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OPTIMAL QUADRATURE FORMULAS WITH RESPECT TO THE ERROR

GH. COMAN, A. OPRIŞAN and I. SOMOGYI

Dedicated to Professor Ştefan Cobzaş at his 60^{th} *anniversary*

Abstract. Using the connection between the optimal approximation of linear operators and spline interpolation, estabilished by I.J. Schoenberg [12], is studied the optimality problem with respect to the error, for some quadrature formulas. Concrete examples are given.

Suppose that $f \in C^r[a,b]$ and $a = x_0 < x_1 < ... < x_n = b$. By $\varphi-$ function method [8], one obtains

$$\int_a^b f(x)dx = \sum_{k=0}^{n} \sum_{j=0}^{r-1} A_{kj} f^{(j)}(x_k) + R_n(f) \tag{1}$$

with

$$R_n(f) = (-1)^r \int_a^b \varphi(x) f^{(r)}(x) dx \tag{2}$$

where

$$\varphi(x) = \frac{(x-x_n)^r}{r!} + (-1)^{r+1} \sum_{k=0}^{n} \sum_{j=0}^{r-1} A_{kj} \frac{(x_k - x)_+^{r-j-1}}{(r-j-1)!} \tag{3}$$

and

$$A_{0v} = (-1)^{v+1} \varphi_1^{(r-v-1)}(x_0), v = 0, ..., r-1 \tag{4}$$

$$A_{iv} = (-1)^{v} (\varphi_i - \varphi_{i+1})^{(r-v-1)}(x_i), i = 1, ..., n-1, v = 0, ..., r-1$$

$$A_{nv} = (-1)^{v} \varphi_n^{(r-v-1)}(x_n), v = 0, ..., r-1,$$

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with

$$\varphi_i = \varphi\mid_{[x_{i-1},x_i]}$$

i.e.

$$\varphi_i(x) = \frac{(x-x_n)^r}{r!} + (-1)^{r+1}\sum_{k=i}^{n}\sum_{j=0}^{r-1} A_{kj}\frac{(x_k-x)^{r-j-1}}{(r-j-1)!}. \tag{5}$$

Indeed, applying the integration by parts method, for $\varphi_k^{(r)} = 1, k = 1, ..., n$, one obtains

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

$$= \sum_{k=1}^{n}\Big\{\Big[\varphi_k^{(r-1)}(x)f\,(x) - \varphi_k^{(r-2)}(x)f'\,(x) + ... + (-1)^{r-1}$$

$$\varphi_k^{'}(x)f^{(r-1)}\,(x)\Big]_{x_{k-1}}^{x_k} + (-1)^r\int_{x_{k-1}}^{x_k}\varphi_k(x)f^{(r)}\,(x)\,dx\Big\}$$

$$= \sum_{v=0}^{r-1}(-1)^{v+1}\varphi_1^{(r-v-1)}(x_0)f^{(v)}(x_0)$$

$$+ \sum_{i=1}^{n-1}\sum_{v=0}^{r-1}(-1)^v[\varphi_i - \varphi_{i+1}]^{(r-v-1)}(x_i)f^{(v)}(x_i)$$

$$+ \sum_{v=0}^{r-1}(-1)^v\varphi_n^{(r-v-1)}(x_n) + (-1)^r\int_a^b \varphi(x)f^{(r)}(x)dx$$

and $(2)-(4)$ follows.

Remark 1. *φ_i is an algebraic polynomial of the degree r.*

Now, if $f \in H^{r,2}[a,b]$ then, from (2), one obtains

$$|R_n(f)| \le \left\|f^{(r)}\right\|_2\left(\int_a^b |\varphi(x)|^2\,dx\right)^{1/2}$$

Definition 2. *The quadrature formula (1) for which*

$$F(A,X) := \int_a^b |\varphi(x)|^2\,dx$$

takes the minimum value, with respect to the coefficients $A := (A_{kj})_{k=\overline{o,n};j=\overline{0,r-1}}$ *and the nodes* $X := (x_k)_{k=1,n-1}$, *is called optimal with respect to the approximation error (or simple error).*

Remark 3. *From (2) it follows that the degree of exactness of the quadrature formula (1) is at least* $r-1$.

There are different ways to construct an optimal quadrature formula.

One of this way is based on the relationship between the optimal approximation of linear operators problem and the problem of spline interpolation, established by I.J.Schoemberg [12].

More precisely, if $S : H^{r,2}[a,b] \to \Im_{2r-1}(\Lambda_H)$ is the natural spline interpolation operator of the order $2r-1$, suitable to Λ_H:

$$\Lambda_H(f) = \left\{\lambda_{kj}(f) := f^{(j)}(x_k) \mid k=0,...,n; j=0,...,r-1\right\},$$

and

$$f = S_r f + R_r f$$

is the natural spline interpolation formula generated by S then

$$\int_a^b f(x)dx = \int_a^b (S_r f)(x)dx + \int_a^b (R_r f)(x)dx$$

is the corresponding optimal quadrature formula.

Now, if $s_{kj}, k=0,...,n; j=0,...,r-1$ are the corresponding cardinal splines, i.e.

$$S_r f = \sum_{k=0}^{n}\sum_{j=0}^{r-1} s_{kj} f^{(j)}(x_k) \tag{6}$$

then the optimal coefficients for fixed nodes $x_k, k=1,...,n$ are

$$\bar{A}_{kj} = \int_a^b s_{kj}(x)dx, k=0,...,n; j=0,...,r-1 \tag{7}$$

and

$$\bar{R}_n(f) = \int_a^b \bar{K}_r(t) f^{(r)}(t)dt$$

with

$$\bar{K}_r(t) := \int_a^b (Rf)(x)dx = \frac{(b-t)^r}{r!} - \sum_{k=0}^{n}\sum_{j=0}^{r-1} \bar{A}_{kj} \frac{(x_k-t)_+^{r-j-1}}{(r-j-1)!} \tag{8}$$

Remark 4. *If the quadrature nodes* $x_k, k = 1, ..., n-1$ *are given (fixed), then the quadrature formula*

$$\int_a^b f(x)\,dx = \sum_{k=0}^{n}\sum_{j=0}^{r-1} \bar{A}_{kj} f^{(j)}(x_k) + \bar{R}_n(f)$$

with

$$\left|\bar{R}_n(f)\right| \le \left\|f^{(r)}\right\|_2 (\int_a^b \bar{K}_r^2(t)dt)^{1/2},$$

is optimal in sense of Sard and the optimality problem is solved.

Suppose, next, that the quadrature nodes $x_k, k = 1, ..., n$ are free. In this case, the optimality problem can be continued, in a secered step, by minimizing with respect to the free parameters $x_k, k = 1, ..., n$ the functional

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

Such, the optimal nodes, say $x_k^*, k = 1, ..., n-1$, are obtained as a solution of the system

$$\frac{\partial F\left(\bar{A}, X\right)}{\partial x_i} := 2\int_a^b \bar{K}_r(t)\left[-\sum_{j=0}^{r-1} \bar{A}_{ij}\frac{(x_i - t)_+^{r-j-2}}{(r-j-2)!}\right] dt = 0, i = 1, ..., n-1$$

Substituting in (7) the nodes x_k by x_k^* for all $k = 1, ..., n-1$, are obtained also the optimal coefficients $A_{kj}^*, k = 1, ..., n-1; j = 0, ..., r-1$.

Finally, for the optimal error, we have

$$|R_n^*(f)| \le \left\|f^{(r)}\right\|_2 (\int_a^b [K_r^*(t)]^2 dt)^{1/2}$$

where

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

Next, two examples are given:

E1. Find the quadrature formula

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

that is optimal with respect to the error.

In the first step, one construct the linear spline function

$$S_1 f = \sum_{k=0}^{n} s_k f(x_k)$$

that interpolates the data $\Lambda(f) = \{f(0), f(x_1), ..., f(x_{n-1}), f(1)\}$, where $s_k, k = 0, ..., n$ are the corresponding cardinal splines, i.e.:

$$\begin{aligned}
s_0(x) &= 1 - \frac{1}{x_1}x + \frac{1}{x_1}(x - x_1)_+ \\
s_1(x) &= \frac{x}{x_1} - \frac{x_2}{x_1(x_2 - x_1)}(x - x_1)_+ + \frac{1}{x_2 - x_1}(x - x_2)_+ \\
s_k(x) &= \frac{1}{x_k - x_{k-1}}(x - x_{k-1})_+ - \frac{x_{k+1} - x_{k-1}}{(x_k - x_{k-1})(x_{k+1} - x_k)}(x - x_k)_+ + \\
&\quad + \frac{1}{x_{k+1} - x_k}(x - x_{k+1})_+ ,\ k = 2, ..., n-1 \\
s_n(x) &= \frac{1}{x_n - x_{n-1}}(x - x_{n-1})_+ - \frac{1}{x_n - x_{n-1}}(x - 1)_+
\end{aligned}$$

It follows that the optimal coefficients for fixed nodes $x_k, k = 1, ..., n-1$ and the corresponding kernel, are

$$\begin{aligned}
\bar{A}_0 &= \frac{x_1}{2} \\
\bar{A}_1 &= \frac{x_2}{2} \\
\bar{A}_k &= \frac{x_{k-1} - x_{k+1}}{2}, k = 2, ..., n-1 \\
\bar{A}_n &= \frac{1 - x_{n-1}}{2}
\end{aligned}$$

respectively

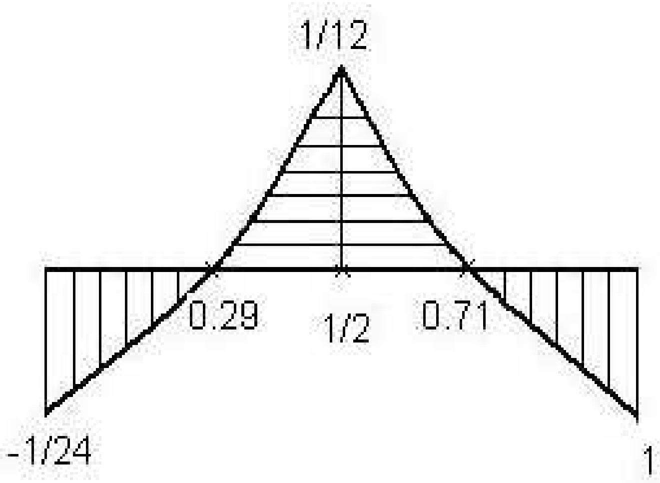
$$\bar{K}_1(t) = 1 - t - \sum_{k=0}^{n} \bar{A}_k (x_k - t)_+^0$$

So,

$$F\left(\bar{A}, X\right) := \int_0^1 \bar{K}_1^2(t)dt = -\frac{1}{12}\sum_{k=1}^{n}(x_k - x_{k-1})^3$$

Now, from the system

$$\frac{\partial F\left(\bar{A}, X\right)}{\partial x_j} := \frac{1}{4}[(x_j - x_{j-1})^2 - (x_{j+1} - x_j)^2] = 0, j = 1, ..., n-1$$



one obtains

$$x_j^* - x_{j-1}^* = x_{j+1}^* - x_j^*, j = 1, ..., n-1$$

i.e. the optimal nodes are

$$x_j^* = \frac{j}{n}, j = 0, 1, ..., n. \tag{9}$$

It follows that

$$A_0^* = \frac{1}{2n}, A_k^* = \frac{1}{n}, k = 1, ..., n-1; A_n^* = \frac{1}{2n} \tag{10}$$

are the optimal coefficients,

$$K_1^*(t) = 1 - t - \sum_{k=0}^{n} A_k^* (\frac{k}{n} - t)_+^0 \tag{11}$$

is the optimal kernel and

$$\int_0^1 (K^*(t))^2 dt = \frac{1}{12n^2}.$$

Finally, for the optimal error, we have

$$|R_n^*(f)| \leq \frac{1}{2n\sqrt{3}} \|f'\|_2$$

This way, is proved the following theorem:

Theorem 5. *If $f \in C^1[0,1]$ then the quadrature formula of the form*

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

which is optimal with respect to the error is given by the nodes and the coefficients of (9), respectively (10). Approximation error is estimated in (12)

Remark 6. *An interesting property of the kernel function K^* (figure 1), is that the domains placed upper respectively under the Ox axis have the equal areas.*

E2. The problem is to construct the quadrature formula of the form

$$\int_a^b f(x)\,dx = A_{01} f'(0) + A_{10} f(\alpha) + A_{11} f'(1) + R_2(f) \tag{12}$$

that is optimal with regard to the error.

Let

$$f = S_3 f + R_3 f$$

be the corresponding cubic spline interpolation formula. We have

$$(S_3 f)(x) = s_{01}(x) f'(0) + s_{10}(x) f(\alpha) + s_{21}(x) f'(1)$$

where

$$\begin{aligned} s_{01}(x) &= \alpha\left(\frac{1}{2}\alpha - 1\right) + x - \frac{1}{2}x^2 + \frac{1}{2}(x-1)_+^2 \\ s_{10}(x) &= 1 \\ s_{21}(x) &= -\frac{1}{2}\alpha^2 + \frac{1}{2}x^2 - \frac{1}{2}(x-1)_+^2 \end{aligned}$$

Then

$$\begin{aligned} \bar{A}_{01} &:= \int_0^1 s_{01}(x)\,dx = \frac{1}{3} + \alpha\left(\frac{1}{2}\alpha - 1\right) \\ \bar{A}_{10} &:= \int_0^1 s_{10}(x)\,dx = 1 \\ \bar{A}_{21} &:= \int_0^1 s_{21}(x)\,dx = \frac{1}{6} - \frac{1}{2}\alpha^2. \end{aligned}$$

One obtains

$$\int_0^1 f(x)\,dx = \bar{A}_{01} f'(0) + \bar{A}_{10} f(\alpha) + \bar{A}_{21} f'(1) + \bar{R}_3(f)$$

with

$$\bar{R}_3(f) = \int_0^1 \bar{K}_3(t) f''(t)\,dt$$

where

$$\bar{K}_3(t) = \frac{(1-t)^2}{2} - (\alpha - t)_+ + \frac{1}{2}\left(\alpha^2 - \frac{1}{3}\right)$$

Taking into account that

$$|R_3(f)| \leq \|f''\|_2 \left(\int_0^1 \bar{K}_3^2(t)\,dt\right)^{1/2}$$

next it must be minimized the function

$$F(\alpha) = \int_0^1 \bar{K}_3^2(t)\,dt$$

with respect to the parameter α.

We have

$$\min_{0<\alpha<1} F(\alpha) = F\left(\frac{1}{2}\right)$$

and

$$F\left(\frac{1}{2}\right) = \frac{1}{2^8 * 15}$$

It follows that the optimal parameters of the quadrature formula (12) are:

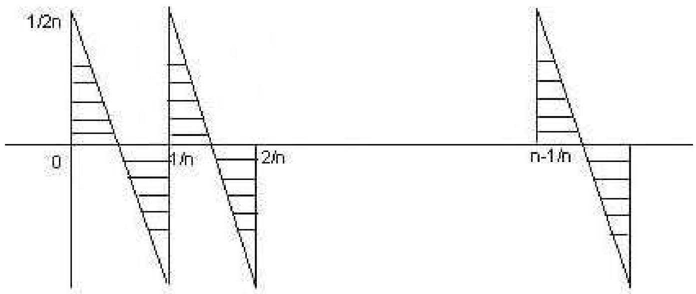
$$\alpha = \frac{1}{2};\, A_{01}^* = -\frac{1}{24};\, A_{10}^* = 1;\, A_{21}^* = \frac{1}{24} \tag{13}$$

and the optimal kernel is:

$$K_3^*(t) = \frac{(1-t)^2}{2} - \left(\frac{1}{2} - t\right)_+ - \frac{1}{24}.$$

Theorem 7. *If* $f \in C^2[0,1]$ *then the quadrature formula of the form* (12), *that is optimal with respect to the error, is given by the parameter of* (13), *while for the optimal error we have*

$$|R_3^*(f)| \leq \frac{1}{16\sqrt{15}} \|f''\|_2$$



Remark 8. *Also, the function K_3^* (figure 2) has the property that the area of the domains placed upper Ox axes is equal to the area of the domain placed under Ox axes.*

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Babeş-Bolyai University,
Faculty of Mathematics and Computer Science,
Str. Kogălniceanu Nr. 1, RO-400084 Cluj-Napoca, Romania
E-mail address: ghcoman@math.ubbcluj.ro

Babeş-Bolyai University,
Faculty of Mathematics and Computer Science,
Str. Kogălniceanu Nr. 1, RO-400084 Cluj-Napoca, Romania
E-mail address: sachaoprisan@yahoo.com

Babeş-Bolyai University,
Faculty of Mathematics and Computer Science,
Str. Kogălniceanu Nr. 1, RO-400084 Cluj-Napoca, Romania
E-mail address: ilkovacs@math.ubbcluj.ro