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SOME PROBLEMS ON OPTIMAL QUADRATURE

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Dedicated to Professor D. D. Stancu on his 80^{th} birthday

Abstract. Using the connection between optimal approximation of linear operators and spline interpolation established by I. J. Schoenberg [35], the φ-function method of D. V. Ionescu [17], and a more general method given by A. Ghizzetti and A. Ossicini [14], the one-to-one correspondence between the monosplines and quadrature formulas given by I. J. Schoenberg [36, 37], and the minimal norm property of orthogonal polynomials, the authors study optimal quadrature formulas in the sense of Sard [33] and in the sense of Nikolski [27], respectively, with respect to the error criterion. Many examples are given.

1. **Introduction**

Optimal quadrature rules with respect to some given criterion represent an important class of quadrature formulas.

The basic optimality criterion is the error criterion. More recently the efficiency criterion has also been used, which is based on the approximation order of the quadrature rule and its computational complexity.

Next, the error criterion will be used.

Let

$$\Lambda = \left\{ \lambda_i \mid \lambda_i \colon H^{m,2}\left[a,b\right] \to \mathbb{R},\ i=\overline{1,N} \right\} \tag{1.1}$$

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be a set of linear functionals and for $f \in H^{m,2}[a,b]$, let

$$\Lambda(f) = \left\{\lambda_i(f) \mid i = \overline{1,N}\right\} \tag{1.2}$$

be the set of information on f given by the functionals of Λ.

Remark 1.1. *Usually, the information $\lambda_i(f)$, $i = \overline{1,N}$, are the pointwise evaluations of f or some of its derivatives at distinct points $x_i \in [a,b]$, $i = \overline{0,n}$, i.e. the pointwise information.*

For $f \in H^{m,2}[a,b]$, one considers the quadrature formula

$$\int_a^b w(x) f(x)\, dx = Q_N(f) + R_N(f), \tag{1.3}$$

where

$$Q_N(f) = \sum_{i=1}^{N} A_i \lambda_i(f),$$

$R_N(f)$ is the remainder, w is a weight function and $\boldsymbol{A} = (A_1, \ldots, A_N)$ are the coefficients. If $\lambda_i(f)$, $i = \overline{1,N}$, represent pointwise information, then $\boldsymbol{X} = (x_0, \ldots, x_n)$ are the quadrature nodes.

Definition 1.1. *The number $r \in \mathbb{N}$ with the property that $Q_N(f) = f$ (or $R_N(f) = 0$) for all $f \in \mathcal{P}_r$ and that there exists $g \in \mathcal{P}_{r+1}$ such that $Q_N(g) \neq g$, (or $R_N(g) \neq 0$) where $\mathcal{P}_s$ is the set of polynomial functions of degree at most s, is called* the degree of exactness *of the quadrature rule Q_N (quadrature formula (1.3)) and is denoted by $\operatorname{dex}(Q_N)$ $(\operatorname{dex}(Q_N) = r)$.*

The problem with a quadrature formula is to find the quadrature parameters (coefficients and nodes) and to evaluate the corresponding remainder (error).

Let

$$E_N(f, \boldsymbol{A}, \boldsymbol{X}) = |R_N(f)|$$

be the quadrature error.

Definition 1.2. *If for a given $f \in H^{m,2}[a,b]$, the parameters $\boldsymbol{A}$ and $\boldsymbol{X}$ are found from the conditions that $E_N(f, \boldsymbol{A}, \boldsymbol{X})$ takes its minimum value, then the quadrature formula is called* locally optimal *with respect to the error.*

If $\boldsymbol{A}$ *and* $\boldsymbol{X}$ *are obtained such that*

$$E_N\left(H^{m,2}[a,b],\boldsymbol{A},\boldsymbol{X}\right)=\sup_{f\in H^{m,2}[a,b]}E_N\left(f,\boldsymbol{A},\boldsymbol{X}\right)$$

takes its minimum value, the quadrature formula is called globally optimal *on the set* $H^{m,2}[a,b]$*, with respect to the error.*

Remark 1.2. *Some of the quadrature parameters can be fixed from the beginning. Such is the case, for example, with quadrature formulas with uniformly spaced nodes or with equal coefficients. Also, the quadrature formulas with a prescribed degree of exactness are frequently considered.*

Subsequently we will study the optimality problem for some classes of quadrature formulas with pointwise information $\lambda_i(f)$, $i=\overline{1,N}$.

2. **Optimality in the sense of Sard**

Suppose that Λ is a set of Birkhoff-type functionals

$$\Lambda:=\Lambda_B=\left\{\lambda_{kj}\mid\lambda_{kj}(f)=f^{(j)}(x_k),\ k=\overline{0,n},\ j\in I_k\right\},$$

where $x_k\in[a,b]$, $k=\overline{0,n}$, and $I_k\subset\{0,1,\ldots,r_k\}$, with $r_k\in\mathbb{N}$, $r_k<m$, $k=\overline{0,n}$.

For $f\in H^{m,2}[a,b]$ and for fixed nodes $x_k\in[a,b]$, $k=\overline{0,n}$, (for example, uniformly spaced nodes), consider the quadrature formula

$$\int_a^b f(x)\,dx=\sum_{k=0}^{n}\sum_{j\in I_k}A_{kj}f^{(j)}(x_k)+R_N(f). \tag{2.1}$$

Definition 2.1. *The quadrature formula* (2.1) *is said to be* optimal in the sense of Sard *if*

(i) $R_N(e_i)=0,\quad i=\overline{0,m-1},\quad$ with $e_i(x)=x^i$,

(ii) $\displaystyle\int_a^b K_m^2(t)\,dt$ is minimum,

where K_m *is Peano's kernel, i.e.*

$$K_m(t):=R_N\left[\frac{(\cdot-t)_+^{m-1}}{(m-1)!}\right]=\frac{(b-t)^m}{m!}-\sum_{k=0}^{n}\sum_{j\in I_k}A_{kj}\frac{(x_k-t)_+^{m-j-1}}{(m-j-1)!}.$$

Such formulas for uniformly spaced nodes ($x_k = a + kh$, $h = (b - a)/n$) and for Lagrange-type functionals, $\lambda_k(f) = f(x_k)$, $k = \overline{0,n}$, were first studied by A. Sard [32] and L. S. Meyers and A. Sard [24], respectively.

In 1964, I. J. Schoenberg [34, 35] has established a connection between optimal approximation of linear operators (including definite integral operators) and spline interpolation operators. For example, if S is the natural spline interpolation operator with respect to the set Λ and

$$f = Sf + Rf$$

is the corresponding spline interpolation formula, then the quadrature formula

$$\int_a^b f(x)\,dx = \int_a^b (Sf)(x)\,dx + \int_a^b (Rf)(x)\,dx \tag{2.2}$$

is optimal in the sense of Sard.

More specifically, let us suppose that the uniqueness condition of the spline operator is satisfied and that

$$(Sf)(x) = \sum_{k=0}^{n} \sum_{j \in I_k} s_{kj}(x)\, f^{(j)}(x_k),$$

where s_{kj}, $k = \overline{0,n}$, $j \in I_k$, are the cardinal splines and S is the corresponding spline operator. Then the optimal quadrature formula (2.2) becomes

$$\int_a^b f(x)\,dx = \sum_{k=0}^{n} \sum_{j \in I_k} A_{kj}^{\star} f^{(j)}(x_k) + R^{\star}(f),$$

with

$$A_{kj}^{\star} = \int_a^b s_{kj}(x)\,dx, \quad k = \overline{0,n}, \quad j \in I_k,$$

and

$$R^{\star}(f) = \int_a^b (Rf)(x)\,dx.$$

Example 2.1. *Let $f \in H^{2,2}[0,1]$ and let the set of Birkhoff-type functionals $\Lambda_B(f) = \left\{f'(0), f\left(\frac{1}{4}\right), f\left(\frac{3}{4}\right), f'(1)\right\}$ be given. Also, let*

$$\begin{aligned}(S_4 f)(x) = s_{01}(x) f'(0) + s_{10}(x) f\left(\frac{1}{4}\right) \\ + s_{20}(x) f\left(\frac{3}{4}\right) + s_{31}(x) f'(1),\end{aligned}$$

be the corresponding cubic spline interpolation function, where s_{01}, s_{10}, s_{20} and s_{31} are the cardinal splines. For the cardinal splines, we have

$$\begin{aligned}
s_{01}(x) =& -\frac{11}{64} + x - \frac{5}{4}(x-0)_+^2 + \left(x-\frac{1}{4}\right)_+^3 - \left(x-\frac{3}{4}\right)_+^3 \\
& - \frac{1}{4}(x-1)_+^2, \\
s_{10}(x) =& \frac{19}{16} - 3(x-0)_+^2 + 4\left(x-\frac{1}{4}\right)_+^3 - 4\left(x-\frac{3}{4}\right)_+^3 \\
& - 3(x-1)_+^2, \\
s_{20}(x) =& -\frac{3}{16} + 3(x-0)_+^2 - 4\left(x-\frac{1}{4}\right)_+^3 + 4\left(x-\frac{3}{4}\right)_+^3 \\
& + 3(x-1)_+^2, \\
s_{31}(x) =& \frac{1}{64} - \frac{1}{4}(x-0)_+^2 + \left(x-\frac{1}{4}\right)_+^3 - \left(x-\frac{3}{4}\right)_+^3 - \frac{5}{4}(x-1)_+^2,
\end{aligned}$$

while the remainder is

$$(R_4 f)(x) = \int_0^1 \varphi_2(x,t) f''(t)\, dt,$$

with

$$\varphi_2(x,t) = (x-t)_+ - \left(\frac{1}{4}-t\right)_+ s_{10}(x) - \left(\frac{3}{4}-t\right)_+ s_{20}(x) - s_{31}(x).$$

It follows that the optimal quadrature formula is given by

$$\int_0^1 f(x)\, dx = A_{01}^\star f'(0) + A_{10}^\star f\left(\frac{1}{4}\right) + A_{20}^\star f\left(\frac{3}{4}\right) + A_{31}^\star f'(1) + R_4^\star(f),$$

where

$$A_{01}^\star = -\frac{1}{96}, \quad A_{10}^\star = \frac{1}{2}, \quad A_{20}^\star = \frac{1}{2}, \quad A_{31}^\star = \frac{1}{96},$$

and

$$R_4^\star(f) = \int_0^1 K_2^\star(t)\, f''(t)\, dt,$$

with

$$\begin{aligned} K_2^\star(t) &:= \int_0^1 \varphi_2(x,t)\, dx \\ &= \frac{1}{2}(1-t)^2 - \frac{1}{2}\left(\frac{1}{4}-t\right)_+ - \frac{1}{2}\left(\frac{3}{4}-t\right)_+ - \frac{1}{96}\,. \end{aligned}$$

Finally, we have

$$\left|R_4^\star(f)\right| \le \|f''\|_2 \left(\int_0^1 \left[K_2^\star(t)\right]^2 dt\right)^{\frac{1}{2}}$$

i.e.

$$\left|R_4^\star(f)\right| \leqslant \frac{1}{48\sqrt{5}}\, \|f''\|_2\,.$$

3. **Optimality in the sense of Nikolski**

Suppose now, that all the parameters of the quadrature formula (2.1) (the coefficients $\boldsymbol{A}$ and the nodes $\boldsymbol{X}$) are unknown.

The problem is to find the coefficients $\boldsymbol{A}^\star$ and the nodes $\boldsymbol{X}^\star$ such that

$$E_n(f, \boldsymbol{A}^\star, \boldsymbol{X}^\star) = \min_{\boldsymbol{A},\boldsymbol{X}} E_n(f, \boldsymbol{A}, \boldsymbol{X})$$

for local optimality, or

$$E_n\left(H^{m,2}[a,b], \boldsymbol{A}^\star, \boldsymbol{X}^\star\right) = \min_{\boldsymbol{A},\boldsymbol{X}} \sup_{f\in H^{m,2}[a,b]} E_n(f, \boldsymbol{A}, \boldsymbol{X})$$

in the global optimality case.

Definition 3.1. *The quadrature formula with the parameters $\boldsymbol{A}^\star$ and $\boldsymbol{X}^\star$ is called* optimal in the sense of Nikolski *and $\boldsymbol{A}^\star$, $\boldsymbol{X}^\star$ are called* optimal coefficients *and* optimal nodes*, respectively.*

Remark 3.1. *If $f \in H^{m,2}[a,b]$ and the degree of exactness of the quadrature formula (2.1) is $r-1$ ($r < m$) then by Peano's theorem, one obtains*

$$R_N(f) = \int_a^b K_r(t)\, f^{(r)}(t)\, dt, \tag{3.1}$$

where

$$K_r(t) = \frac{(b-t)^r}{r!} - \sum_{k=0}^{n} \sum_{j \in I_k} A_{kj} \frac{(x_k - t)_+^{r-j-1}}{(r-j-1)!}.$$

From (3.1), *one obtains*

$$|R_N(f)| \leqslant \left\| f^{(r)} \right\|_2 \left(\int_a^b K_r^2(t)\, dt \right)^{\frac{1}{2}}. \tag{3.2}$$

It follows that the optimal parameters $\boldsymbol{A}^\star$ and $\boldsymbol{X}^\star$ are those which minimize the functional

$$F(\boldsymbol{A}, \boldsymbol{X}) = \int_a^b K_r^2(t)\, dt.$$

There are many ways to find the functional F.

1. One of them is described above and is based on Peano's theorem.

Remark 3.2. *In this case, the quadrature formula is assumed to have degree of exactness* $r-1$.

2. Another approach is based on the φ-function method [17].

Suppose that $f \in H^{r,2}[a,b]$ and that $a = x_0 < \ldots < x_n = b$. On each interval $[x_{k-1}, x_k]$, $k = \overline{1,n}$, consider a function φ_k, $k = \overline{1,n}$,, with the property that

$$D^r \varphi_k := \varphi_k^{(r)} = 1, \quad k = \overline{1,n}. \tag{3.3}$$

We have

$$\int_a^b f(x)\, dx = \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} \varphi_k^{(r)}(x) f(x)\, dx.$$

Using the integration by parts formula, one obtains

$$\begin{aligned} \int_a^b f(x)\, dx = \sum_{k=1}^{n} \Bigg\{ & \left[\varphi_k^{(r-1)} f - \varphi_k^{(r-2)} f' + \cdots + (-1)^{r-1} \varphi_k f^{(r-1)} \right] \Bigg|_{x_{k-1}}^{x_k} \\ & + (-1)^r \int_{x_{k-1}}^{x_k} \varphi_k(x) f^{(r)}(x)\, dx \Bigg\} \end{aligned}$$

and subsequently,

$$\begin{aligned}\int_a^b f(x)dx = &\sum_{j=1}^{r} (-1)^j \varphi_1^{(r-j)}(x_0) f^{(j-1)}(x_0) \\ &+ \sum_{k=1}^{n-1}\sum_{j=1}^{r} (-1)^{j-1} (\varphi_k - \varphi_{k+1})^{(r-j)}(x_k) f^{(j-1)}(x_k) \\ &+ \sum_{j=1}^{r} (-1)^{j-1} \varphi_n^{(r-j)}(x_n) f^{(j-1)}(x_n) \\ &+ (-1)^r \int_a^b \varphi(x) f^{(r)}(x)\, dx,\end{aligned} \tag{3.4}$$

where

$$\varphi\Big|_{[x_{k-1},x_k]} = \varphi_k, \quad k = \overline{1,n}. \tag{3.5}$$

For

$$\begin{aligned}(-1)^j \varphi_1^{(r-j)}(x_0) &= \begin{cases} A_{0j}, & j \in I_0, \\ 0, & j \in J_0, \end{cases} \\ (-1)^{j-1} (\varphi_k - \varphi_{k+1})^{(r-j)}(x_k) &= \begin{cases} A_{kj}, & j \in I_k, \\ 0, & j \in J_k, \end{cases} \\ (-1)^{j-1} \varphi_n^{(r-j)}(x_n) &= \begin{cases} A_{nj}, & j \in I_n, \\ 0, & j \in J_n, \end{cases}\end{aligned} \tag{3.6}$$

with $J_k = \{0, 1, \ldots, r_k\} \setminus I_k$, formula (3.4) becomes the quadrature formula (2.1), with the remainder

$$R_N(f) = (-1)^r \int_a^b \varphi(x) f^{(r)}(x)\, dx.$$

It follows that

$$K_r = (-1)^r \varphi$$

and

$$F(\boldsymbol{A}, \boldsymbol{X}) = \int_a^b \varphi^2(x)\, dx.$$

Remark 3.3. *From* (3.3)*, it follows that* φ_k *is a polynomial of degree* $r : \varphi_k(x) = \frac{x^r}{r!} + P_{r-1,k}(x)$*, with* $P_{r-1,k} \in \mathcal{P}_{r-1}$, $k = \overline{1,n}$*, satisfying the conditions of* (3.6)*.*

Example 3.1. *Let* $f \in H^{2,2}[0,1]$, $\Lambda(f) = \left\{ f(x_k) \mid k = \overline{0,n} \right\}$, *with* $0 = x_0 < x_1 < \cdots < x_{n-1} < x_n = 1$, *and let*

$$\int_0^1 f(x)\,dx = \sum_{k=0}^{n} A_k f(x_k) + R_n(f) \tag{3.7}$$

be the corresponding quadrature formula. Find the functional $F(\boldsymbol{A}, \boldsymbol{X})$, *where* $\boldsymbol{A} = (A_0, \ldots, A_n)$ *and* $\boldsymbol{X} = (x_0, \ldots, x_n)$.

Using the φ*-function method, on each interval* $[x_{k-1}, x_k]$ *one considers a function* φ_k, *with* $\varphi_k'' = 1$.

Formula (3.4) *becomes*

$$\begin{aligned}
\int_0^1 f(x)\,dx = &-\varphi_1'(0) f(0) + \sum_{k=1}^{n-1} \left(\varphi_k' - \varphi_{k+1}'\right)(x_k) f(x_k) \\
&+ \varphi_n'(1) f(1) + \varphi_1(0) f'(0) \\
&- \sum_{k=1}^{n-1} (\varphi_k - \varphi_{k+1})(x_k) f'(x_k) - \varphi_n(1) f'(1) \\
&+ \int_0^1 \varphi(x) f''(x)\,dx.
\end{aligned} \tag{3.8}$$

Now, for

$$\begin{aligned}
&\varphi_1'(0) = -A_0,\ \left(\varphi_k' - \varphi_{k+1}'\right)(x_k) = A_k,\ k = \overline{1, n-1},\ \varphi_n'(1) = A_n, \\
&\varphi_1(0) = 0, \qquad \varphi_k(x_k) = \varphi_{k+1}(x_k),\ k = \overline{1, n-1},\ \varphi_n(1) = 0,
\end{aligned} \tag{3.9}$$

formula (3.8) *becomes the quadrature formula of* (3.7)*.*

From the conditions $\varphi_k'' = 1$, $k = \overline{1,n}$, *and using* (3.9), *it follows that*

$$\begin{aligned}
\varphi_1(x) &= \frac{x^2}{2} - A_0 x,\\
\varphi_2(x) &= \frac{x^2}{2} - A_0 x - A_1(x - x_1),\\
&\vdots\\
\varphi_n(x) &= \frac{x^2}{2} - A_0 x - A_1(x - x_1) - \cdots - A_{n-1}(x - x_{n-1}).
\end{aligned}$$

Finally, we have

$$F(\boldsymbol{A}, \boldsymbol{X}) = \int_0^1 \varphi^2(x)\,dx = \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} \varphi_k^2(x)\,dx$$

or

$$F(\boldsymbol{A}, \boldsymbol{X}) = \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} \left[\frac{x^2}{2} - x\sum_{i=0}^{k-1} A_i + \sum_{i=1}^{k-1} A_i x_i\right]^2 dx.$$

Remark 3.4. *A generalization of the* φ*-function method was given in the book of A. Ghizzetti and A. Ossicini* [14], *where a more general linear differential operator of order* r *is used instead of the differential operator* D^r.

3. A third method was given by I. J. Schoenberg [36, 37, 38] and it uses the one-to-one correspondence between the set of so called monosplines

$$M_r(x) = \frac{x^r}{r!} + \sum_{k=0}^{n} \sum_{j\in I_k} A_{kj}(x - x_k)_+^j$$

and the set of quadrature formulas of the form (2.1), with degree of exactness $r-1$.

The one-to-one correspondence is described by the relations

$$\begin{aligned}
A_{0j} &= (-1)^{j+1} M_r^{(r-j-1)}(x_0), \quad j \in I_0,\\
A_{kj} &= (-1)^j \left[M_r^{(r-j-1)}(x_k - 0) - M_r^{(r-j-1)}(x_k + 0)\right], k = \overline{1, n-1}, j \in I_k,\\
A_{nj} &= (-1)^{j+1} M_r^{(r-j-1)}(x_n), \quad j \in I_n,
\end{aligned}$$

and the remainder is given by

$$R_N(f) = (-1)^r \int_a^b M_r(x) f^{(r)}(x)\, dx.$$

So

$$F(\boldsymbol{A}, \boldsymbol{X}) = \int_a^b M_r^2(x)\, dx.$$

In fact, there is a close relationship between monosplines and φ-functions.

Remark 3.5. *One of the advantages of the φ-function method is that the* degree of exactness *condition is not necessary, it follows from the remainder representation*

$$R_N(f) = (-1)^r \int_a^b \varphi(x) f^{(r)}(x)\, dx.$$

3.1. **Solutions for the optimality problem.** In order to obtain an optimal quadrature formula, in the sense of Nikolski, we have to minimize the functional $F(\boldsymbol{A}, \boldsymbol{X})$.

1. A two-step procedure

First step. The functional $F(\boldsymbol{A}, \boldsymbol{X})$ is minimized with respect to the coefficients, the nodes being considered fixed. For this, we use the relationship with spline interpolation.

So let

$$f = Sf + Rf$$

be the spline interpolation formula with $\boldsymbol{X} = (x_0, \ldots, x_n)$ the interpolation nodes. If

$$(Sf)(x) = \sum_{k=0}^{n} \sum_{j \in I_k} s_{kj}(x) f^{(j)}(x_k)$$

is the interpolation spline function, then

$$\overline{A}_{kj} := \overline{A}_{kj}(x_0, \ldots, x_n) = \int_a^b s_{kj}(x)\, dx, \quad k = \overline{0, n}, \;\; j \in I_k,$$

are the corresponding optimal (in the sense of Sard) coefficients for the fixed nodes $\boldsymbol{X}$ and

$$\overline{R}_N(f) = \int_a^b (Rf)(x)\, dx$$

is the remainder. So

$$\overline{R}_N(f) = \int_a^b \overline{K}_r(t) f^{(r)}(t)\, dt,$$

with

$$\overline{K}_r(t) = \frac{(b-t)^r}{r!} - \sum_{k=0}^{n} \sum_{j \in I_k} \overline{A}_{kj} \frac{(x_k - t)_+^{r-j-1}}{(r-j-1)!}.$$

Second step. The functional

$$F\left(\overline{\boldsymbol{A}}, \boldsymbol{X}\right) := \int_a^b \overline{K}_r^2(t)\, dt$$

is minimized with respect to the nodes $\boldsymbol{X}$.

Let $\boldsymbol{X}^\star = (x_0^\star, \ldots, x_n^\star)$ be the minimum point of $F\left(\overline{\boldsymbol{A}}, \boldsymbol{X}\right)$, i.e. the optimal nodes of the quadrature formula. It follows that $A_{kj}^\star := \overline{A}_{kj}(x_0^\star, \ldots, x_n^\star)$, $k = \overline{0,n}$, $j \in I_k$, are the optimal coefficients and that

$$R_N^\star(f) = \int_a^b K_r^\star(t) f^{(r)}(t)\, dt,$$

with

$$K_r^\star(t) = \frac{(b-t)^r}{r!} - \sum_{k=0}^{n} \sum_{j \in I_k} A_{kj}^\star \frac{(x_k^\star - t)_+^{r-j-1}}{(r-j-1)!},$$

is the optimal error. We also have

$$\left|R_N^\star(f)\right| \leqslant \left\|f^{(r)}\right\|_2 \left(\int_a^b \left[K_r^\star(t)\right]^2 dt\right)^{\frac{1}{2}}.$$

Example 3.2. *For $f \in H^{2,2}[0,1]$ and $\Lambda_B = \{f'(0), f(x_1), f'(x_1), f'(1)\}$, with $x_1 \in (0,1)$, find the quadrature formula of the type*

$$\int_0^1 f(x)\, dx = A_{01} f'(0) + A_{10} f(x_1) + A_{11} f'(x_1) + A_{21} f'(1) + R_3(f)$$

that is optimal in the sense of Nikolski, i.e. find the optimal coefficients

$$\boldsymbol{A}^\star = (A_{01}^\star, A_{10}^\star, A_{11}^\star, A_{21}^\star)$$

and the optimal nodes $\boldsymbol{X}^\star = (0, x_1^\star, 1)$.

First step. *The spline interpolation formula is given by*

$$f(x) = s_{01}(x) f'(0) + s_{10}(x) f(x_1) + s_{11}(x) f'(x_1) + s_{21}(x) f'(1) + (R_4 f)(x),$$

where

$$\begin{aligned} s_{01}(x) &= -\frac{x_1}{2} + x - \frac{(x-0)_+^2}{2x_1} + \frac{(x-1)_+^2}{2x_1}, \\ s_{10}(x) &= 1, \\ s_{11}(x) &= -\frac{x_1}{2} + \frac{(x-0)_+^2}{2x_1} - \frac{(x-x_1)_+^2}{2x_1(1-x_1)} - \frac{(x-1)_+^2}{1-x_1}, \\ s_{21}(x) &= \frac{(x-x_1)_+^2}{2(1-x_1)} - \frac{(x-1)_+^2}{2(1-x_1)}. \end{aligned}$$

It follows that

$$\overline{A}_{01} = -\frac{x_1^2}{6},\ \overline{A}_{10} = 1, \quad \overline{A}_{11} = \frac{1-2x_1}{3},\ \overline{A}_{21} = \frac{(1-x_1)^2}{6}, \tag{3.10}$$

$$\overline{K}_2(t) = \frac{(1-t)^2}{2} - (x_1 - t)_+ - \frac{1-2x_1}{3}(x_1-t)_+^0 - \frac{(1-x_1)^2}{6}$$

and

$$F\left(\overline{\boldsymbol{A}}, \boldsymbol{X}\right) = \int_0^1 \overline{K}_2^2(t)\,dt = \frac{1}{45} - \frac{1}{9} x_1(1-x_1)\left(1-x_1+x_1^2\right).$$

Second step. *We have to minimize $F\left(\overline{\boldsymbol{A}}, \boldsymbol{X}\right)$ with respect to x_1. From the equation*

$$\frac{\partial F\left(\overline{\boldsymbol{A}}, \boldsymbol{X}\right)}{\partial x_1} = -\frac{1}{9}(1-2x_1)\left[x_1^2 + (1-x_1)^2\right] = 0,$$

we obtain $x_1 = \frac{1}{2}\cdot$ Also, (3.10) *implies that*

$$A_{01}^\star = -\frac{1}{24}, \quad A_{10}^\star = 1, \quad A_{11}^\star = 0, \quad A_{21}^\star = \frac{1}{24}.$$

Finally, we have

$$\left|R_4^\star(f)\right| \leqslant \left\|f''\right\|_2 \left(\int_0^1 \left[K_2^\star(t)\right]^2 dt\right)^{\frac{1}{2}} = \frac{1}{12\sqrt{5}}\left\|f''\right\|_2.$$

3.2. **Minimal norm of orthogonal polynomials.** Let $\widetilde{\mathcal{P}}_n \subset \mathcal{P}_n$ be the set of polynomials of degree n with leading coefficient equal to one. If $P_n \in \widetilde{\mathcal{P}}_n$ and $P_n \perp \mathcal{P}_{n-1}$ on $[a,b]$ with respect to the weight function w, then

$$\|P_n\|_{w,2} = \min_{P\in\widetilde{\mathcal{P}}_n} \|P\|_{w,2}\,,$$

where

$$\|P\|_{w,2} = \left(\int_a^b w\left(x\right) P^2\left(x\right) dx\right)^{\frac{1}{2}}.$$

It follows that the parameters of the functional $F\left(\boldsymbol{A},\boldsymbol{X}\right)$ can be determined such that the restriction of the kernel K_r to the interval $[x_{k-1},x_k]$ is identical to the orthogonal polynomial on the same interval with respect to the corresponding weight function.

Example 3.3. *Consider the functional of Example 3.1*

$$F\left(\boldsymbol{A},\boldsymbol{X}\right) = \sum_{k=1}^{n} \int_{x_{k-1}}^{x_k} \varphi_k^2\left(x\right) dx,$$

with

$$\begin{aligned}
\varphi_1\left(x\right) &= \frac{x^2}{2} - A_0 x,\\
\varphi_k\left(x\right) &= \frac{x^2}{2} - x\sum_{i=0}^{k-1} A_i + \sum_{i=1}^{k-1} A_i x_i, \quad k=\overline{2,n-1},\\
\varphi_n\left(x\right) &= \frac{\left(1-x\right)^2}{2} - A_n\left(1-x\right).
\end{aligned}$$

Since for $w=1$ the corresponding orthogonal polynomial on $[x_{k-1},x_k]$ is the Legendre polynomial of degree two

$$\ell_{2,k}\left(x\right) = \frac{x^2}{2} - \frac{x_{k-1}+x_k}{2}x + \frac{\left(x_{k-1}+x_k\right)^2}{8} - \frac{\left(x_k-x_{k-1}\right)^2}{24}$$

and

$$\int_{x_{k-1}}^{x_k} \ell_{2,k}^2\left(x\right) dx = \frac{1}{720}\left(x_k-x_{k-1}\right)^5,$$

from $\varphi_k \equiv \ell_{2,k}$, $k = \overline{2, n-1}$, *one obtains*

$$\begin{aligned} \sum_{i=0}^{k-1} \overline{A}_i &= \frac{x_{k-1} + x_k}{2}, \\ \sum_{i=0}^{k-1} \overline{A}_i x_i &= \frac{(x_{k-1} + x_k)^2}{8} - \frac{(x_k - x_{k-1})^2}{24}, \quad k = \overline{2, n-1} \end{aligned} \tag{3.11}$$

and thus

$$\sum_{k=2}^{n-1} \int_{x_{k-1}}^{x_k} \varphi_k^2 (x)\, dx = \frac{1}{720} \sum_{k=2}^{n-1} (x_k - x_{k-1})^5 . \tag{3.12}$$

Taking into account that φ_1 *and* φ_n *are particular polynomials of second degree to which the above identities do not apply, from the equations*

$$\frac{\partial}{\partial A_0} \left[\int_0^{x_1} \varphi_1^2 (x)\, dx \right] = 0, \quad \frac{\partial}{\partial A_n} \left[\int_{x_{n-1}}^{1} \varphi_n^2 (x)\, dx \right] = 0,$$

one obtains

$$\overline{A}_0 = \frac{3}{8} x_1, \quad \overline{A}_n = \frac{3}{8} (1 - x_{n-1}) \tag{3.13}$$

and hence

$$\begin{aligned} \int_0^{x_1} \left(\frac{x^2}{2} - \overline{A}_0 x \right)^2 dx &= \frac{1}{320} x_1^5, \\ \int_{x_{n-1}}^{1} \left[\frac{(1-x)^2}{2} - \overline{A}_n (1-x) \right]^2 dx &= \frac{1}{320} (1 - x_{n-1})^5 . \end{aligned} \tag{3.14}$$

From (3.12) *and* (3.14), *it follows that*

$$F\left(\overline{\boldsymbol{A}}, \boldsymbol{X}\right) = \frac{1}{320} x_1^5 + \frac{1}{720} \sum_{k=2}^{n-1} (x_k - x_{k-1})^5 + \frac{1}{320} (1 - x_{n-1})^5 ,$$

which can be minimized with respect to the nodes $\boldsymbol{X}$.

First, we have that

$$\frac{\partial}{\partial x_k} \left[\sum_{i=2}^{n-1} (x_i - x_{i-1})^5 \right] = 5 \left[(x_k - x_{k-1})^4 - (x_{k+1} - x_k)^4 \right] = 0,$$

which implies that

$$x_k - x_{k-1} = \frac{x_{n-1} - x_1}{n-2}, \quad k = \overline{2, n-1}, \tag{3.15}$$

and thus

$$F\left(\overline{\boldsymbol{A}},\boldsymbol{X}\right)=\frac{1}{320}x_1^5+\frac{1}{720\,(n-2)^4}\,(x_{n-1}-x_1)^5 + \frac{1}{320}\,(1-x_{n-1})^5\,. \tag{3.16}$$

Next, the minimum value of $F\left(\overline{\boldsymbol{A}},\boldsymbol{X}\right)$ *with respect to* x_1 *and* x_{n-1} *is attained for*

$$x_1^\star=1-x_{n-1}^\star=2\mu,$$

where

$$\mu=\frac{1}{4+(n-2)\sqrt{6}}\,.$$

Finally, from (3.15), (3.11), (3.13) *and* (3.16), *one obtains*

$$x_0^\star=0;\quad x_k^\star=\left[2+(k-1)\sqrt{6}\right]\mu,\ k=\overline{1,n-1};\quad x_n^\star=1;$$

$$A_0^\star=A_n^\star=\frac{3}{4}\mu;\ A_1^\star=A_{n-1}^\star=\frac{5+2\sqrt{6}}{4}\mu;\ A_k^\star=\mu\sqrt{6},\ k=\overline{2,n-2};$$

and

$$F\left(\boldsymbol{A}^\star,\boldsymbol{X}^\star\right)=\frac{1}{20}\mu^4,$$

which is the minimum value of $F\left(\boldsymbol{A},\boldsymbol{X}\right)$.

4. Optimal quadrature formulas generated by Lagrange interpolation formula

Let $\Lambda(f)=\left\{f(x_i)\mid i=\overline{0,n}\right\}$, with $x_i\in[a,b]$, be a set of Lagrange-type information.

Consider the Lagrange interpolation formula

$$f=L_nf+R_nf, \tag{4.1}$$

where

$$(L_nf)(x)=\sum_{k=0}^{n}\frac{u(x)}{(x-x_k)\,u'(x_k)}f(x_k)\,,$$

with $u(x)=(x-x_0)\dots(x-x_n)$ and for $f\in C^{n+1}[a,b]$,

$$(R_nf)(x)=\frac{u(x)}{(n+1)!}f^{(n+1)}(\xi)\,,\quad a<\xi<b.$$

If $w\colon\ [a,b] \to \mathbb{R}$ is a weight function, from (4.1) one obtains

$$\int_a^b w(x) f(x)\, dx = \sum_{k=0}^{n} A_k f(x_k) + R_n(f), \tag{4.2}$$

where

$$A_k = \int_a^b w(x) \frac{u(x)}{(x - x_k) u'(x_k)} dx \tag{4.3}$$

and

$$R_n(f) = \frac{1}{(n+1)!} \int_a^b w(x) u(x) f^{(n+1)}(\xi)\, dx.$$

We also have

$$\left|R_n(f)\right| \leqslant \frac{1}{(n+1)!} \left\|f^{(n+1)}\right\|_\infty \int_a^b w(x) |u(x)|\, dx. \tag{4.4}$$

Theorem 4.1. *Let $w\colon\ [a,b] \to \mathbb{R}$ be a weight function and $f \in C^{n+1}[a,b]$. If $u \perp \mathcal{P}_n$, then the quadrature formula (4.2), with the coefficients (4.3) and the nodes $\boldsymbol{X} = (x_0, \ldots, x_n)$ - the roots of the polynomial u, is optimal with respect to the error.*

Proof. From (4.4), we have

$$\left|R_n(f)\right| \leqslant \frac{1}{(n+1)!} \left\|f^{(n+1)}\right\|_\infty \int_a^b \sqrt{w(x)}\sqrt{w(x)}\, |u(x)|\, dx \tag{4.5}$$

or

$$\left|R_n(f)\right| \leqslant \frac{1}{(n+1)!} \left\|f^{(n+1)}\right\|_\infty \left[\int_a^b w(x)\, dx\right]^{\frac{1}{2}} \left[\int_a^b w(x) |u(x)|^2\, dx\right]^{\frac{1}{2}}.$$

So

$$|R_n(f)| \leqslant C_{w,2}^f \|u\|_{w,2}, \tag{4.6}$$

where

$$C_{w,2}^f = \frac{1}{(n+1)!} \left\|f^{(n+1)}\right\|_\infty \left\|\sqrt{w}\right\|_2.$$

If $u \perp \mathcal{P}_n$ on $[a,b]$ with respect to the weight function w, then $\|u\|_{w,2}$ is minimum, i.e. the error $|R_n(f)|$ is minimum. $\square$

Remark 4.1. *Theorem 4.1 implies that the optimal nodes* $x_k^\star$, $k=\overline{0,n}$, *are the roots of the orthogonal polynomial on* $[a,b]$ *with respect to the weight function* w, *say* P_{n+1}, *and the optimal coefficients* $A_k^\star$, $k=\overline{0,n}$, *are given by*

$$A_k^\star = \int_a^b w(x) \frac{\tilde{P}_{n+1}(x)}{(x-x_k^\star)\tilde{P}'_{n+1}(x_k^\star)} dx, \quad k=\overline{0,n}.$$

For the optimal error, we have

$$|R_n^\star(f)| \leqslant C_{w,2}^f \left\| \tilde{P}_{n+1} \right\|_{w,2}.$$

4.1. **Particular cases.** *Case 1.* $[a,b]=[-1,1]$ and $w=1$.

The orthogonal polynomial is the Legendre polynomial

$$\tilde{\ell}_{n+1}(x) = \frac{(n+1)!}{(2n+2)!} \frac{d^{n+1}}{dx^{n+1}} \left[\left(x^2-1\right)^{n+1} \right].$$

The corresponding optimal quadrature formula has the nodes $x_k^\star$, $k=\overline{0,n}$, and the coefficients $A_k^\star$, $k=\overline{0,n}$, of the Gauss quadrature rule. For the error, we have

$$\left| R_n^\star(f) \right| \leqslant \frac{(n+1)!2^{n+2}}{(2n+2)!\sqrt{2n+3}} \left\| f^{(n+1)} \right\|_\infty.$$

Case 2. $[a,b]=[-1,1]$ and $w(x)=\frac{1}{\sqrt{1-x^2}}$.

The orthogonal polynomial is the Chebyshev polynomial of the first kind

$$T_{n+1}(x) = \cos\left[(n+1)\arccos(x)\right].$$

The optimal parameters are

$$x_k^\star = \cos\frac{2k+1}{2(n+1)}\pi, \quad k=\overline{0,n},$$

$$A_k^\star = \int_{-1}^1 \frac{1}{\sqrt{1-x^2}} \frac{\tilde{T}_{n+1}(x)}{(x-x_k^\star)\tilde{T}'_{n+1}(x_k^\star)} dx = \frac{\pi}{n+1}, \quad k=\overline{0,n},$$

and we have

$$\begin{aligned} \left| R_n^\star(f) \right| &\leqslant \frac{1}{(n+1)!} \left\| f^{(n+1)} \right\|_\infty \left(\int_{-1}^1 \frac{1}{\sqrt{1-x^2}} dx \right)^{\frac{1}{2}} \left\| \tilde{T}_{n+1} \right\|_{w,2} \\ &= \frac{\pi}{\sqrt{2}(n+1)!2^n} \left\| f^{(n+1)} \right\|_\infty. \end{aligned}$$

Case 3. $[a,b]=[-1,1]$ and $w(x)=\sqrt{1-x^2}$.

The orthogonal polynomial is the Chebyshev polynomial of the second kind

$$Q_{n+1}(x) = \frac{1}{\sqrt{1-x^2}} \sin\left[(n+2)\arccos(x)\right].$$

We have

$$x_k^\star = \cos\frac{k+1}{n+2}\pi, \quad k = \overline{0,n},$$

$$\begin{aligned} A_k^\star &= \int_{-1}^{1} \sqrt{1-x^2}\frac{\tilde{Q}_{n+1}(x)}{(x-x_k^\star)\,\tilde{Q}'_{n+1}(x_k^\star)}dx \\ &= \frac{\pi}{n+2}\sin^2\left(\frac{k+1}{n+2}\pi\right), \quad k = \overline{0,n}, \end{aligned}$$

and

$$\begin{aligned} \left|R_n^\star(f)\right| &\leqslant \frac{1}{(n+1)!}\left\|f^{(n+1)}\right\|_\infty \left(\int_{-1}^{1}\sqrt{1-x^2}\,dx\right)^{\frac{1}{2}} \left\|\tilde{Q}_{n+1}\right\|_{w,2} \\ &= \frac{\pi}{(n+1)!2^{n+2}}\left\|f^{(n+1)}\right\|_\infty. \end{aligned}$$

4.2. **Special cases.** $[a,b]=[-1,1]$ and $w=1$.

Case 4. From (4.4), we obtain

$$|R_n(f)| \leqslant \frac{2}{(n+1)!}\left\|f^{(n+1)}\right\|_\infty \|u\|_\infty.$$

Since

$$\left\|\tilde{T}_{n+1}\right\|_\infty \leqslant \|P\|_\infty, \quad P \in \tilde{\mathcal{P}}_{n+1},$$

it follows that for $u = \tilde{T}_{n+1}$, the error $|R_n(f)|$ is minimum. So

$$x_k^\star = \cos\frac{2k+1}{2(n+1)}\pi, \quad k = \overline{0,n},$$

$$\begin{aligned} A_k^\star &= \int_{-1}^{1}\frac{\tilde{T}_{n+1}(x)}{(x-x_k^\star)\,\tilde{T}'_{n+1}(x_k^\star)}dx \\ &= \frac{2}{n+1}\left[1 - 2\sum_{i=1}^{\left[\frac{n}{2}\right]}\frac{1}{4i^2-1}\cos\frac{(2k+1)\,i}{n+1}\pi\right], \quad k = \overline{0,n}, \end{aligned} \tag{4.7}$$

and

$$\left|R_n^\star(f)\right| \leqslant \frac{1}{(n+1)!2^{n-1}}\left\|f^{(n+1)}\right\|_\infty.$$

Case 5. From (4.4), we also have

$$\left|R_n\left(f\right)\right| \leqslant \frac{1}{(n+1)!} \left\|f^{(n+1)}\right\|_\infty \left\|u\right\|_1.$$

In this case the minimum $L_1\left[-1,1\right]$-norm is given by the Chebyshev polynomial of the second kind Q_{n+1}. So

$$x_k^\star = \cos\frac{k+1}{n+2}\pi, \quad k=\overline{0,n},$$

$$\begin{aligned} A_k^\star &= \int_{-1}^{1} \frac{\tilde{Q}_{n+1}\left(x\right)}{\left(x-x_k^\star\right)\tilde{Q}_{n+1}'\left(x_k^\star\right)}dx \\ &= \frac{4\sin\left(\frac{k+1}{n+2}\pi\right)}{n+2} \sum_{i=0}^{\left[\frac{n}{2}\right]} \frac{\sin\left[\frac{(2i+1)(k+1)}{n+2}\pi\right]}{2i+1}, \quad k=\overline{0,n}, \end{aligned} \tag{4.8}$$

and

$$\left|R_n^\star\left(f\right)\right| \leqslant \frac{1}{(n+1)!}\left\|f^{(n+1)}\right\|_\infty \left\|\tilde{Q}_{n+1}\right\|_1 = \frac{1}{(n+1)!2^n}\left\|f^{(n+1)}\right\|_\infty.$$

4.3. **Other cases.** Let

$$\int_a^b f\left(x\right)dx = \sum_{k=0}^{n} A_k f\left(x_k\right) + R_n\left(f\right) \tag{4.9}$$

be the quadrature formula generated by the Lagrange interpolation formula

$$f\left(x\right) = \sum_{k=0}^{n} \frac{u\left(x\right)}{\left(x-x_k\right)u'\left(x_k\right)} f\left(x_k\right) + \left(R_n f\right)\left(x\right),$$

with $u\left(x\right) = \left(x-x_0\right)\ldots\left(x-x_n\right)$ and

$$\left(R_n f\right)\left(x\right) = \frac{u\left(x\right)}{(n+1)!} f^{(n+1)}\left(\xi\right), \quad a<\xi<b.$$

We have

$$\left|R_n\left(f\right)\right| \leqslant \frac{1}{(n+1)!}\left\|f^{(n+1)}\right\|_\infty \int_a^b \left|u\left(x\right)\right| dx.$$

If w is a weight function, then

$$\int_a^b \left|u\left(x\right)\right| dx = \int_a^b \frac{1}{\sqrt{w\left(x\right)}}\sqrt{w\left(x\right)}\left|u\left(x\right)\right| dx \leqslant \left[\int_{-1}^{1}\frac{dx}{w\left(x\right)}\right]^{\frac{1}{2}} \left\|u\right\|_{w,2}.$$

Finally, we have

$$\left|R_n\left(f\right)\right| \leqslant C_{f,w}\left\|u\right\|_{w,2},$$

with

$$C_{f,w}=\frac{1}{(n+1)!}\left\|f^{(n+1)}\right\|_{\infty}\left[\int_{-1}^{1}\frac{1}{w(x)}dx\right]^{\frac{1}{2}}.$$

It follows that the quadrature formula (4.9) is optimal when $\|u\|_{w,2}$ is minimum, i.e. u is orthogonal on $[a,b]$ with respect to the weight function w.

Case 6. $[a,b]=[-1,1]$ and $w(x)=\frac{1}{\sqrt{1-x^2}}$.

We get

$$x_k^\star=\cos\frac{2k+1}{2(n+1)}\pi,\quad k=\overline{0,n},$$

$$A_k^\star=\int_{-1}^{1}\frac{\tilde{T}_{n+1}(x)}{(x-x_k^\star)\,\tilde{T}_{n+1}'(x_k^\star)}dx,\quad k=\overline{0,n},\quad (\text{see } (4.7)),$$

and hence

$$\begin{aligned}\left|R_n^\star(f)\right| &\leqslant \frac{1}{(n+1)!}\left\|f^{(n+1)}\right\|_{\infty}\left(\int_{-1}^{1}\sqrt{1-x^2}\,dx\right)^{\frac{1}{2}}\left\|\tilde{T}_{n+1}\right\|_{w,2}\\ &=\frac{\pi}{(n+1)!2^{n+1}}\left\|f^{(n+1)}\right\|_{\infty}.\end{aligned}$$

Case 7. $[a,b]=[-1,1]$ and $w(x)=\sqrt{1-x^2}$.

It follows that

$$x_k^\star=\cos\frac{k+1}{n+2}\pi,\quad k=\overline{0,n},$$

$$A_k^\star=\int_{-1}^{1}\frac{\tilde{Q}_{n+1}(x)}{(x-x_k^\star)\,\tilde{Q}_{n+1}'(x_k^\star)}dx,\quad k=\overline{0,n},\quad (\text{see } (4.8)),$$

and thus

$$\begin{aligned}\left|R_n^\star(f)\right| &\leqslant \frac{1}{(n+1)!}\left\|f^{(n+1)}\right\|_{\infty}\left(\int_{-1}^{1}\frac{1}{\sqrt{1-x^2}}\,dx\right)^{\frac{1}{2}}\left\|\tilde{Q}_{n+1}\right\|_{w,2}\\ &=\frac{\pi}{\sqrt{2}\,(n+1)!2^{n+1}}\left\|f^{(n+1)}\right\|_{\infty}.\end{aligned}$$

Remark 4.2. *From* (4.5)*, we also have*

$$|R_n(f)|\leqslant C_{w,\infty}^{f}\,\|u\|_{w,2}\,,$$

with

$$C_{w,\infty}^{f}=\frac{\sqrt{b-a}}{(n+1)!}\left\|f^{(n+1)}\right\|_{\infty}\left\|\sqrt{w}\right\|_{\infty}.$$

For particular orthogonal polynomials, we can obtain new upper bounds for the quadrature error.

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