On natural cubic splines, with an application to numerical integration formulae

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by

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Introduction and summary

0. By $C[0,1]$ we denote the set of real-valued continuous functions defined on the interval $[0,1]$. Let the numbers $x_0, x_1, \ldots, x_n$ be prescribed with $0 = x_0 < x_1 < \ldots < x_{n-1} < x_n = 1$. Then to every division of the unit interval into n subintervals $[x_{i-1}, x_i]$ there corresponds an (n+1)-dimensional subspace $S \equiv S(x_0, x_1, \ldots, x_n)$ 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 1 in [7], p. 158.

The object of this report is twofold. *Always assuming that the nodes are equally spaced on* $[0,1]$, we first show how explicit formulae may be given for the n.c.s. This approach is based upon the solutions of a set of linear equations from which the so-called cardinal natural cubic spline functions (c.n.c.s.) may be calculated. As an application of these basic functions we present a new way to derive some familiar results of Meyers-Sard [4] and Holladay [3].

In the second part of the paper 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, p. 99) and establish it in its definite form. In the course of the proof use is made of recent work of Sonneveld [8].

On cardinal natural cubic spline functions

1.1. 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. $s(x_i) = f(x_i)$ for $i = 0,1,\ldots,n$. If we write

$$f_i = f(x_i) \ , \quad \bar{\mu}_i = s''(x_i) \ ,$$

then on the interval $[x_{i-1},x_i]$ the function s can be written in the following form:

$$(1.1) \qquad s(x) = f_{i-1}\, A_i(x) + f_i\, B_i(x) + \bar{\mu}_{i-1}\, C_i(x) + \bar{\mu}_i\, D_i(x) \ .$$

Here $A_i(x),\ldots,D_i(x)$ are certain cubic polynomials with suitable chosen properties. In fact, we have

$$(1.2) \qquad A_i(x) = 1 - n(x - x_{i-1}) \ ,$$

$$(1.3) \qquad B_i(x) = n(x - x_{i-1}) \ ,$$

$$(1.4) \qquad C_i(x) = -\frac{1}{6n}(x - x_{i-1})\{2 - 3n(x - x_{i-1}) + n^2(x - x_{i-1})^2\} \ ,$$

$$(1.5) \qquad D_i(x) = -\frac{1}{6n}(x - x_{i-1})\{1 - n^2(x - x_{i-1})^2\} \ .$$

It is obvious from these formulae that $A_i(x),B_i(x) \geq 0$, whereas $C_i(x),D_i(x) \leq 0$ on $[x_{i-1},x_i]$. Moreover,

$$(1.6) \qquad A_i(x) + B_i(x) = 1 \ ,$$

$$(1.7) \qquad \int_{x_{i-1}}^{x_i} A_i(x)dx = \int_{x_{i-1}}^{x_i} B_i(x)dx = \frac{1}{2n} \ ,$$

$$(1.8) \qquad \int_{x_{i-1}}^{x_i} C_i(x)dx = \int_{x_{i-1}}^{x_i} D_i(x)dx = -\frac{1}{24n^3} \ .$$

In view of the conditions (i) and (ii) the parameters $\bar{\mu}_i$ have to satisfy some particular relations, which can be found for instance in [9]. They take the form

$$(1.9) \qquad \bar{\mu}_{i-1} + 4\bar{\mu}_i + \bar{\mu}_{i+1} = 6n^2(f_{i+1} - 2f_i + f_{i-1}) \ , \qquad (i = 1,2,\ldots,n-1) \ ,$$

with

(1.10) $\overline{\mu}_0 = \overline{\mu}_n = 0$.

There exists a unique solution for the parameters $\overline{\mu}_i$, because the matrix associated with system (1.9) is diagonally dominant. Together with (1.1) this establishes a proof of the fact that the interpolating n.c.s. exists and is unique.

Besides (1.1) there is another way of representing the interpolating n.c.s. s(x). If $s^i(x) \in S$ denotes the i-th c.n.c.s. (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

(1.11) $$s(x) = \sum_{i=0}^{n} f_i\, s^i(x) ;$$

this is a formula of Lagrange-type.

1.2. As usual we write for $m \geq 0$

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

Moreover, let

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

In the sequel we will need a result which is due to Atkinson. It reads as follows:

<u>THEOREM 1</u> (Atkinson [1])

(i) $L(x,t)$ is symmetric, i.e. $L(x,t) = L(t,x)$. For each x, it is an n.c.s. in t with nodes $x_0,x_1,\dots,x_n$, and x; for $i = 0,1,\dots,n$, $L(x,x_i) = 0$.

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

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

with

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

As an obvious consequence of (1.13) we have

COROLLARY 1

$$
(1.15)\qquad \int_0^1 f(x)dx - \sum_{i=0}^{n} f_i \int_0^1 s^i(x)dx = c_0 f''(1) + c_1 f''(0) + \int_0^1\int_0^1 L(x,t) f^{(4)}(t)dtdx ,
$$

where

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

Under the assumption that the nodes are equally spaced, it is true (cf. formula (1.34)) that $c_0 = c_1$. Relation (1.15) is of some interest because Schoenberg [6] has shown that of all numerical integration formulae of type

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

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

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

In his paper [5] Sard also included a short table of weights w_i in case the nodes are equally spaced. Actually it is possible to determine explicit formulae for the weights. This was done for the first time in 1950 by Meyers and Sard [4] without using the concept of spline function. We refer the reader to their paper for more extensive data on the numbers w_i. In this respect one also has to mention a paper by Holladay [3]. In 1957 he proved a fundamental result in the theory of n.c.s., apparently without knowing of the work of Schoenberg in this area. He also derived formulae for the numbers w_i using (1.17), exhibited a table for the weights and formulated some simple rules to calculate them. Schoenberg noted that the data given by Holladay are exactly the same as those of Meyers-Sard and this led him to establish a close connection between the problems of spline interpolation and mechanical quadratures, which culminates in his fundamental theorem 1 in [7].

In view of Schoenberg's theorem, it seems to be of some interest to get hold of the c.n.c.s. $s^i(x)$ $(i = 0,1,\ldots,n)$. They also enable us to calculate the weights w_i in a different way as was done before by Sard, Meyers-Sard and Holladay. These two subjects will be dealt with in the next two sections.

1.3. The calculation of the c.n.c.s. can be based upon formulae (1.1), (1.9) and (1.10). Putting

$$\mu_i^{(k)} = (s^k)''(x_i) ,$$

then according to (1.1) we have on the interval $[x_{i-1},x_i]$:

$$(1.18) \qquad s^k(x) = \delta_{i-1}^k \, A_i(x) + \delta_i^k \, B_i(x) + \mu_{i-1}^{(k)} \, C_i(x) + \mu_i^{(k)} \, D_i(x) , \qquad (k = 0,1,\ldots,n) .$$

In order to compute $s^k(x)$, we first have to write equations (1.9) in their appropriate form. We get

$$(1.19) \qquad \mu_{i-1}^{(k)} + 4\mu_i^{(k)} + \mu_{i+1}^{(k)} = 6n^2(\delta_{i+1}^k - 2\delta_i^k + \delta_{i-1}^k) , \quad \begin{pmatrix} k = 0,1,\ldots,n; \\ i = 1,2,\ldots,n-1 \end{pmatrix} ,$$

with

$$(1.20) \qquad \mu_0^{(k)} = \mu_n^{(k)} = 0 , \quad (k = 0,1,2,\ldots,n) .$$

In view of (1.18) and together with formulae (1.2), (1.3), (1.4), (1.5), the c.n.c.s. will be completely determined if we can solve the systems of linear equations (1.19) for n = 2,3,... . Before we go into this, we first state an elementary lemma which will be needed for the proof of the next theorem.

<u>LEMMA 1</u> The solution of the difference equation

$$(1.21) \qquad a_{i+2} - 4a_{i+1} + a_i = 0 , \quad (i = 0,1,2,\ldots) ,$$

with initial conditions $a_0 = 0$, $a_1 = 1$, is given by

(1.22) $$a_i = \frac{1}{6}\sqrt{3}(\alpha^i - \alpha^{-i}) , \qquad (i = 0,1,2,\ldots) ,$$

where $\alpha = 2 + \sqrt{3}$. Moreover, we have

(1.23) $$a_i\, a_{n-i} = a_{n-1} + a_{n-3} + \ldots + a_{n-2i+1} , \qquad (1 \le i \le [\tfrac{n}{2}]) ,$$

(1.24) $$a_{i+1}\, a_{n-i} - a_i\, a_{n-i-1} = a_n , \qquad (0 \le i \le n-1) .$$

Some other particular solutions are

(1.25) $$b_0 = 1 , \; b_1 = 1 , \; b_i = \frac{1}{6}\{(\alpha^{-1} + 1)\alpha^i + (\alpha + 1)\alpha^{-i}\} , \quad (i = 0,1,2,\ldots) ,$$

(1.26) $$c_0 = 1 , \; c_1 = 5 , \; c_i = \frac{1}{2}\{(\alpha - 1)\alpha^i + (\alpha^{-1} - 1)\alpha^{-i}\} , \quad (i = 0,1,2,\ldots) ,$$

(1.27) $$d_0 = 2 , \; d_1 = 4 , \; d_i = \alpha^i + \alpha^{-i} , \qquad (i = 0,1,2,\ldots) .$$

PROOF Using the standard technique for solving difference equations with constant coefficients we easily deduce the formulae (1.22), (1.25), (1.26), (1.27). Relation (1.23) can be proved by using mathematical induction. Equality (1.24) is a straightforward calculation. ∎

THEOREM 2 Let n = 2m, respectively n = 2m + 1 (m = 1,2,...). Then for an arbitrary but fixed number m the unique solution of the set of equations (1.19), always assuming that (1.20) holds, takes the form

(1.28) $$\mu_i^{(0)} = (-1)^{i-1} \frac{6n^2\, a_{n-i}}{a_n} , \qquad (i = 1,2,\ldots,n-1) ,$$

(1.29) $$\mu_i^{(k)} = (-1)^{i-k-1} \frac{36n^2\, a_k\, a_{n-i}}{a_n} , \qquad (k = 1,2,\ldots,m;\; i = k+1,k+2,\ldots,n-1) ,$$

(1.30) $$\mu_i^{(k)} = \mu_k^{(i)} , \qquad (k = 1,2,\ldots,m;\; i = 1,2,\ldots,k-1) ,$$

(1.31) $$\mu_1^{(1)} = -\,2\mu_1^{(0)} + \mu_2^{(0)} ,$$

(1.32) $$\mu_k^{(k)} = \mu_{k-1}^{(k-1)} + \mu_{2k-1}^{(1)} , \qquad (k = 2,3,\ldots,m) ,$$

(1.33) $$\mu_{n-i}^{(n-k)} = \mu_i^{(k)} , \qquad (k = 0,1,\ldots,m;\; i = 1,2,\ldots,n-1) .$$

Here a_i is given by (1.22).

PROOF It is sufficient to consider the systems (1.19) only for $k = 0,1,\dots,m$, because in case of $k = m+1,\dots,n$ we can proceed by replacing k by n-k and i by n-i. Then we get a system of equations which we encounter in case $k = 0,1,\dots,m$. Therefore we have formula (1.33) which has as a consequence, together with (1.18) and (1.2), (1.3), (1.4), (1.5), that

$$(1.34)\qquad s^{n-i}(x) = s^{i}(1 - x) , \qquad (i = 0,1,\dots,m) ;$$

this was to be expected because the nodes are equally spaced.

As for the proof of theorem 2, let m be an arbitrary but fixed positive integer. Then k can be one of the integers $0,1,\dots,m$ and we have to distinguish between several cases. If $k = 0$, then it follows from (1.19) that we have to deal with

$$(1.35)\qquad \begin{cases} \mu_0^{(0)} + 4\mu_1^{(0)} + \mu_2^{(0)} = 6n^2 , \\ \mu_i^{(0)} + 4\mu_{i+1}^{(0)} + \mu_{i+2}^{(0)} = 0 , \qquad (i = 1,2,\dots,n-2) . \end{cases}$$

Together with (1.20), it is an immediate consequence of the difference equation (1.21) that (1.28) is the solution of system (1.35). (If the last element of the set through which the index variable i runs is smaller than the first element, we will always assume that the set of equations under consideration is void.) Now we turn to the case $k = 1$. Then in view of (1.19) one has for $n > 2$

$$(1.36)\qquad \begin{cases} \mu_0^{(1)} + 4\mu_1^{(1)} + \mu_2^{(1)} = -\ 12n^2 , \\ \mu_1^{(1)} + 4\mu_2^{(1)} + \mu_3^{(1)} = 6n^2 , \\ \mu_i^{(1)} + 4\mu_{i+1}^{(1)} + \mu_{i+2}^{(1)} = 0 , \qquad (i = 2,3,\dots,n-2) . \end{cases}$$

Using (1.20), (1.31), (1.21) and the fact that $a_1 = 1$, it is easily verified that the expressions for $\mu_i^{(1)}$ as exhibited in (1.29), together with (1.31), are the solution of system (1.36). The case $k = 2$, when appropriate, can be dealt with in an analogous way. The main part of the proof of theorem 2 comes in when $k = 3,4,\dots,m$; these cases can be considered all together. Let k be an arbitrary but fixed element of the set $\{3,4,\dots,m\}$. From (1.19) we obtain

$$
(1.37)\quad \begin{cases}
\mu_i^{(k)} + 4\mu_{i+1}^{(k)} + \mu_{i+2}^{(k)} = 0 , & (i = 0,1,\ldots,k-3) , \\
\mu_{k-2}^{(k)} + 4\mu_{k-1}^{(k)} + \mu_k^{(k)} = 6n^2 , & \\
\mu_{k-1}^{(k)} + 4\mu_k^{(k)} + \mu_{k+1}^{(k)} = -12n^2 , & \\
\mu_k^{(k)} + 4\mu_{k+1}^{(k)} + \mu_{k+2}^{(k)} = 6n^2 , & \\
\mu_i^{(k)} + 4\mu_{i+1}^{(k)} + \mu_{i+2}^{(k)} = 0 , & (i = k+1,k+2,\ldots,n-2) .
\end{cases}
$$

In the first set of equations of system (1.37) we can make use of (1.30). Then one has to show that

$$4\mu_k^{(1)} + \mu_k^{(2)} = 0$$

and

$$\mu_k^{(i)} + 4\mu_k^{(i+1)} + \mu_k^{(i+2)} = 0 , \qquad (i = 1,2,\ldots,k-3) .$$

In order to do this we apply (1.29). Then both equalities are a consequence of relation (1.21) if we take into account the accompanying initial conditions. Using (1.30) the second equation of system (1.37) can be written in the form

$$(1.38)\qquad \mu_k^{(k-2)} + 4\mu_k^{(k-1)} + \mu_k^{(k)} = 6n^2 .$$

In view of (1.32) and then applying (1.31), the left-hand side of this equality is equal to

$$\mu_k^{(k-2)} + 4\mu_k^{(k-1)} - 2\mu_1^{(0)} + \mu_2^{(0)} + \mu_3^{(1)} + \ldots + \mu_{2k-1}^{(1)} .$$

Now the formulae (1.28) and (1.29) can be used. If we proceed in this way, then the verification of (1.38) amounts to showing that

$$(1.39)\qquad a_k\, a_{n-k} = a_{n-1} + a_{n-3} + \ldots + a_{n-2k+1} , \quad (n = 6,7,\ldots;\ k = 3,4,\ldots,m) .$$

And this is true because of (1.23) of lemma 1.

The third and fourth equation of system (1.37) can be dealt with in the same way. We do not carry out the details of these calculations, but remark that in both derivations it is advantageous to use relation (1.39). For instance, the validity of the third equation of (1.37) then stems from (1.24) of lemma 1. Finally, it is obvious that in the last set of equations of system (1.37) the appropriate formulae of (1.29) can be applied. Then it is sufficient to refer to (1.21) and the proof of theorem 2 is complete. ∎

Taking into account (1.22), the whole set of formulae of theorem 2 is rather complicated and one may have some doubts whether they are suited for a rapid calculation of the second derivatives of the c.n.c.s. Fortunately, this is the case. We will now first give some examples by way of illustration. On the basis of this we will supply an algorithm which can be used to calculate the numbers $\mu_i^{(k)}$ recursively by going from n nodes to n+1 nodes. In the following tables we only exhibit the numbers $\mu_i^{(k)}$ for $k = 0,1,\dots,[\frac{n}{2}]$ and $i = 1,2,\dots,n-1$ because of (1.20) and the symmetry relations (1.33). We remark that for a specific number n all data in the table have to be multiplied by $\frac{6n^2}{a_n}$, where a_n is given by (1.22). This number, together with the value of n, is placed in the first row.

As is apparent from theorem 2 the sequence $\{a_i\}$ as given in (1.22) plays a prominent role in our calculations. Starting out with the initial conditions $a_0 = 0$, $a_1 = 1$, the elements are easily generated by means of the recurrence relation (1.21). We so obtain

$$(1.40)\quad \begin{cases} a_0 = 0,\ a_1 = 1,\ a_2 = 4,\ a_3 = 15,\ a_4 = 56,\ a_5 = 209, \\ a_6 = 780,\ a_7 = 2911,\ a_8 = 10864,\ a_9 = 40545,\ \dots\ . \end{cases}$$

Formula (1.40), together with the contents of theorem 2, gives rise to the data for $\mu_i^{(k)}$ as exhibited in tables 1,2,...,7.

	n = 2	$\frac{6n^2}{4}$
i \ k	0	1
1	1	-2

Table 1

	n = 3	$\frac{6n^2}{15}$
i \ k	0	1
1	4	-9
2	-1	6

Table 2

	n = 4		$\frac{6n^2}{56}$
i \ k	0	1	2
1	15	-34	24
2	- 4	24	-40
3	1	- 6	24

Table 3

	n = 5		$\frac{6n^2}{209}$
i \ k	0	1	2
1	56	-127	90
2	-15	90	-151
3	4	- 24	96
4	- 1	6	- 24

Table 4

	n = 6			$\frac{6n^2}{780}$
i \ k	0	1	2	3
1	209	-474	336	- 90
2	- 56	336	-564	360
3	15	- 90	360	-570
4	- 4	24	- 96	360
5	1	- 6	24	- 90

Table 5

	n = 7			$\frac{6n^2}{2911}$
i \ k	0	1	2	3
1	780	-1769	1254	- 336
2	-209	1254	-2105	1344
3	56	- 336	1344	-2129
4	- 15	90	- 360	1350
5	4	- 24	96	- 360
6	- 1	6	- 24	90

Table 6

	n = 8				$\frac{6n^2}{10864}$
i \ k	0	1	2	3	4
1	2911	-6602	4680	-1254	336
2	- 780	4680	-7856	5016	-1344
3	209	-1254	5016	-7946	5040
4	- 56	336	-1344	5040	-7952
5	15	- 90	360	-1350	5040
6	- 4	24	- 96	360	-1344
7	1	- 6	24	- 90	336

Table 7

Based on the formulae of theorem 2 we will now give an algorithm for the calculation of the data $\mu_i^{(k)}$ $(k = 0,1,\ldots,[\frac{n}{2}];\ i = 1,2,\ldots,n-1)$ for an arbitrary number of nodes. For a specific value of n let us denote the quantities in the tables by $b_{i,k}^{(n)}$ $(k = 0,1,\ldots,[\frac{n}{2}];\ i = 1,2,\ldots,n-1)$. Then in going from n to n+1 one has the following procedure, which is easy to apply, and which can serve to calculate the numbers $b_{i,k}^{(n+1)}$.

ALGORITHM 1

step 1

$$b_{i+1,k}^{(n+1)} = -\,b_{i,k}^{(n)}\ , \qquad (i = 1,2,\ldots,n-1;\ k = 0,1,\ldots,\min(i-1,[\tfrac{n}{2}]))\ .$$

The next step has only to be applied when going from n is odd to n+1 is even.

step 2

$$b_{i+1,[\frac{n}{2}]+1}^{(n+1)} = -\left(4b_{i+1,[\frac{n}{2}]}^{(n+1)} + b_{i+1,[\frac{n}{2}]-1}^{(n+1)}\right)\ ,$$

$$(i = [\tfrac{n+1}{2}] + 1, [\tfrac{n+1}{2}] + 2, \ldots, n-1)\ .$$

step 3

$$b_{i,i-1}^{(n+1)} = -\left(4b_{i+1,i-1}^{(n+1)} + b_{i+2,i-1}^{(n+1)}\right)\ , \qquad (i = 1,2,\ldots,[\tfrac{n+1}{2}] + 1)\ ,$$

with

$$b_{2,1}^{(3)} = 6\ ,\ b_{3,2}^{(4)} = 24\ ,\ b_{n+1,k}^{(n+1)} = 0\ , \qquad (k = 0,1,\ldots,[\tfrac{n+1}{2}])\ .$$

step 4

$$b_{i,k}^{(n+1)} = b_{k,i}^{(n+1)}\ , \qquad (i = 1,2,\ldots,[\tfrac{n+1}{2}] - 1;\ k = i+1,i+2,\ldots,[\tfrac{n+1}{2}])\ .$$

step 5

$$b_{1,1}^{(n+1)} = -\,2b_{1,0}^{(n+1)} + b_{2,0}^{(n+1)}\ .$$

step 6

$$b_{i,i}^{(n+1)} = b_{i-1,i-1}^{(n+1)} + b_{2i-1,1}^{(n+1)}\ , \qquad (i = 2,3,\ldots,[\tfrac{n+1}{2}])\ .$$

step 7

$$\mu_i^{(k)} = \frac{6(n+1)^2}{a_{n+1}}\, b_{i,k}^{(n+1)}\ , \qquad (i = 1,2,\ldots,n;\ k = 0,1,\ldots,[\tfrac{n+1}{2}])\ ,$$

where a_{n+1} is given by (1.22).

REMARK The process of the algorithm is initiated with the data of table 1. If one of the variables i or k runs through a sequence of values the last of which is smaller than the first one, then it is understood that the corresponding instructions are not to be executed. An examination of the structure of the algorithm reveals that the first three steps are a consequence of formulae (1.28), (1.29). Step 2 is only to be applied in case n is odd, because then in going from n to n+1 the value of m (and thus the number of columns of the matrix) is increased by 1. The steps 4, 5 and 6 immediately follow from (1.30), (1.31), (1.32) respectively. Relation (1.33) does not find its analogue in the algorithm because we have restricted the values of k to $0,1,\ldots,[\frac{n+1}{2}]$.

An important consequence is that now, together with the formulae (1.2), (1.3), (1.4), (1.5) and (1.18), the c.n.c.s. are completely at our disposal for an arbitrary number of (equally spaced) nodes. By way of illustration we exhibit these basic functions in cases n = 2 and n = 3, using the data from tables 1, 2 and the symmetry relations (1.33).

n = 2

$$s^0(x) = \begin{cases} A_1(x) + 6D_1(x), & (0 \le x \le \frac{1}{2}), \\ 6C_2(x), & (\frac{1}{2} \le x \le 1). \end{cases}$$

$$s^1(x) = \begin{cases} B_1(x) - 12D_1(x), & (0 \le x \le \frac{1}{2}), \\ A_2(x) - 12C_2(x), & (\frac{1}{2} \le x \le 1). \end{cases}$$

$$s^2(x) = \begin{cases} 6D_1(x), & (0 \le x \le \frac{1}{2}), \\ B_2(x) + 6C_2(x), & (\frac{1}{2} \le x \le 1). \end{cases}$$

n = 3

$$s^0(x) = \begin{cases} A_1(x) + \frac{72}{5} D_1(x), & (0 \le x \le \frac{1}{3}), \\ \frac{72}{5} C_2(x) - \frac{18}{5} D_2(x), & (\frac{1}{3} \le x \le \frac{2}{3}), \\ -\frac{18}{5} C_3(x), & (\frac{2}{3} \le x \le 1). \end{cases}$$

$$s^1(x) = \begin{cases} B_1(x) - \frac{162}{5} D_1(x) , & (0 \le x \le \frac{1}{3}) , \\ A_2(x) - \frac{162}{5} C_2(x) + \frac{108}{5} D_2(x) , & (\frac{1}{3} \le x \le \frac{2}{3}) , \\ \frac{108}{5} C_3(x) , & (\frac{2}{3} \le x \le 1) . \end{cases}$$

$$s^2(x) = \begin{cases} \frac{108}{5} D_1(x) , & (0 \le x \le \frac{1}{3}) , \\ B_2(x) + \frac{108}{5} C_2(x) - \frac{162}{5} D_2(x) , & (\frac{1}{3} \le x \le \frac{2}{3}) , \\ A_3(x) - \frac{162}{5} C_3(x) , & (\frac{2}{3} \le x \le 1) . \end{cases}$$

$$s^3(x) = \begin{cases} - \frac{18}{5} D_1(x) , & (0 \le x \le \frac{1}{3}) , \\ - \frac{18}{5} C_2(x) + \frac{72}{5} D_2(x) , & (\frac{1}{3} \le x \le \frac{2}{3}) , \\ B_3(x) + \frac{72}{5} C_3(x) , & (\frac{2}{3} \le x \le 1) . \end{cases}$$

REMARK Using various properties of the numbers $\mu_i^{(k)}$ $(k = 0,1,\dots,n;$ $i = 0,1,\dots,n)$ and taking into account (1.18), one can show that the c.n.c.s. $s^k(x)$ $(k = 0,1,\dots,n)$ do not change sign on the subintervals and have simple zeros at the nodes. We omit the details of this verification.

1.4. Besides the derivation of the c.n.c.s. we recall that at the end of section 1.2 we set ourselves the task of calculating the weights w_k $(k = 0,1,\dots,n)$, which numbers appear in the numerical integration formula (1.15). One has (cf. (1.17))

$$w_k = \int_0^1 s^k(x)dx , \qquad (k = 0,1,\dots,n) ,$$

where $s^k(x)$ is the k-th c.n.c.s., the nodes being equally spaced. These integrals can be expressed in terms of the numbers $\mu_i^{(k)}$ $(i = 0,1,\dots,n)$, the second derivatives of the function $s^k(x)$ at the nodes. Because of (1.34) it is sufficient to restrict ourselves to values of k for which $0 \le k \le m$, where $n = 2m$, respectively $n = 2m + 1$. It is a consequence of (1.18), together with (1.7), (1.8) and (1.20), that one has

$$
(1.41)\quad \begin{cases} w_0 = \dfrac{1}{2n} - \dfrac{1}{12n^3} \displaystyle\sum_{i=1}^{n-1} \mu_i^{(0)} , \\[2ex] w_k = \dfrac{1}{n} - \dfrac{1}{12n^3} \displaystyle\sum_{i=1}^{n-1} \mu_i^{(k)} , \qquad (k = 1,2,\dots,m) , \\[2ex] w_{n-k} = w_k , \qquad (k = 0,1,\dots,m) . \end{cases}
$$

For some explicit formulae of the underlying functions $s^k(x)$ we refer to the examples given at the end of the preceding section. The sums which appear in (1.41) can be dealt with in the following way. Taking into account (1.20) it is an easy consequence of (1.19) that $\sum_{i=1}^{n-1} \mu_i^{(k)}$ can be written in terms of $\mu_1^{(k)}$ and $\mu_{n-1}^{(k)}$. This fact, together with the information supplied by theorem 2, actually gives rise to the following expressions:

$$
\sum_{i=1}^{n-1} \mu_i^{(0)} = n^2 + \frac{\mu_1^{(0)} + \mu_{n-1}^{(0)}}{6} =
$$

$$
(1.42)\qquad = n^2 + \frac{\dfrac{6n^2\, a_{n-1}}{a_n} + \dfrac{(-1)^n\, 6n^2\, a_1}{a_n}}{6} = \frac{n^2}{a_n} \{a_n + a_{n-1} + (-1)^n\} ,
$$

$$
\sum_{i=1}^{n-1} \mu_i^{(1)} = -\, n^2 + \frac{\mu_1^{(1)} + \mu_{n-1}^{(1)}}{6} = \qquad (n \geq 3)
$$

$$
(1.43)\qquad = -\, n^2 + \frac{-2\mu_1^{(0)} + \mu_2^{(0)} + \mu_{n-1}^{(1)}}{6} = -\,\frac{6n^2}{a_n} \{a_{n-1} + (-1)^n\} .
$$

This formula holds also in case $n = 2$; in the course of its derivation use is made of (1.21). When $k = 2,3,\dots,m$ we obtain

$$
\sum_{i=1}^{n-1} \mu_i^{(k)} = \frac{\mu_1^{(k)} + \mu_{n-1}^{(k)}}{6} = \frac{\mu_k^{(1)} + \mu_{n-1}^{(k)}}{6} =
$$

$$
= (-1)^k \frac{36n^2\, a_1\, a_{n-k}}{6a_n} + (-1)^{n-2+k} \frac{36n^2\, a_k\, a_1}{6a_n} =
$$

$$
(1.44)\qquad = (-1)^k \frac{6n^2}{a_n} \{a_{n-k} + (-1)^n\, a_k\} .
$$

As usual, a_i $(i = 0,1,\ldots)$ is given by (1.22). We note that in view of (1.43) formula (1.44) can also be used in case $k = 1$.

Formulae (1.42) and (1.44), together with (1.22), can be used to give explicit expressions for the sums $\sum_{i=1}^{n-1} \mu_i^{(k)}$ $(k = 0,1,\ldots,m)$. It turns out to be advantageous to consider the cases n is even and n is odd separately. We omit the somewhat tedious but elementary calculations and state only the results. In case n is even $(n = 2m)$ one has

$$(1.45) \qquad \sum_{i=1}^{n-1} \mu_i^{(0)} = \frac{n^2\{(\alpha^{-1}+1)\alpha^{n/2} + (\alpha+1)\alpha^{-n/2}\}}{\alpha^{n/2}+\alpha^{-n/2}} ,$$

$$(1.46) \qquad \sum_{i=1}^{n-1} \mu_i^{(k)} = \frac{(-1)^k\, 6n^2\{\alpha^{\frac{n}{2}-k} + \alpha^{-\frac{n}{2}+k}\}}{\alpha^{n/2}+\alpha^{-n/2}} , \qquad (k = 1,2,\ldots,m) ,$$

whereas in case n is odd $(n = 2m + 1)$ we obtain

$$(1.47) \qquad \sum_{i=1}^{n-1} \mu_i^{(0)} = \frac{2\sqrt{3}\, n^2\{\alpha^{\frac{n-1}{2}} - \alpha^{-\frac{(n-1)}{2}}\}}{(\alpha-1)\alpha^{\frac{n-1}{2}} + (\alpha^{-1}-1)\alpha^{-\frac{(n-1)}{2}}} ,$$

$$(1.48) \qquad \sum_{i=1}^{n-1} \mu_i^{(k)} = \frac{(-1)^k\, 6n^2\{(\alpha-1)\alpha^{\frac{n-1}{2}-k} + (\alpha^{-1}-1)\alpha^{-\frac{(n-1)}{2}+k}\}}{(\alpha-1)\alpha^{\frac{n-1}{2}} + (\alpha^{-1}-1)\alpha^{-\frac{(n-1)}{2}}} ,$$

$$(k = 1,2,\ldots,m) .$$

To give the reader an idea what the sums $\sum_{i=1}^{n-1} \mu_i^{(k)}$ $(k = 0,1,\ldots,m)$ look like for the first few values of n, we use the expressions (1.42) and (1.44) instead of (1.45)-(1.48). We arrive at the following table; to obtain the value of the sum $\sum_{i=1}^{n-1} \mu_i^{(k)}$ for a particular n and k, the element in the top row and (n-1)-th column has to be multiplied by the entry in the k-th row and (n-1)-th column.

	$\frac{6n^2}{4}$	$\frac{6n^2}{5}$	$\frac{6n^2}{14}$	$\frac{6n^2}{19}$	$\frac{6n^2}{52}$	$\frac{6n^2}{71}$	$\frac{6n^2}{194}$	$\frac{6n^2}{265}$	$\frac{6n^2}{724}$	$\frac{6n^2}{989}$
k \ n	2	3	4	5	6	7	8	9	10	11
0	1	1	3	4	11	15	41	56	153	209
1	-2	-1	-4	-5	-14	-19	-52	-71	-194	-265
2			2	1	4	5	14	19	52	71
3					- 2	- 1	- 4	- 5	- 14	- 19
4							2	1	4	5
5									- 2	- 1

Table 8

We note that there are several striking recurrences in this table. When n is even the sequence of numbers {2,4,14,52,...} plays a dominant role. In case n is odd the same is true for the sequence {1,5,19,71,...}. Both sequences are characterized by property (1.21).

Using the set of formulae (1.45)-(1.48) one can show that the recurrence features of the entries exhibited in table 8 for n = 2,...,11 do hold in general. Using these properties an algorithm can be deduced for the calculation of the sums $\sum_{i=1}^{n-1} \mu_i^{(k)}$. It is apparent from the data of the table that the cases n is even and n is odd have to be considered separately. Assume first that $n = 2m$ ($m = 1,2,\ldots$) and let the value of m be increased by 1; further let the numbers b_i and d_i be defined by (1.25), respectively (1.27).

ALGORITHM 2

step 1

$$d_{m+1} = 4d_m - d_{m-1}\ , \quad b_{m+1} = 4b_m - b_{m-1}\ .$$

step 2

$$e_k^{(m+1)} = (-1)^k\, d_{m-k+1}\ , \qquad (k = 1,2,\ldots,m+1)\ .$$

step 3

$$\sum_{i=1}^{2m+1} \mu_i^{(0)} = \frac{24(m+1)^2}{d_{m+1}} b_{m+1} ,$$

$$\sum_{i=1}^{2m+1} \mu_i^{(k)} = \frac{24(m+1)^2}{d_{m+1}} e_k^{(m+1)} , \qquad (k = 1,2,\ldots,m+1) .$$

Now let $n = 2m + 1$ $(m = 1,2,\ldots)$ and let the value of m be increased by 1; the numbers a_i and c_i are given by (1.22), respectively (1.26).

ALGORITHM 3

step 1

$$c_{m+1} = 4c_m - c_{m-1} , \quad a_{m+1} = 4a_m - a_{m-1} .$$

step 2

$$g_k^{(m+1)} = (-1)^k c_{m-k+1} , \qquad (k = 1,2,\ldots,m+1) .$$

step 3

$$\sum_{i=1}^{2m+2} \mu_i^{(0)} = \frac{6(2m+3)^2}{c_{m+1}} a_{m+1} ,$$

$$\sum_{i=1}^{2m+2} \mu_i^{(k)} = \frac{6(2m+3)^2}{c_{m+1}} g_k^{(m+1)} , \qquad (k = 1,2,\ldots,m+1) .$$

REMARK Since there corresponds a uniquely determined n.c.s. to each $f \in C[0,1]$, and taking into account (1.11), it follows that

$$\sum_{k=0}^{n} s^k(x) \equiv 1 .$$

This, together with (1.6) and the representation formula (1.18) for $s^k(x)$, has as a consequence that at an arbitrary node the sum of the second derivatives of the c.n.c.s. is zero, i.e.

$$\sum_{k=0}^{n} \mu_i^{(k)} = 0 , \qquad (i = 0,1,\ldots,n) ,$$

and thus (cf. table 8)

$$\sum_{k=0}^{n} \sum_{i=1}^{n-1} \mu_i^{(k)} = 0 .$$

The ultimate aim of the first part of this paper is the calculation of the weights in the numerical integration formula (1.15). This can now be accomplished by using (1.41) and the set of formulae (1.45)-(1.48). As is to be expected the calculations involved are rather lengthy and therefore omitted here. We obtain the following results.

Assume first that $n = 2m$. If, as usual, $\alpha = 2 + \sqrt{3}$ then

$$(1.49) \qquad w_0 = \frac{1}{4n} + \frac{\sqrt{3}}{12n} \frac{(\alpha^n + \alpha^{-n} - 2)}{(\alpha^n - \alpha^{-n})} ,$$

$$(1.50) \qquad w_k = \frac{1}{n} + \frac{(-1)^{k+1}}{2n} \frac{(\alpha^{\frac{n}{2}-k} + \alpha^{-\frac{n}{2}+k})}{(\alpha^{n/2} + \alpha^{-n/2})} , \qquad (k = 1,2,\dots,m) .$$

If $n = 2m + 1$, then one has

$$(1.51) \qquad w_0 = \frac{1}{4n} + \frac{\sqrt{3}}{12n} \frac{(\alpha^n + \alpha^{-n} + 2)}{(\alpha^n - \alpha^{-n})} ,$$

$$(1.52) \qquad w_k = \frac{1}{n} + \frac{(-1)^{k+1}}{2n} \frac{(\alpha^{\frac{n}{2}-k} - \alpha^{-\frac{n}{2}+k})}{(\alpha^{n/2} - \alpha^{-n/2})} , \qquad (k = 1,2,\dots,m) .$$

Apart from a normalization factor, these formulae can be proved to be identical with similar ones given by Meyers-Sard ([4], p. 121-122) and Holladay ([3], p.237-238). It is of some interest to gather together the weights for the first few values of n. This is done in table 9 (a more extensive one may be found in [4]).

	$\frac{1}{8n}$	$\frac{1}{10n}$	$\frac{1}{28n}$	$\frac{1}{38n}$	$\frac{1}{104n}$	$\frac{1}{142n}$	$\frac{1}{388n}$	$\frac{1}{530n}$	$\frac{1}{1448n}$	$\frac{1}{1978n}$
k \ n	2	3	4	5	6	7	8	9	10	11
0	3	4	11	15	41	56	153	209	571	780
1	10	11	32	43	118	161	440	601	1642	2243
2			26	37	100	137	374	511	1396	1907
3					106	143	392	535	1462	1997
4							386	529	1444	1973
5									1450	1979

Table 9

For an arbitrary value of n and k ($0 \le k \le m$) the weight w_k is equal to the product of the element in the top row of the n-th column and the entry in the k-th row and the n-th column.

We do not hesitate to say that the structure of table 9 is beautiful. As Meyers-Sard remark ([4], p. 121) there are several kinds of striking regularities. For instance, minus any entry plus four times the entry two places on its right equals the entry four places on its right. This is, in fact, relation (1.21) and shows again that it is appropriate to distinguish between n is even and n is odd. Moreover, if n is odd, say, then the difference between the entry in the second row and the entry in the first row is just $7a_m$, where a_m is defined by (1.22). A similar statement holds when n is even.

On the basis of formulae (1.49), (1.50), (1.51) and (1.52) it can be shown that the various recurrences which may be observed when n = 2,3,...,11 hold in general. This makes it possible to construct an easily applicable algorithm for the calculation of the weights (cf. also Holladay's paper). We first assume that n is even (n = 2m). Using (1.25) and (1.27) of lemma 1 we have

ALGORITHM 4

step 1

$$d_{m+1} = 4d_m - d_{m-1} \ , \quad b_{m+2} = 4b_{m+1} - b_m \ .$$

step 2

$$\beta_1^{(m+1)} = b_{m+2} + 7b_{m+1} .$$

step 3

$$\beta_{k+1}^{(m+1)} = \beta_k^{(m+1)} + (-1)^k \, 6b_{m+1-k} , \qquad (k = 1,2,\dots,m) .$$

step 4

$$w_0 = \frac{b_{m+2}}{4(m+1)d_{m+1}} , \quad w_k = \frac{\beta_k^{(m+1)}}{4(m+1)d_{m+1}} , \qquad (k = 1,2,\dots,m+1) .$$

Let now n be odd ($n = 2m + 1$). If a_i and c_i are defined as in lemma 1, then one has to apply

ALGORITHM 5

step 1

$$c_{m+1} = 4c_m - c_{m-1} , \quad a_{m+2} = 4a_{m+1} - a_m .$$

step 2

$$\gamma_1^{(m+1)} = a_{m+2} + 7a_{m+1} .$$

step 3

$$\gamma_{k+1}^{(m+1)} = \gamma_k^{(m+1)} + (-1)^k \, 6a_{m+1-k} , \qquad (k = 1,2,\dots,m) .$$

step 4

$$w_0 = \frac{a_{m+2}}{2(2m+3)c_{m+1}} , \quad w_k = \frac{\gamma_k^{(m+1)}}{2(2m+3)c_{m+1}} , \qquad (k = 1,2,\dots,m+1) .$$

REMARK Because (1.15) is exact for linear functions it follows that

$$\sum_{i=0}^{n} w_i = 1 , \quad \sum_{i=0}^{n} i w_i = n/2 .$$

Also it can be shown that for an arbitrary value of n the weights with even subscripts form an increasing sequence, whereas on the other hand $w_1 > w_3 > \dots$; moreover, $\max_i w_{2i} < \min_i w_{2i+1}$. We omit the verification of this result.

An application to numerical integration formulae

2.1. Whereas in the first part of the paper we were mainly concerned with the calculation of the c.n.c.s. and the weights w_i appearing in the integration formula (1.15), we now fix the attention to the right-hand side of (1.15). The purpose of this second part is an improvement in its definite form of the following result due to Atkinson.

THEOREM 3 ([1], p. 99) Let the nodes be equally spaced and let c_0 (= c_1) be given by (1.16). Then

$$(2.1) \qquad \frac{.0219}{n^3} < -c_0 < \frac{.0277}{n^3} .$$

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

$$\left| \int_0^1 f(x)dx - \sum_{i=0}^{n} w_i f_i \right| \le \frac{.0277}{n^3} \left| f''(0) + f''(1) \right| + \frac{.2}{n^4} \| f^{(4)} \| ,$$

where $\|f^{(4)}\| = \max\limits_{0 \le x \le 1} |f^{(4)}(x)|$. The lower bound of (2.1) implies that no greater an order than $\frac{1}{n^3}$ is possible when

$$f''(0) + f''(1) \ne 0 .$$

The derivation of this theorem (and also our improvement of it) is based upon corollary 1 of section 1.2. From this corollary we conclude that

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

$$(2.2) \qquad \le |c_0| \left| f''(0) + f''(1) \right| + \|f^{(4)}\| \int_0^1 \left| \int_0^1 L(x,t)dt \right| dx .$$

To calculate the constant c_0 we may note that it is an immediate consequence of (1.15), (1.14) and (1.17) that we have

$$c_0 = \frac{1}{4} \left\{ \frac{1}{3} - \frac{1}{n^2} \sum_{i=0}^{n} i^2 w_i \right\} ,$$

$$(2.3) \qquad c_0 = \frac{1}{6}\left\{\frac{1}{4} - \frac{1}{n^3}\sum_{i=0}^{n} i^3 w_i\right\},$$

where the weights w_i are given by formulae (1.49)-(1.52). But the expressions just exhibited for c_0 do not seem to be so suitable for calculation. *) Therefore we proceed in a different way. Using formula (1.12) for $L(x,t)$ one has

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

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

But

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

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

---

*) Atkinson shows that

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

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

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

and

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

Using this he arrives at inequality (2.1). (Actually, the lower bound of (2.1) is not valid for $n = 2$, cf. (2.15).) 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).

Using this it is then easily verified that

$$(2.4)\qquad \int_0^1 L(x,t)dt = \frac{1}{24}\left\{x^4 - 2x^3 - \sum_{i=0}^{n}(x_i^4 - 2x_i^3)s^i(x)\right\}.$$

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 (1.17) 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

$$(2.5)\qquad \int_0^1 L(x,t)dx = \frac{1}{6}\left\{- 6c_0(1-t) + \frac{1}{4}(1-t)^4 - \sum_{i=0}^{n} w_i(x_i-t)_+^3\right\}$$

because of (2.3).

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 (2.5) is equivalent to the right-hand side of (2.4) if the variable t is replaced by x. The expression in (2.4) can be regarded as the difference of the function $\frac{1}{24}(x^4 - 2x^3)$ and its interpolating n.c.s. Taking into account (2.5) 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.

2.2. Returning to (2.2), 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 $n \geq 2$. In order to calculate and estimate these numbers accurately one needs information about the function in (2.4), especially where it changes sign on [0,1]. As we already noticed the right-hand side of (2.4) can be seen as the difference of the function $\frac{1}{24}(x^4 - 2x^3)$ and its interpolating n.c.s. Because of the fact that the second derivative of $\frac{1}{24}(x^4 - 2x^3)$ 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 [8]. 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

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

the subscript $1/n$ means that we assume the nodes to be 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) $y_H(f;x_i) = f_i$, $(i = 0,1,\dots,n)$,

(iiii) $y'_H(f;x_i) = f'_i$, $(i = 0,1,\dots,n)$.

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

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

$$(x_i \le x \le x_{i+1},\ x_i < \xi_i < x_{i+1},\ 0 \le i \le n-1) .$$

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

$$(2.6) \qquad f(x) - y_{1/n}(f;x) = f(x) - y_H(f;x) + y_H(f;x) - y_{1/n}(f;x) =$$

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

Let us now take in particular $f(x) = \frac{1}{24}(x^4 - 2x^3)$ 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 (2.6) 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 [8]) 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 $[x_i, x_{i+1}]$

$$(2.7)\qquad \frac{1}{24}\left\{x^4 - 2x^3 - \sum_{i=0}^{n}(x_i^4 - 2x_i^3)s^i(x)\right\} =$$

$$= \frac{1}{24}(x - x_i)(x_{i+1} - x)\left[(x - x_i)(x_{i+1} - x) + n^2\{z_i'(x_{i+1} - x) - z_{i+1}'(x - x_i)\}\right] ,$$

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

$$(2.8)\qquad \begin{cases} 2z_0' + z_1' = \frac{1}{n^3} , \\ \frac{1}{2}z_0' + 2z_1' + \frac{1}{2}z_2' = 0 , \\ \quad\vdots \\ \frac{1}{2}z_{n-2}' + 2z_{n-1}' + \frac{1}{2}z_n' = 0 , \\ z_{n-1}' + 2z_n' = -\frac{1}{n^3} . \end{cases}$$

For the investigation of (2.7) we need the solution of the set (2.8).

<u>THEOREM 4</u> Let n be even $(n = 2m)$ and $\alpha = 2 + \sqrt{3}$. Then the unique solution of the system of linear equations (2.8) is given by

$$(2.9)\qquad \begin{cases} z_i' = \frac{(-1)^i\sqrt{3}}{3n^3}\,\frac{(\alpha^{\frac{n}{2}-i} - \alpha^{-\frac{n}{2}+i})}{(\alpha^{n/2} + \alpha^{-n/2})} , \qquad (i = 0,1,\ldots,m) , \\ \\ z_{n-i}' = -z_i' , \qquad (i = 0,1,2,\ldots,m) ; \end{cases}$$

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

$$(2.10)\quad \begin{cases} z_i' = \dfrac{(-1)^i\sqrt{3}}{3n^3}\dfrac{(\alpha^{\frac{n}{2}-i} + \alpha^{-\frac{n}{2}+i})}{(\alpha^{n/2} - \alpha^{-n/2})}, & (i = 0,1,\ldots,m), \\ z_{n-i}' = -z_i', & (i = 0,1,\ldots,m). \end{cases}$$

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 (2.8) is diagonally dominant. Assuming $n = 2m$, it is sufficient to show that the exhibited numbers z_i' of (2.9) satisfy the first m+1 equations of (2.8). 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 (2.8) 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

$$\tfrac{1}{2}z_{i-1}' + 2z_i' + \tfrac{1}{2}z_{i+1}' =$$

$$= \frac{\sqrt{3}}{48m^3(\alpha^m + \alpha^{-m})}\{\alpha^{m-i+1} - \alpha^{-m+i-1} - 4(\alpha^{m-i} - \alpha^{-m+i}) + \alpha^{m-i-1} - \alpha^{-m+i+1}\},$$

and the expression between brackets vanishes because $\alpha - 4 + \alpha^{-1} = 0$. The (m+1)-th equation of (2.8) is also satisfied because $z_m' = 0$ and $z_{m-1}' = -z_{m+1}'$. This proves theorem 4. ∎

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 2 Let the numbers z_i' $(i = 0,1,\ldots,m)$ be given by (2.9), respectively (2.10). Then the following assertions are true:

(i) when n is even, then $n^3 z_0'$ is increasing with n and

(2.11) $$\frac{1}{2n^3} \le z_0' < \frac{\sqrt{3}}{3n^3} ,$$

(ii) when n is odd, then $n^3 z_0'$ is decreasing with n and

(2.12) $$\frac{\sqrt{3}}{3n^3} < z_0' \le \frac{3}{5n^3} ,$$

(2.13) (iii) $|z_0'| \ge 3|z_1'| \ge 3^2|z_2'| \ge \ldots \ge 3^m|z_m'|$.

PROOF All three statements can be verified by elementary calculations based upon theorem 4. We omit the details. ∎

REMARK In view of (2.4) and (2.7) 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 23 this suffices for the calculation of the constant c_0 appearing in (2.2). Using (2.5), together with (2.9) and (2.10) we obtain

(2.14) $$c_0 = -\frac{1}{24} z_o' = -\frac{\sqrt{3}}{72n^3} \frac{(\alpha^n + \alpha^{-n} - 2(-1)^n)}{(\alpha^n - \alpha^{-n})} .$$

Moreover, using (2.11) and (2.12), it is a consequence of (2.14) that

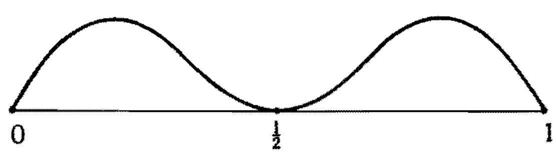
(2.15) $$\frac{1}{48n^3} \le -c_0 \le \frac{1}{40n^3} .$$

2.3. Theorem 4, together with formula (2.7), 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 (2.2) it is our purpose to give an estimate of $\int_0^1 |\int_0^1 L(x,t)dt|dx$ which holds for all positive integer values of $n \ge 2$ 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 $x = \frac{1}{2}$. This follows from (2.7) 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 (2.7) 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

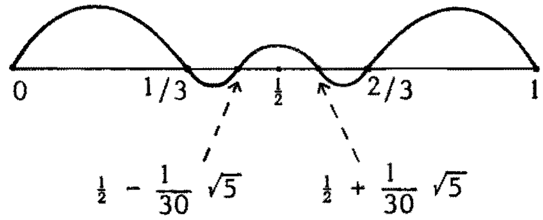
(2.16) $\quad (x - x_i)(x_{i+1} - x) + n^2[z_i'(x_{i+1} - x) - z_{i+1}'(x - x_i)]$

on the interval $[x_i, x_{i+1}]$, which occurs in (2.7). Due to symmetry we may restrict ourselves to $0 \le i \le m-1$. If i is even, then according to theorem 4 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 (2.16) is pulled down, but due to the fact that $|z_i'| < \frac{1}{5n^3}$ for $i = 1,2,\ldots,m$ (this is a consequence of lemma 2), the function remains positive when $x = \frac{1}{2}(x_i + x_{i+1})$. 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 $x = \frac{1}{2}$ 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 $\frac{1}{24}$, 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 (2.7) and theorem 4.

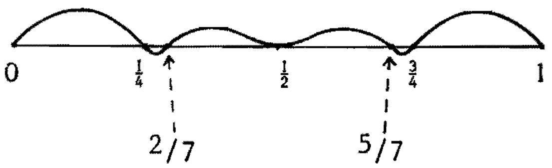
n = 2



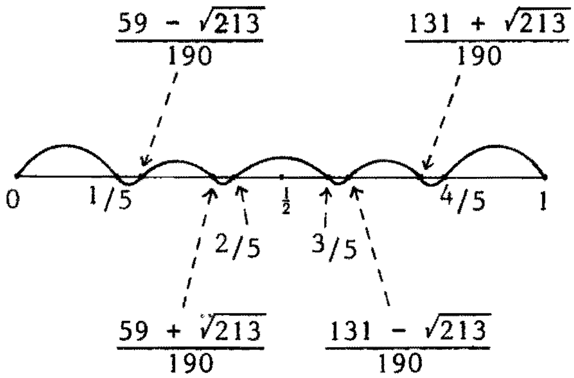
n = 3



n = 4



n = 5



Using the information provided by the pictures, formula (2.7) and theorem 4, we can evaluate 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:

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

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

(2.19) $\quad$ 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,... 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 (2.7). As a preliminary result we need the integrals

$$(2.20)\qquad \int_{x_i}^{x_{i+1}} (x - x_i)^2 (x_{i+1} - x)^2 dx = \frac{1}{30n^5},$$

$$(2.21)\qquad \int_{x_i}^{x_{i+1}} (x - x_i)(x_{i+1} - x)^2 dx = \int_{x_i}^{x_{i+1}} (x - x_i)^2 (x_{i+1} - x) dx = \frac{1}{12n^4}.$$

An estimate of $\int_0^1 \left| \int_0^1 L(x,t)dt \right| dx$ may now be derived from (2.7) as follows. Taking together all contributions to the integral over the n subintervals and using (2.20), (2.21) and theorem 4, we obtain

(2.22)

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

We will show that for an arbitrary but fixed positive integer $n \ge 5$ the right-hand side of (2.22) is smaller than $\frac{1}{320n^4}$ (cf. (2.17)). Accordingly, it is sufficient to establish that

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

Using $z_0' \le \frac{3}{5n^3}$ and taking into account (2.13) we obtain

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

$$(n \ge 5).$$

This, together with (2.18) and (2.19), shows that

$$(2.23)\qquad \int_0^1 \left| \int_0^1 L(x,t)dt \right| dx \le \frac{1}{320n^4}, \qquad (n = 2,3,4,\ldots),$$

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

2.4. Now we can state our definite result. Taking into account formula (2.2), together with (2.15) and (2.23), one has the following theorem, which is an improvement of Atkinson's result as formulated on p. 21.

THEOREM 5 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 (1.17), then for $n = 2,3,\ldots$

$$(2.24) \qquad \left| \int_0^1 f(x)dx - \sum_{i=0}^{n} w_i\, f_i \right| \le \frac{1}{40n^3} \left| f''(0) + f''(1) \right| + \frac{1}{320n^4} \|f^{(4)}\|$$

with $\|f^{(4)}\| = \max_{0 \le x \le 1} |f^{(4)}(x)|$. In this inequality the constants

$$\frac{1}{40} = 0.025$$

and

$$\frac{1}{320} = 0.003125$$

are best possible.

PROOF 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 (1.15) we obviously have

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

and it is a consequence of (2.15) that $|c_0| = \dfrac{1}{40n^3}$ when $n = 3$. So the constant $\frac{1}{40}$ in (2.24) cannot be replaced by any smaller number.

It is also easy to show that the constant $\frac{1}{320}$ in (2.24) is best possible. For this purpose take $n = 2$ and consider the function f_2 on $[0,1]$, defined by $f_2(x) = \frac{1}{24}(x^4 - 2x^3)$. 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 (2.4) is non-negative on $[0,1]$ (cf. p. 28), it follows from (1.15) and (2.17) that we have

$$\int_0^1 f_2(x)dx - \sum_{i=0}^{2} w_i\, f_2(x_i) = \frac{1}{320.2^4} \,.$$

This proves our assertion. ∎

REMARK If $f''(0) + f''(1) \neq 0$, then the first two terms in the right-hand side of formula (1.15) behave like $\frac{1}{n^3}$ as $n \to \infty$; this is a consequence of (2.15). Using (2.7) and theorem 4 it can also be shown that no greater an order than $\frac{1}{n^4}$ is possible for the last term in (1.15). We omit the details.

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