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AN APPLICATION OF NATURAL CUBIC SPLINE FUNCTIONS TO NUMERICAL INTEGRATION FORMULAE

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Summary. By $C[0,1]$ we denote the set of real-valued continuous functions defined on the interval $[0, 1]$. Let numbers $x_0, x_1, \dots, x_n$ be prescribed with $0=x_0<x_1<\dots<x_{n-1}<x_n=1$. Then to each division of the unit interval into n subintervals $[x_{i-1}, x_i]$ there corresponds an $(n+1)$-dimensional subspace $S\equiv S(x_0, x_1, \dots, x_n)$ of $C[0,1]$ whose members are the natural cubic spline functions (hereafter referred to as n. c. s.) with nodes x_i. So, $s\in S$ if and only if this function satisfies the following three conditions: (i) $s\in C^2[0,1]$; (ii) $s''(0)=s''(1)=0$; (iii) the restriction of s to an arbitrary subinterval $[x_{i-1}, x_i]$ is a polynomial of degree at most three.

In a number of papers (see for instance [6] and [7]), Schoenberg has brought out the important role which n. c. s. play when approximating linear functionals. (We particularly want to mention here his fundamental theorem I in [7], p. 158]). The contents of this note may be summarized as follows. Assuming that the nodes are equally spaced on [0,1], we carry on research done by Atkinson [1] concerning the application of n. c. s. to numerical integration formulae. We improve on one of his results (theorem 7 of [1, p. 99]) and establish it in its definite form. In the course of the proof use is made of recent work of Sonneveld [9].

1. It is known ([2], lemma 1) that with each $f\in C[0,1]$ there can be associated a uniquely determined element $s\in S$ with the interpolation property, i. e. $s(x_i)=f(x_i)$, $i=0,1,\dots,n$. This interpolating n. c. s. can be represented as follows. Let $s^i(x)\in S$ denote the i-th cardinal natural cubic spline (this function is defined by the equations $s^i(x_j)=\delta^i_j$ for $i,j=0,1,\dots,n$), then in terms of these functions we have

$$s(x)=\sum_{i=0}^{n} f(x_i)s^i(x).$$

We now proceed by stating some results of Atkinson, which will be needed in the sequel of this paper. In order to do this we introduce the function

$$L(x,t)=\frac{1}{6}\left[(x-t)_+^3-(1-t)x^3-\sum_{i=0}^{n}\{(x_i-t)_+^3-(1-t)x_i^3\}s^i(x)\right], \tag{1}$$

where, as usual,

$$(x-t)_+^3=\begin{cases}(x-t)^3 & \text{if } x\geq t,\\ 0 & \text{if } x<t.\end{cases}$$

We have

Theorem 1 (Atkinson [1]).

(i) $L(x,t)$ is symmetric, i. e. $L(x, t)=L(t,x)$; moreover, for each x, it is an n. c. s. in t with nodes $x_0, x_1, \ldots, x_n$ and x.

(ii) Let $f\in C^4[0, 1]$. Then

$$f(x)-\sum_{i=0}^{n} f(x_i)s^i(x)=e_0(x)f''(1)+e_1(x)f''(0)+\int_0^1 L(x, t)f^{(4)}(t)dt$$

with

$$(2)\qquad \begin{cases} e_0(x)=\dfrac{1}{6}\left\{x^3-\displaystyle\sum_{i=0}^{n} x_i^3 s^i(x)\right\}, \\ e_1(x)=\dfrac{1}{6}\left\{(1-x)^3-\displaystyle\sum_{i=0}^{n}(1-x_i)^3 s^i(x)\right\}. \end{cases}$$

As an obvious consequence one gets

Corollary 1.

$$(3)\qquad \int_0^1 f(x)dx-\sum_{i=0}^{n} f(x_i)\int_0^1 s^i(x)\,dx=c_0f''(1)+c_1f''(0)+\int_0^1\int_0^1 L(x, t)f^{(4)}(t)\,dt\,dx,$$

where

$$(4)\qquad c_0=\int_0^1 e_0(x)dx,\quad c_1=\int_0^1 e_1(x)dx.$$

Relation (3) is of some importance because Schoenberg [6] has shown that of all numerical integration formulae of type

$$\int_0^1 f(x)dx\approx\sum_{i=0}^{n} w_i f(x_i),$$

which are exact for linear functions, the best one in the sense of Sard (cf. [5]) is obtained by integrating the n. c. s. that interpolates f at the points $x_0, x_1, \ldots x_n$, i. e.

$$(5)\qquad w_i=\int_0^1 s^i(x)dx,\quad i=0, 1, \ldots, n.^*$$

2. As we already indicated in the introductory section the purpose of this note is an improvement in its definite form of the following theorem due to Atkinson.

Theorem 2 ([1], p. 99). Let the nodes be equally spaced and let $c_0(=c_1)$ be given by (4). Then

* In case the nodes are equally spaced it is possible to determine explicit formulae for the weights w_i. We refer the reader to the references [5], [4], [3] and [8] for information about these interesting numbers (Tables with numerical data for w_i are also given there).

$$(6) \qquad \frac{0.0219}{n^3} < -c_0 < \frac{0.0277}{n^3}.$$

Furthermore, if $f \in C^4[0, 1]$, then one has

$$\left| \int_0^1 f(x)dx - \sum_{i=0}^n w_i f(x_i) \right| \leq \frac{0.0277}{n^3} \left| f''(0)+f''(1) \right| + \frac{0.2}{n^4} \| f^{(4)} \|$$

with $\| f^{(4)} \| = \max_{0 \leq x \leq 1} | f^{(4)}(x) |$. The lower bound of (6) implies that no greater an order than $1/n^3$ is possible when $f''(0)+f''(1) \neq 0$.

In accordance with the formulation of this theorem we will from now on assume that the nodes are equally spaced on $[0, 1]$. The derivation of theorem 2 (and also our improvement of it) is based upon Corollary 1. From this corollary we conclude that

$$(7) \qquad \left| \int_0^1 f(x)dx - \sum_{i=0}^n w_i f(x_i) \right| \leq |c_0| \, |f''(0)+f''(1)| + \left| \int_0^1 \int_0^1 L(x,t) f^{(4)}(t) dt \, dx \right|$$

$$\leq |c_0| \, |f''(0)+f''(1)| + \| f^{(4)} \| \int_0^1 \left| \int_0^1 L(x,t) dt \right| dx.$$

To calculate the constant c_0 we may note that it is an immediate consequence of (3), (2) and (5) that we have

$$(8) \qquad c_0 = \frac{1}{6} \left\{ \frac{1}{4} - \frac{1}{n^3} \sum_{i=0}^n i^3 w_i \right\}.$$

But the expression just exhibited for c_0 does not seem to be so suitable for calculation.* Therefore we proceed in a different way. Using formula (1) for $L(x, t)$ one gets

$$\int_0^1 L(x,t)dt = \frac{1}{6} \int_0^1 \left[(x-t)_+^3 - (1-t)x^3 - \sum_{i=0}^n \{ (x_i - t)_+^3 - (1-t) x_i^3 \} s^i(x) \right] dt$$

* Atkinson shows that

$$\text{(i)} \qquad c_0 = \frac{1}{24 n^3 \delta_n} \sum_{i=1}^n \frac{(-1)^{n-i+1}(6+\delta_{i-1})}{k_{i-1} \ldots k_{n-1}},$$

where the constants δ_i, $i=0, 1, 2, \ldots$, and k_i, $i=0, 1, 2, \ldots$, are defined recursively by the relations

$$\text{(ii)} \qquad \delta_{i+1} = 4 \frac{3+\delta_i}{4+\delta_i}, \quad \delta_0 = 0,$$

and

$$\text{(iii)} \qquad k_{i+1} = 4 - 1/k_i, \quad k_0 = 2.$$

Using this he arrives at inequality (6). (Actually, the lower bound of (6) is not valid for $n=2$, cf. (20).) It is possible to calculate the exact value of c_0 on the basis of the expressions (i), (ii), (iii). This was pointed out to me by F. Göbel and F. W. Steutel (Twente University of Technology).

$$=\frac{1}{6}\left\{\int_0^x (x-t)^3 dt - x^3\int_0^1 (1-t)dt + \sum_{i=0}^n x_i^3 s^i(x)\int_0^1 (1-t)dt - \int_0^1 \sum_{i=0}^n (x_i-t)_+^3 s^i(x)dt\right\}.$$

But

$$\sum_{i=0}^n s^i(x)\int_0^1 (x_i-t)_+^3\,dt$$

$$=s^1(x)\int_0^{x_1}(x_1-t)^3dt+s^2(x)\int_0^{x_2}(x_2-t)^3dt+\ldots+s^n(x)\int_0^1(1-t)^3dt=\frac{1}{4}\sum_{i=0}^n x_i^4 s^i(x).$$

Using this it is then easily verified that

$$\int_0^1 L(x,t)dt=\frac{1}{24}\left\{x^4-2x^3-\sum_{i=0}^n (x_i^4-2x_i^3)s^i(x)\right\}. \tag{9}$$

In order to find the constant c_0 it turns out to be worthwhile to consider the integral $\int_0^1 L(x,t)dx$. Using (5) we obtain

$$\int_0^1 L(x,t)dx=\frac{1}{6}\left\{\frac{1}{4}(1-t)^4-\frac{1}{4}(1-t)+(1-t)\sum_{i=0}^n w_i x_i^3-\sum_{i=0}^n w_i(x_i-t)_+^3\right\},$$

which can be written in the form

$$\int_0^1 L(x,\,t)dx=\frac{1}{6}\left\{-6c_0(1-t)+\frac{1}{4}(1-t)^4-\sum_{i=0}^n w_i(x_i-t)_+^3\right\}, \tag{10}$$

because of (8).

At this junction we need one of the results of theorem 1 which says that the function $L(x,t)$ is symmetric, i. e. $L(x,t)=L(t,x)$. This property has as an important consequence that the right-hand side of (10) is equivalent to the right-hand side of (9) if the variable t is replaced by x. The expression in (9) can be regarded as the difference of the function $(x^4-2x^3)/24$ and its interpolating n. c. s. Taking into account (10) the constant c_0 will be determined if we know the first derivative of the function

$$\frac{1}{24}\left\{x^4-2x^3-\sum_{i=0}^n (x_i^4-2x_i^3)s^i(x)\right\}$$

at the point $x=1$. We will come to this later.

3. Returning to (7), one is led to consider the integral

$$\int_0^1 \left| \int_0^1 L(x,t)dt \right| dx$$

for positive integer values of $n \geqq 2$. In order to calculate and estimate these numbers accurately one needs information about the function in (9), especially where it changes sign on [0, 1]. As we already noticed the right-hand side of (9) can be seen as the difference of the function $(x^4-2x^3)/24$ and its interpolating n. c. s. Because of the fact that the second derivative of $(x^4-2x^3)/24$ vanishes at the end points of the unit interval, the corresponding interpolating n. c. s. is equivalent to a type of spline functions as considered by Sonneveld in his paper [9]. Therefore his results are applicable and we will use them to examine the behaviour of the function $\int_0^1 L(x,t)dt$. Following Sonneveld we denote by $y_{1/n}(f;x)$ the unique cubic spline associated with $f(x)$ and having the properties

$$\begin{cases} y_{1/n}(f;x_i)=f_i, & 0 \leqq i \leqq n, \\ y''_{1/n}(f;x_i)=f''_i, & i=0,\ i=n; \end{cases}$$

the subscript $1/n$ means that the nodes are equally spaced on [0, 1].

In his paper Sonneveld establishes a relation between cubic spline interpolation and cubic Hermite interpolation. Assuming $f(x) \in C^1[0, 1]$, this classical approximation function $y_H(f;x)$ satisfies the following conditions:

(i) $y_H(f;x) \in C^1[0, 1]$,
(ii) $y_H(f;x)$ is a polynomial of degree at most three on each subinterval $[x_{i-1}, x_i]$,
(iii) $y_H(f;x_i)=f_i, \quad i=0, 1, \ldots, n,$
(iiii) $y'_H(f;x_i)=f'_i. \quad i=0, 1, \ldots, n.$

Furthermore, if $f \in C^4[0, 1]$, then it is well known that one has

$$f(x)-y_H(f;x)=\frac{(x-x_i)^2(x_{i+1}-x)^2}{24} f^{(4)}(\xi_i),\ x_i \leqq x \leqq x_{i+1};\ x_i < \xi_i < x_{i+1};\ 0 \leqq i \leqq n-1.$$

In view of this we can write on $[x_i, x_{i+1}]$

$$(11) \qquad f(x)-y_{1/n}(f;x)=f(x)-y_H(f;x)+y_H(f;x)-y_{1/n}(f;x)$$

$$=\frac{(x-x_i)^2(x_{i+1}-x)^2}{24} f^{(4)}(\xi_i)+y_H(f;x)-y_{1/n}(f;x), \quad x_i < \xi_i < x_{i+1}.$$

Let us now take in particular $f(x)=(x^4-2x^3)/24$ on [0, 1]. Then the spline functions $\frac{1}{24}\sum_{i=0}^{n}(x_i^4-2x_i^3)s^i(x)$ and $y_{1/n}(f;x)$ are identical and it follows from (11) that we have

$$\frac{1}{24}\left\{x^4-2x^3-\sum_{i=0}^{n}(x_i^4-2x_i^3)s^i(x)\right\}=\frac{(x-x_i)^2(x_{i+1}-x)^2}{24}+y_H(f;x)-y_{1/n}(f;x).$$

Using Sonneveld's results (in particular (2.25.b) and the set of formulae on p. 113 of [9]) the difference of the cubics $y_H(f; x)$ and $y_{1/n}(f; x)$ can be evaluated. Proceeding in this way we get on $[x_i, x_{i+1}]$

$$(12)\quad \frac{1}{24}\left\{x^4-2x^3-\sum_{i=0}^{n}(x_i^4-2x_i^3)s^i(x)\right\}=\frac{1}{24}(x-x_i)(x_{i+1}-x)\,[(x-x_i)(x_{i+1}-x)$$
$$+n^2\{z_i'(x_{i+1}-x)-z_{i+1}'(x-x_i)\}],$$

where the numbers z_i', $i=0, 1, \ldots, n$, are the solution of a system of linear equations of the form

$$(13)\quad \begin{cases} 2z_0'+z_1'=\frac{1}{n^3}, \\ \frac{1}{2}z_0'+2z_1'+\frac{1}{2}z_2'=0, \\ \ldots\ldots\ldots \\ \frac{1}{2}z_{n-2}'+2z_{n-1}'+\frac{1}{2}z_n'=0, \\ z_{n-1}'+2z_n'=-\frac{1}{n^3}. \end{cases}$$

For the investigation of (12) we need the solution of the set (13).

Theorem 3. Let n be even $(n=2m)$ and $\alpha=2+\sqrt{3}$. Then the unique solution of the system of linear equations (13) is given by

$$(14)\quad \begin{cases} z_i'=\dfrac{(-1)^i\sqrt{3}\left(\alpha^{\frac{n}{2}-i}-\alpha^{-\frac{n}{2}+i}\right)}{3n^3\left(\alpha^{\frac{n}{2}}+\alpha^{-\frac{n}{2}}\right)}, & i=0, 1, \ldots, m; \\ z_{n-i}'=-z_i', & i=0, 1, 2, \ldots, m; \end{cases}$$

however, if n is odd $(n=2m+1)$ then we have

$$(15)\quad \begin{cases} z_i'=\dfrac{(-1)^i\sqrt{3}\left(\alpha^{\frac{n}{2}-i}+\alpha^{-\frac{n}{2}+i}\right)}{3n^3\left(\alpha^{\frac{n}{2}}-\alpha^{-\frac{n}{2}}\right)}, & i=0, 1, \ldots, m; \\ z_{n-i}'=-z_i', & i=0,1,\ldots, m. \end{cases}$$

Proof. We will only verify the contents of the theorem in case n is even; the proof in case n is odd may be given in a similar way. First of all we remark that there is a unique solution because the matrix of (13) is diagonally dominant. Assuming $n=2m$, it is sufficient to show that the exhibited numbers z_i' of (12) satisfy the first $m+1$ equations of (13). If this is true, then the symmetry relations $z_{2m-i}'=-z_i'$, $i=0, 1, \ldots, m$, will guarantee that the remaining equations of (13) are also satisfied. Taking into account $\alpha=2+\sqrt{3}$ we have

$$2z_0'+z_1'=\frac{\sqrt{3}}{12m^3}\,\frac{\alpha^m-\alpha^{-m}}{\alpha^m+\alpha^{-m}}-\frac{\sqrt{3}}{24m^3}\,\frac{\alpha^{m-1}-\alpha^{-m+1}}{\alpha^m+\alpha^{-m}}$$

$$=\frac{\sqrt{3}}{24m^3}\left\{\frac{2(\alpha^m-\alpha^{-m})-(2-\sqrt{3})\alpha^m+(2+\sqrt{3})\alpha^{-m}}{\alpha^m+\alpha^{-m}}\right\}=\frac{1}{8m^3}.$$

In case $i=1, 2, \ldots, m-1$ we get

$$\frac{1}{2}z'_{i-1}+2z'_i+\frac{1}{2}z'_{i+1}=\frac{\sqrt{3}}{48m^3(\alpha^m+\alpha^{-m})}\{\alpha^{m-i+1}-\alpha^{-m+i-1}$$

$$-4(\alpha^{m-i}-\alpha^{-m+i})+\alpha^{m-i-1}-\alpha^{-m+i+1}\},$$

and the expression between brackets vanishes because $\alpha-4+\alpha^{-1}=0$. The $(m+1)$-th equation of (13) is also satisfied because $z'_m=0$ and $z'_{m-1}=-z'_{m+1}$. This proves Theorem 3.

In the sequel we will need some information about the magnitude of the numbers z'_i, $i=0, 1, \ldots, m$. This we state in the form of a lemma.

Lemma 1. Let the numbers $z'_i, i=0,1,\ldots,m$, be given by (14), respectively (15). Then the following assertions are true:

(i) when n is even then $n^3z'_0$ is increasing with n and

(16) $$\frac{1}{2n^3}\leq z'_0<\frac{\sqrt{3}}{3n^3},$$

(ii) when n is odd, then $n^3z'_0$ is decreasing with n and

(17) $$\frac{\sqrt{3}}{3n^3}<z'_0\leq\frac{3}{5n^3},$$

(iii)

(18) $$|z'_0|\geq 3|z'_1|\geq 3^2|z'_2|\geq\ldots\geq 3^m|z'_m|.$$

Proof. All three statements can be verified by elementary calculations based upon Theorem 3. We omit the details.

Remark. In view of (9) and (12) the first derivative of the function $\int_0^1 L(x,t)dt$ at the point $x=1$ is equal to $\frac{1}{24}z'_n=-\frac{1}{24}z'_0$. As we remarked on page 318 this suffices for the calculation of the constant c_0 appearing in (7). Using (10), together with (14) and (15) we obtain

(19) $$c_0=-\frac{1}{24}z'_0=-\frac{\sqrt{3}}{72n^3}\,\frac{(\alpha^n+\alpha^{-n}-2(-1)^n)}{(\alpha^n-\alpha^{-n})}.$$

Moreover, using (16) and (17), it is a consequence of (19) that

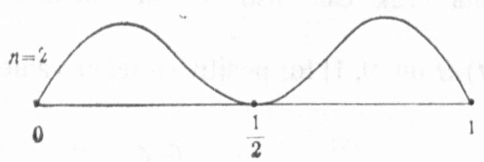
(20) $$\frac{1}{48n^3}\leq -c_0\leq\frac{1}{40n^3}.$$

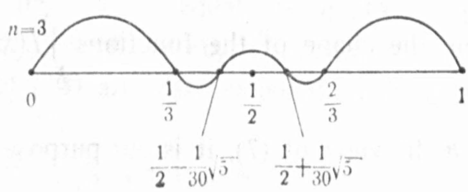
4. Theorem 3, together with formula (12), can also be used to determine the shape of the functions $\int_0^1 L(x,t)\,dt$ on $[0, 1]$ for positive integer values of n. In view of (7), it is our purpose to give an estimate of $\int_0^{\frac{1}{2}}\left|\int_0^1 L(x,t)dt\right|dx$ which holds for all positive integer values of $n\geq 2$ and which is best

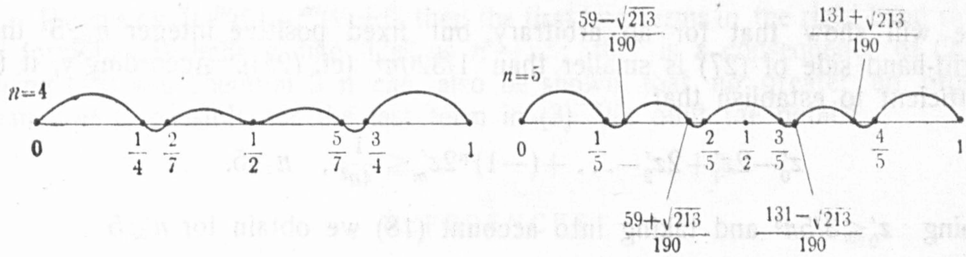
possible. Therefore we are particularly interested where the functions $\int_0^1 L(x,t)dt$ change sign on [0, 1]. Before we go into this, we first want to remark that the functions under consideration are symmetric on the unit interval with respect to $x=1/2$. This follows from (12) and the relations $z'_{n-i}=-z'_i$, $i=0, 1, \ldots, m$. As for the sign changes of $\int_0^1 L(x,t)dt$, we note from (12) that on every subinterval we deal with a polynomial of degree four which vanishes at both end points. Now let n be arbitrary, but fixed and consider the expression

$$(x-x_i)(x_{i+1}-x)+n^2[z'_i(x_{i+1}-x)-z'_{i+1}(x-x_i)] \tag{21}$$

on the interval $[x_i, x_{i+1}]$, which occurs in (12). Due to symmetry we may restrict ourselves to $0 \leq i \leq m-1$. If i is even, then according to theorem 3 we have $z'_i>0$ and $z'_{i+1}<0$ and thus is $\int_0^1 L(x,t)dt$ positive definite on (x_i,x_{i+1}). However, if i is odd, then we obtain $z'_i<0$, $z'_{i+1}>0$. So the parabola in (21) is pulled down, but due to the fact that $|z'_i|<1/5n^3$ for $i=1, 2, \ldots, m$ (this is a consequence of lemma 1), the function remains positive when $x=(x_i+x_{i+1})/2$. Therefore the function $\int_0^1 L(x,t)\,dt$ has two simple zeros on the open interval (x_i, x_{i+1}), assuming i is odd. In case n is even, finally, there is a double zero in $x=1/2$ because $z'_m=0$; moreover, the fourth zero will lie on the inside of $[x_{m-1}, x_m]$ when m is even and stay outside when m is odd. These observations, together with the fact that the coefficient of the leading term of the polynomial on each subinterval is 1/24, completely, determine the shape of the functions $\int_0^1 L(x, t)dt$ on [0, 1]. By way of illustration we exhibit the graphs of these functions for $n=2, 3, 4, 5$. The values which are given for the zeros on the inside of a subinterval may be verified by simple calculations based on (12) and Theorem 3.







Using the information provided by the pictures, formula (12) and Theorem 3, we have evaluated the integrals $\int_0^1 \left| \int_0^1 L(x,t)dt \right| dx$ in cases $n=2, 3, 4$. Elementary calculations lead to the following results:

(22) $\qquad$ if $n=2$, then $\displaystyle\int_0^1 \left| \int_0^1 L(x,t)dt \right| dx = \frac{1}{320n^4} = \frac{0.003125}{n^4}$,

(23) $\qquad$ if $n=3$, then $\displaystyle\int_0^1 \left| \int_0^1 L(x,t)dt \right| dx = \frac{125+2\sqrt{5}}{45000n^4} = \frac{0.00283\ldots}{n^4}$,

(24) $\qquad$ if $n=4$, then $\displaystyle\int_0^1 \left| \int_0^1 L(x,t)dt \right| dx = \frac{19349}{8067360n^4} = \frac{0.00239\ldots}{n^4}$.

In cases $n=5, 6, \ldots$ the integrals under consideration can be dealt with in the following way. For our purpose it is not necessary to calculate them exactly; estimates will be sufficient. To this end we use the representation of $\int_0^1 L(x,t)dt$ on the interval $[x_i, x_{i+1}]$ as given in (12). As a preliminary result we need the integrals

(25) $$\int_{x_i}^{x_{i+1}} (x-x_i)^2(x_{i+1}-x)^2 dx = \frac{1}{30n^5},$$

(26) $$\int_{x_i}^{x_{i+1}} (x-x_i)(x_{i+1}-x)^2 dx = \int_{x_i}^{x_{i+1}} (x-x_i)^2(x_{i+1}-x) dx = \frac{1}{12n^4}.$$

An estimate of $\int_0^1 \left| \int_0^1 L(x,t)dt \right| dx$ may now be derived from (12) as follows. Taking together all contributions to the integral over the n subintervals and using (25), (26) and theorem 3, we obtain

(27) $$\int_0^1 \left| \int_0^1 L(x,t)dt \right| dx \le \frac{1}{24}\left\{\frac{1}{30n^4} + \frac{1}{6n^2}\left[z_0' - 2z_1' + 2z_2' - \ldots + (-1)^m 2z_m'\right]\right\}.$$

We will show that for an arbitrary, but fixed positive integer $n \geqq 5$ the right-hand side of (27) is smaller than $1/320n^4$ (cf. (22)). Accordingly, it is sufficient to establish that

$$z_0' - 2z_1' + 2z_2' - \ldots + (-1)^m 2z_m' \leqq \frac{1}{4n^2}, \quad n \geqq 5.$$

Using $z_0' \leqq 3/5n^3$ and taking into account (18) we obtain for $n \geqq 5$

$$z_0' - 2z_1' + 2z_2' - \ldots + (-1)^m 2z_m' < \frac{3}{5n^3} + \frac{2}{5n^3}\left\{1 + \frac{1}{3} + \frac{1}{3^2} + \ldots\right\} = \frac{6}{5n^3} < \frac{1}{4n^2}.$$

This, together with (23) and (24), shows that

$$\int_0^1 \left| \int_0^1 L(x,t)dt \right| dx \leqq \frac{1}{320n^4}, \quad n = 2, 3, 4, \ldots, \tag{28}$$

and the equality sign holds if and only if $n=2$.

5. Now we can state our definite result. Taking into account formula (7), together with (20) and (28), one has the following theorem, which is an improvement of Aktinson's result as formulated on p. 317.

Theorem 4. Let $f \in C^4[0, 1]$ and let the nodes x_i, $i = 0, 1, \ldots, n$, be equally spaced on $[0, 1]$. If the weights w_i are defined by (5), then for $n = 2, 3, \ldots$

$$\left| \int_0^1 f(x)dx - \sum_{i=0}^n w_i f(x_i) \right| \leqq \frac{1}{40n^3} |f''(0) + f''(1)| + \frac{1}{320n^4} \| f^{(4)} \| \tag{29}$$

with $\| f^{(4)} \| = \max\limits_{0 \leqq x \leqq 1} |f^{(4)}(x)|$. In this inequality the constants $1/40 = 0.025$ and $1/320 = 0.003125$ are best possible.

P r o o f. Only the last assertion needs to be verified. This will be done by choosing two extremal functions f_1 and f_2 having the property that $\|f_1^{(4)}\| = 0$ and $f_2''(0) + f_2''(1) = 0$. In fact, f_1 can be set equal to x^3 on $[0,1]$. Applying the numerical integration formula (3) we obviously have

$$\frac{1}{4} - \sum_{i=0}^n w_i x_i^3 = 6c_0,$$

and it is a consequence of (20) that $|c_0| = 1/40n^3$ when $n=3$. So the constant $1/40$ in (29) cannot be replaced by any smaller number.

It is also easy to show that the constant $1/320$ in (29) is best possible. For this purpose take $n=2$ and consider the function f_2 on $[0, 1]$, defined by $f_2(x) = (x^4 - 2x^3)/24$. Then $f_2''(0) + f_2''(1) = 0$ and $f_2^{(4)}(x) \equiv 1$. Because of this and the fact that for $n=2$ the right-hand side of (9) is non-negative on $[0, 1]$ (cf. p. 322), it follows from (3) and (22) that we have

$$\int_0^1 f_2(x)dx - \sum_{i=0}^2 w_i f_2(x_i) = \frac{1}{320 \cdot 2^4}.$$

This proves our assertion.

R e m a r k. If $f''(0)+f''(1)\neq 0$, then the first two terms in the right-hand side of formula (3) behave like $1/n^3$ as $n\to\infty$; this is a consequence of (20). Using (12) and Theorem 3 it can also be shown that no greater an order than $1/n^4$ is possible for the last term in (3). We omit the details.

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