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Sard's Best Quadrature Formulas of Order Two

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1. INTRODUCTION

The concept of best quadrature was introduced by Sard in [5] and elaborated on by him in [6]. More recently Schoenberg [8] has presented a general theory of this type of quadrature and the interested reader is referred to that paper for details and further references.

The present paper is concerned with two problems which arise for second-order best quadrature formulae. The main problem is that of convergence, and it is shown, with suitable assumptions, that the formula has $O(h^{5/2})$ convergence in general and $O(h^4)$ convergence for a particular class of functions. The proof of these results utilizes in an essential fashion the Rodrigues function which was introduced by Schoenberg in [8].

Sard in [6] presents tables of the weights for his equal interval formulae together with the L_2-norm of the corresponding Peano kernels. The other objective in this paper is to give simple explicit formulas for each of these.

2. PRELIMINARY DEFINITIONS AND RESULTS

The set of real numbers $t_0, t_1, \ldots, t_N$ will be called *quadrature points* or *knots* and will satisfy

$$0 = t_0 < t_1, \ldots, < t_N = 1, \text{ where } N \geqslant 1; \text{ let } h_j = t_{j+1} - t_j,\ j = 0, 1, N-1.$$

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The *truncated power* K_n^+ is defined for $n = 1, 2, \ldots$, by

$$K_n^+(s) = s^n/n!, \qquad s \geqslant 0$$
$$= 0 \quad \text{otherwise.}$$

Let $w \in C[0, 1]$, $x \in C^2[0, 1]$. The equation

$$\int_0^1 w(t)\, x(t)\, dt = \sum_{j=0}^{N} H_j x(t_j) + R(x) \tag{2.1}$$

will be called a *best quadrature formula of second order* with *remainder* R if

(i)
$$R(x) = \int_0^1 k(t)\, x^{(2)}(t)\, dt, \tag{2.2}$$

where k is the *Peano kernel* for the quadrature formula and is given by

$$k(t) = \int_0^1 w(s)\, K_1^+(s - t)\, ds - \sum_{j=0}^{N} H_j K_1^+(t_j - t), \tag{2.3}$$

(ii) the weights $H_0, H_1, \ldots, H_N$ are chosen so as to minimize

$$\int_0^1 [k(t)]^2\, dt. \tag{2.4}$$

Clearly, from (2.1), (2.2), the weights must satisfy

$$\int_0^1 w(t)\, t^r\, dt = \sum_{j=0}^{N} H_j t_j^r, \qquad r = 0, 1. \tag{2.5}$$

Intimately connected with best quadrature formulas are *natural splines.* For second order quadrature the relevant spline is the *natural cubic spline* with the quadrature points as knots. The theory of splines is dealt with in detail in [1]; it will be sufficient to state that a natural cubic spline with the knots $t_0, t_1, \ldots, t_N$ is in $C^2(-\infty, \infty)$ and such that outside (t_0, t_N) it is linear and in each interval $(t_j, t_{j+1}), j = 0, 1, N - 1$ it is at most a cubic. It is shown in [1] that a natural cubic spline is determined uniquely by its values at the knots. Further, from [1], if y is the natural cubic spline with the knots $t_0, t_1, \ldots, t_N$, then

$$\begin{aligned} 2\lambda_0 + \lambda_1 &= 3[t_0, t_1]\, y, \\ (1 - \alpha_j)\, \lambda_{j-1} + 2\lambda_j + \alpha_j \lambda_{j+1} & \\ = 3(1 - \alpha_j)[t_{j-1}, t_j]\, y &+ 3\alpha_j[t_j, t_{j+1}]\, y, \qquad j = 1, 1, N - 1 \\ \lambda_{N-1} + 2\lambda_N &= 3[t_{N-1}, t_N]\, y, \end{aligned} \tag{2.6}$$

where, for simplicity, $\lambda_j = y^{(1)}(t_j)$, $\alpha_j = h_{j-1}/(h_{j-1} + h_j)$ and $[t_i, t_{i+1}]\,y$ denotes, in Ostrowski's notation, the first divided difference of y at the knots t_i, t_{i+1}. The *cardinal natural cubic spline* L_i is a natural cubic spline such that

$$L_i(t_j) = \delta_{ij}, \qquad j = 0, 1, N.$$

The last definition which will be made is of T_r, U_r. These are the r-th degree Chebyshev polynomials of the first and second kinds *each with argument* -2.

The following is a special case of a theorem which was proved by Schoenberg in [7] and generalized by him in [8].

THEOREM 2.1. *A best quadrature formula of second order integrates exactly any natural cubic spline which has the quadrature points as knots.*

The following is an immediate consequence of this theorem and the definition of the cardinal cubic spline.

COROLLARY 2.1.1. *The quadrature weights in* (2.1) *are given by*

$$H_i = \int_0^1 w(t)\, L_i(t)\, dt, \qquad i = 0, 1, N. \tag{2.7}$$

A less obvious result is

COROLLARY 2.1.2.

$$\int_0^1 [k(t)]^2\, dt = \int_0^1 w(t)[z(t) - y_0(t)]\, dt,$$

where

$$z(t) = \int_0^1 w(s)\, K_3{}^+(s - t)\, ds - K_3{}^+(-t) \int_0^1 (1 - s)\, w(s)\, ds - K_3{}^+(1 - t) \int_0^1 sw(s)\, ds \tag{2.8}$$

and y_0 is the natural cubic spline which agrees with z at the knots.

(The function $z - y_0$ is the Rodrigues function which was introduced in [8] by Schoenberg.)

Proof.

Let $u = z - v$ where z is defined by (2.8) and

$$v(t) = \sum_{j=0}^{N} H_j K_3{}^+(t_j - t) - K_3{}^+(-t) \int_0^1 (1 - s)\, w(s)\, ds - K_3{}^+(1 - t) \int_0^1 sw(s)\, ds.$$

It is easily verified with the aid of (2.5) that v is in fact a natural cubic spline, whence $R(v) = 0$. Further it is seen that $u^{(2)} = k$; consequently,

$$\int_0^1 [k(t)]^2\, dt = R(u) = R(z - v) = R(z).$$

It remains to take y_0 as stated in the corollary; for then, as $R(y_0) = 0$,

$$R(z) = R(z - y_0) = \int_0^1 w(t)[z(t) - y_0(t)]\, dt.$$

A proof of the next theorem will be found in [4]

THEOREM 2.2. *Let $x \in C^4[0, 1]$, and let y be the natural cubic spline such that*

$$y(t_i) = x(t_i), \qquad i = 0, 1, N.$$

If $x^{(2)}(0) = x^{(2)}(1) = 0$, then, with the uniform norm on $[0, 1]$,

$$\| x - y \| \leqslant \tfrac{3}{64} M h^4, \qquad \| x^{(2)} - y^{(2)} \| \leqslant \tfrac{3}{8} M h^2,$$

where $M = \| x^{(4)} \|$ and $h = \max(t_{i+1} - t_i)$.

The next lemma is a consequence of a result proved in [2].

LEMMA 2.1. *If $a_0, a_1, \ldots, b_{N-1}, b_N$ are numbers which satisfy*

$$\begin{aligned} 2a_0 + a_1 &= b_0, \\ a_{j-1} + 4a_j + a_{j+1} &= b_j, \qquad j = 1, 1, N - 1, \\ a_{N-1} + 2a_N &= b_N, \end{aligned}$$

then

$$a_0 = -\tfrac{1}{3} \sum_{k=0}^{N} b_k T_{N-k} / U_{N-1}, \qquad a_N = -\tfrac{1}{3} \sum_{k=0}^{N} b_k T_k / U_{N-1}.$$

The final result which will be needed will now be proved.

LEMMA 2.2. *If $p(t) = [(1 - t)^3 a_0 + t^3 a_N]/6$, and if z is the natural cubic spline which agrees with z at the knots, then*

$$\int_0^1 [p^{(2)}(t) - z^{(2)}(t)]^2\, dt < \tfrac{1}{3}\{h_0 a_0^2 + h_{N-1} a_N^2 + (h_0 + h_{N-1}) \mid a_0 a_N \mid 2^{-N}\}.$$

Proof. Two careful integration by parts shows that

$$\int_0^1 [p^{(2)}(t) - z^{(2)}(t)]^2\, dt = a_N[p^{(1)}(1) - z^{(1)}(1)] - a_0[p^{(1)}(0) - z^{(1)}(0)]. \quad (2.9)$$

Let $z^{(1)}(t_j) = \lambda_j$, $p^{(1)}(t_j) = \pi_j$, $j = 0, 1, N$, and so $p^{(1)}(1) = \pi_N$, $p^{(1)}(0) = \pi_0$. Now (2.6) can be rewritten

$$2(\lambda_0 - \pi_0) + (\lambda_1 - \pi_1) = \tfrac{1}{2}h_0 a_0$$

$$(1 - \alpha_j)(\lambda_{j-1} - \pi_{j-1}) + 4(\lambda_j - \pi_j) + \alpha_j(\lambda_{j+1} - \pi_{j+1}) = 0, \ \ j = 1, 1, N-1,$$

$$(\lambda_{N-1} - \pi_{N-1}) + 2(\lambda_N - \pi_N) = -\tfrac{1}{2}h_{N-1}a_N .$$

The use of a result in [3] produces the inequalities

$$| \lambda_0 - \pi_0 | < \tfrac{1}{3}[h_0 \mid a_0 \mid + h_{N-1} \mid a_N \mid 2^{-N}],$$

$$| \lambda_N - \pi_N | < \tfrac{1}{3}[h_0 \mid a_0 \mid 2^{-N} + h_{N-1} \mid a_N \mid].$$

The proof of the lemma is completed by inserting these inequalities in (2.9).

3. Equal Interval Quadrature

In this section it will be assumed that

$$w(t) = 1, \ 0 \leqslant t \leqslant 1, \text{ and } t_i = ih, \ i = 0, 1, N, \text{ where } h = 1/N. \quad (3.1)$$

THEOREM 3.1.

(i) $H_0 = H_N = \tfrac{1}{4}h[1 + \tfrac{1}{3}(1 - T_N)/U_{N-1}]$,

(ii) $H_i = h[1 - \tfrac{1}{2}(U_{i-1} + U_{N-i-1})/U_{N-1}]$, $\quad i = 1, 1, N-1$,

(iii) $\displaystyle\int_0^1 [k(t)]^2\, dt = \tfrac{1}{144}h^4[\tfrac{1}{5} + \tfrac{1}{3}h(1 - T_N)/U_{N-1}]$.

Proof. If y is a natural cubic spline with the knots defined by (3.1) then, from the Euler–Maclaurin sum formula,

$$\int_0^1 y(t)\, dt = h\left[\tfrac{1}{2}y(0) + \sum_{j=1}^{N-1} y(jh) + \tfrac{1}{2}y(1)\right] - \tfrac{1}{12}h^2[y^{(1)}(t)]_0^1 , \quad (3.2)$$

whence, when $y = L_0$, it follows that

$$H_0 = \tfrac{1}{2}h - \tfrac{1}{12}h^2[L_0^{(1)}(1) - L_0^{(1)}(0)]. \quad (3.3)$$

For simplicity let $\lambda_j = L_0^{(1)}(jh)$, then from (2.6) with $\alpha_j = \tfrac{1}{2}, j = 1, 1, N-1$,

$$\begin{aligned} 2\lambda_0 + \lambda_1 &= -3/h, \qquad \lambda_0 + 4\lambda_1 + \lambda_2 = -3/h, \\ \lambda_{i-1} + 4\lambda_i + \lambda_{i+1} &= 0, \qquad i = 2, 1, N-1, \\ \lambda_{N-1} + 2\lambda_N &= 0. \end{aligned} \quad (3.4)$$

These equations can be solved for λ_0, λ_N, by the use of Lemma 2.1, to give

$$\lambda_0 = (T_N + T_{N-1})/(hU_{N-1}), \qquad \lambda_N = (T_0 + T_1)/(hU_{N-1}).$$

When these are substituted in (3.3) the expression for H_0 will be obtained after some simple manipulation. By symmetry, $H_N = H_0$.

The calculation of H_i, $i = 1, 1, N - 1$ proceeds in the same fashion and will not be given.

In order to prove (iii) use will be made again of the Euler–Maclaurin formula. From corollary 2.1.2 it is necessary to calculate

$$\int_0^1 [z(t) - y_0(t)]\, dt, \tag{3.5}$$

where

$$z(t) = (1 - t)^4/24 - (1 - t)^3/12 = (t^4 - 2t^3 + 2t - 1)/24 \tag{3.6}$$

and y_0 is the natural cubic spline which agrees with z at the quadrature points. It follows with the use of the Euler–Maclaurin sum formula that

$$\int_0^1 [z(t) - y_0(t)]\, dt = -\frac{h^2}{12} [z^{(1)}(t) - y_0^{(1)}(t)]_0^1 + h^4/720. \tag{3.7}$$

Let, for convenience, $\lambda_i = y_0^{(1)}(t_i)$, $\zeta_i = z^{(1)}(t_i)$, $i = 0, 1, N$. Then it is easily verified that (2.6) can be written (again $\alpha_j = \frac{1}{2}$) as

$$\begin{aligned}
&2(\zeta_0 - \lambda_0) + (\zeta_1 - \lambda_1) = h^3/24,\\
&(\zeta_{j-1} - \lambda_{j-1}) + 4(\zeta_j - \lambda_j) + (\zeta_{j+1} - \lambda_{j+1}) = 0, \qquad j = 1, 1, N - 1,\\
&(\zeta_{N-1} - \lambda_{N-1}) + 2(\zeta_N - \lambda_N) = -h^3/24.
\end{aligned}$$

Whence, with the use of Lemma 2.1,

$$72(\zeta_0 - \lambda_0) = h^3(1 - T_N)/U_{N-1} \text{ and } 72(\zeta_N - \lambda_N) = h^3(T_N - 1)/U_{N-1}.$$

The result follows when these are substituted in (3.7).

COROLLARY 3.1.1.

$$H_i > 0, \qquad i = 0, 1, N, \qquad \int_0^1 [k(t)]^2\, dt = O(h^4) \qquad \text{as} \quad h \to 0.$$

The proof is straightforward and is omitted, as is the proof of the next result.

COROLLARY 3.1.2.

$$H_{i-1} + 4H_i + H_{i+1} = 6h, \qquad i = 2, 1, N-2. \tag{3.8}$$

This provides an alternative method for calculating the internal quadrature weights. For it is easy to see that

$$4H_1 + H_2 = 11h/2 = H_{N-2} + 4H_{N-1}.$$

Thus if these equations are adjoined to (3.8) the result will be a tridiagonal set of linear algebraic equations for $H_1, \ldots, H_{N-1}$. When these have been calculated, H_0, H_N can be found from

$$H_0 = H_N = [7h - 2H_1]/12.$$

4. CONVERGENCE

The general second order quadrature formula (2.1) will be considered in this section and the quadrature points will be required to satisfy only

$$0 = t_0 < t_1 < \cdots < t_N = 1.$$

The norms which will be used are defined by

$$\| \cdot \| = \max_{0 \leqslant t \leqslant 1} | \cdot |, \qquad \| \cdot \|_2^2 = \int_0^1 | \cdot |^2 \, dt.$$

LEMMA 4.1. $\int_0^1 [k(t)]^2 \, dt = 3h^4 \| w \|^2/64.$

Proof. From Corollary 2.1.2,

$$\int_0^1 [k(t)]^2 \, dt \leqslant \| w \| \cdot \| z - y_0 \|.$$

Now it is easily verified that $z^{(2)}(0) = z^{(2)}(1) = 0$ (in fact this property was built in to z). Thus, from Theorem 2.2,

$$\| z - y_0 \| \leqslant \tfrac{3}{64} h^4 \| z^{(4)} \| = 3h^4 \| w \|/64.$$

The result follows.

The convergence of Sard's second order best quadrature formula can now be proved

THEOREM 4.1. *If* $x \in C^4[0, 1]$, $M = \| x^{(4)} \|$ *and* R *is the remainder given by* (2.2), *then* $| R(x)| \leqslant Kh^{5/2}$, *where* K *is a constant.*

Proof. Let p be as in Lemma 2.2 with $a_0 = x^{(2)}(0)$, $a_N = x^{(2)}(1)$.
Now

$$R(x) = R(x - p) + R(p) = R(x - p - y) + R(p - z), \tag{4.1}$$

where y and z are the natural cubic splines which agree with $x - p$ and p, respectively, at the quadrature points. Hence, with the use of Schwartz's inequality the following inequality holds:

$$| R(x)| \leqslant | R(x - p - y)| + | R(p - z)| ,$$

which gives

$$| R(x)| \leqslant \| k \|_2 [\| x^{(2)} - p^{(2)} - y^{(2)} \|_2 + \| p^{(2)} - z^{(2)} \|_2]. \tag{4.2}$$

But

$$x^{(2)}(0) - p^{(2)}(0) = x^{(2)}(1) - p^{(2)}(1) = 0;$$

consequently from Theorem 2.2,

$$\| x^{(2)} - p^{(2)} - y^{(2)} \| \leqslant \tfrac{3}{8}Mh^2. \tag{4.3}$$

Further, Lemma 2.2 gives

$$\begin{aligned} \| p^{(2)} - z^{(2)} \|_2^2 \leqslant \tfrac{1}{3}[h_0 \, | x^{(2)}(0)|^2 &+ h_{N-1} \, | x^{(2)}(1)|^2 \\ &+ (h_0 + h_{N-1}) \, | x^{(2)}(0) \, x^{(2)}(1)| \, 0.2^{-N}]. \end{aligned} \tag{4.4}$$

It remains to note that

$$\| \cdot \|_2 \leqslant \| \cdot \| ,$$

then the insertion of (4.3), (4.4) in (4.2) together with the result of Lemma 4.1 completes the proof of the theorem.

COROLLARY 4.1.

If, in addition, $x^{(2)}(0) = x^{(2)}(1) = 0$, *then*

$$| R(x)| \leqslant \frac{3\sqrt{3}}{64} M \cdot \| w \| \, h^4.$$

This follows from the proof of the theorem with (4.2) replaced by

$$| R(x)| \leqslant \| k \|_2 \cdot \| x^{(2)} - p^{(2)} - y^{(2)} \|_2 .$$

5. Remarks

It is clear from the proof of convergence that the Rodrigues function was essential to the argument. A systematic use of this function together with convergence estimates for generalized splines should provide a simple way of proving the convergence of the optimum quadrature formulae discussed in [8].

References

1. J. H. Ahlberg, E. N. Nilson, and J. L. Walsh, "The Theory of Splines and Their Applications," Academic Press, New York, 1967.
2. D. Kershaw, The explicit inverses of two commonly occurring matrices, *Math. Comp.* **23** (1969), 189–191.
3. D. Kershaw, Inequalities on the elements of the inverse of a certain tridiagonal matrix, *Math. Comp.* **24** (1970), 155–158.
4. D. Kershaw, A note on the convergence of interpolatory cubic splines, *SIAM J. Numer. Anal.* **8** (1971), 67–74.
5. A. Sard, Best approximate integration formulas; best approximation formulas, *Amer. J. Math.* **71** (1949), 80–91.
6. A. Sard, "Linear Approximation," American Mathematical Society, Providence, RI, 1963.
7. I. J. Schoenberg, Spline interpolation and best quadrature formulae, *Bull. Amer. Math. Soc.* **70** (1964), 143–148.
8. J. Schoenberg, A second look at approximate quadrature formulae and spline interpolation, *Advances in Math.* **4** (1970), 277–300.