j) = -\left\{ \int_{x_j}^{x_{j+1}} f(x)\,dx - I_j(h) \right\} \Big/ [(23h^6/7! \cdot 12) \cdot \{f_{j+1}^{(5)} - f_j^{(5)}\}] \qquad (0 \leqslant j \leqslant n-1)$$

$$\kappa = -\left\{ \int_0^1 f(x)\,dx - \sum_{j=0}^{n-1} I_j(h) \right\} \Big/ [(23h^6/7! \cdot 12) \cdot \{f^{(5)}(1) - f^{(5)}(0)\}]$$

$$\varepsilon = -\left\{ \int_0^1 f(x)\,dx - \sum_{j=0}^{n-1} I_j(h) \right\}.$$

Then, by means of the theorem and its corollary, $\kappa(j)$ and κ tend to 1 as $h \to 0$. Except for i near 0 and n, $\kappa(j)$ are nearly to 1. For example, $0.99 \leqslant \kappa(j) \leqslant 1.01$ $(5 \leqslant j \leqslant n-1)$ with $n = 64$, 128 for e^{5x}.

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