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Exactness Conditions in Numerical Quadrature*

By

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The integral

$$I = \int_a^b f(x)\,dx \tag{1}$$

is usually computed numerically by means of a formula of the type

$$I = H_1 f(x_1) + \cdots + H_n f(x_n) + E. \tag{2}$$

The weights $H_1, \ldots, H_n$ and abcissae $x_1, \ldots, x_n$ are determined by selecting a family $\mathscr{F}$ of functions $f(x)$ and requiring that

$$E = 0 \qquad (f \in \mathscr{F}). \tag{3}$$

We propose here to modify this last restriction by requiring only that the average error be as small as possible over the family $\mathscr{F}$. It will be seen that this condition leads to extremely simple error estimates in certain cases as well as permitting considerable enlargement of the families of functions considered. We specialize at once to the interval $(a, b) = (0, 1)$ and the family

$$\mathscr{F} = \{x^n\}_{n=0}^{\infty}. \tag{4}$$

Generalizations will be obvious.

The error committed in integrating x^j is

$$\frac{1}{j+1} - \sum_{k=1}^{n} H_k x_k^j$$

and so we consider the question of minimizing

$$W(H_1, \ldots, H_n; x_1, \ldots, x_n) = \sum_{j=0}^{\infty} \left\{ \frac{1}{j+1} - \sum_{k=1}^{n} H_k x_k^j \right\}^2. \tag{5}$$

Geometrically speaking we wish to find the vector of approximate moments

$$\mu_j = \sum_{k=\varphi}^{n} H_k x_k^j \qquad (j = 0, 1, 2, \ldots),$$

which is nearest to the true moment vector

$$\mu_j = \frac{1}{j+1} \qquad (j = 0, 1, \ldots)$$

in the usual Euclidean (l^2) norm, the integer n being fixed.

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Suppose for the present that this has been done, and that W of equation (5) assumes its minimum value W_n at $H_1^*, \ldots, H_n^*$; $x_1^*, \ldots, x_n^*$. Now let

$$f(x) = \sum_{n=0}^{\infty} a_n x^n \tag{6}$$

be analytic in $|x| < 1$ and $\mathscr{L}^2$ on the unit circle; i.e.,

$$\|f\|^2 = \frac{1}{2\pi} \int_0^{2\pi} |f(e^{i\vartheta})|^2 d\vartheta = \sum_{n=0}^{\infty} |a_n|^2 < \infty. \tag{7}$$

Then the error committed in integrating $f(x)$ is

$$\begin{aligned}
&\left|\int_0^1 f(x)\,dx - \sum_{k=1}^{n} H_k^* f(x_k^*)\right| \\
&\quad = \left|\sum_{m=0}^{\infty} a_m \left\{\frac{1}{m+1} - \sum_{k=1}^{n} H_k^* x_k^{*\,n}\right\}\right| \\
&\quad \leqq \left\{\sum_{m=0}^{\infty} |a_m|^2\right\}^{\frac{1}{2}} \left[\sum_{m=0}^{\infty} \left\{\frac{1}{m+1} - \sum_{k=1}^{n} H_k^* x_k^{*\,m}\right\}^2\right]^{\frac{1}{2}} \\
&\quad = W_n^{\frac{1}{2}} \left\{\sum_{m=0}^{\infty} |a_m|^2\right\}^{\frac{1}{2}}.
\end{aligned}$$

Consequently,

$$|\text{Error}| \leqq W_n^{\frac{1}{2}} \|f\| \tag{8}$$

and so the same quantity which we sought to minimize on geometrical grounds in (5) also appears as the coefficient in the error estimate. We emphasize here that W_n is independent of f and so can be (and is below) tabulated as a function of n.

To carry out the minimization, the equations

$$\frac{\partial W}{\partial H_\alpha} = 0 \qquad \frac{\partial W}{\partial x_\alpha} = 0 \qquad (\alpha = 1, \ldots, n)$$

are of the form

$$\frac{1}{x_\alpha} \log \frac{1}{1 - x_\alpha} = \sum_{k=1}^{n} \frac{H_k}{1 - x_\alpha x_k} \qquad (\alpha = 1, \ldots, n), \tag{9}$$

$$\frac{1}{x_\alpha (1 - x_\alpha)} - \frac{1}{x_\alpha^2} \log \frac{1}{1 - x_\alpha} = \sum_{k=1}^{n} H_k \frac{X_k}{(1 - x_k x_\alpha)^2} \qquad (\alpha = 1, \ldots, n) \tag{10}$$

(geomet.).

These are $2n$ simultaneous transcendental equations in the unknowns, $x_1, \ldots, x_n$, $H_1, \ldots, H_n$. An analytic solution does not seem feasible, but these equations do have an interesting geometric interpretation. In fact if we consider the Stieltjes transform of the measure dx,

$$F(x) = \int_0^1 \frac{dt}{1 - xt} = \frac{1}{x} \log \frac{1}{1 - x} \tag{11}$$

and the approximate Stieltjes transform

$$F^*(x) = \sum_{k=1}^{n} \frac{H_k}{1 - x\,x_k} \tag{12}$$

obtained by doing the integral in (11) by the rule (2), then it is easy to verify that equations (9), (10) are precisely the assertions that the curves $y = F(x)$, $y = F^*(x)$ have second order contact at each of the points $x_1, \ldots, x_n$. The same remark holds for more general measures.

The Stieltjes transform also enters into the error estimate (8). Indeed, let us ask when the sign of equality can hold there. From the derivation of (8) it is clear that this will happen if and only if

$$a_m = \lambda \left\{ \frac{1}{m+1} - \sum_{i=1}^{n} H_k^* \, x_k^{*\,m} \right\} \qquad (m = 0, 1, \ldots)$$

which means that the function being integrated is

$$\begin{aligned} f(x) &= \lambda \sum_{m=0}^{\infty} \left\{ \frac{1}{m+1} - \sum_{k=1}^{n} H_k^* \, x_k^{*\,m} \right\} x^m \\ &= \lambda \left[F(x) - F^*(x) \right]. \end{aligned} \tag{13}$$

We may say then that the "hardest" of all functions to integrate by this method is the error in the approximation of (11) by (12). These remarks give a new and simple characterization of the minimum value W_n. For if we have the equality sign in (8) with $f = F - F^*$ then

$$\begin{aligned} \left| \int_0^1 [F(x) - F^*(x)]\, dx \right| &= W_n^{\frac{1}{2}} \left\{ \sum_{m=0}^{\infty} |a_m|^2 \right\}^{\frac{1}{2}} \\ &= W_n^{\frac{1}{2}} \, W_n^{\frac{1}{2}} \\ &= W_n \end{aligned}$$

because the approximate integral of $F(x) - F^*(x)$ is zero since that function vanishes at each of the x_k. It follows that

$$W_n = \left| \frac{\pi^2}{6} - \sum_{k=1}^{n} \frac{H_k}{x_k} \log \frac{1}{1 - x_k} \right| .$$

In words, *W_n is the magnitude of the error in integrating $x^{-1} \log(1 - x)^{-1}$ by our formula.*

Solutions to equations (9), (10) are shown below for $n = 2, 3$.

Table

n	x_j	H_j	W_n
2	.48118 .95477	.83421 .15040	.0198
3	.99378 .89813 .37903	.02002 .24302 .72048	.0044

Concerning the order of magnitude of W_n we can show only that $W_n = O(\log n/n)$ $(n \to \infty)$, which is probably quite conservative. To see this, note that since W_n is the minimum of $W(H_1, \ldots, H_n; x_1, \ldots, x_n)$ we have in particular

$$\begin{aligned}
W_n &\leq W\left(\frac{1}{n}, \ldots, \frac{1}{n}; \frac{1}{n+1}, \ldots, \frac{n}{n+1}\right) \\
&= \sum_{j=0}^{\infty} \left\{\frac{1}{j+1} - \frac{1}{n}\sum_{k=1}^{n} \frac{k^j}{(n+1)^j}\right\}^2 \\
&= \frac{\pi^2}{6} - \frac{2}{n}\sum_{k=1}^{n} \frac{n+1}{k} \log \frac{1}{1-\frac{k}{n+1}} + \frac{1}{n^2}\sum_{k,l=1}^{n} \frac{1}{1-\frac{kl}{(n+1)^2}} \\
&\leq \frac{\pi^2}{6} - \frac{2}{n}\int_0^n \frac{n+1}{t} \log \frac{1}{1-\frac{t}{n+1}}\, dt + \frac{1}{n^2}\int_0^{n+1}\int_0^{n+1} \frac{dx\,dy}{1-\frac{xy}{(n+1)^2}} \\
&= \left(2+\frac{2}{n}\right)\int_{n/n+1}^{1} \frac{1}{t}\log\frac{1}{1-t}\, dt + O(n^{-2}) \\
&= O(\log n/n).
\end{aligned}$$

In particular, of course, $W_n \to 0$ $(n \to \infty)$, and so the sequence of approximate integrals converges to the exact integral for any f with $\|f\| < \infty$.

We conclude by making a few remarks about the use of the method. The principal disadvantage of our scheme appears to be that in the error estimate (8) we require knowledge of $\|f\|$ defined in (7). This may be virtually impossible to obtain for functions which are given only tabularly on $(0, 1)$. For integrands given analytically we are in a much better position. In fact, the estimate

$$\|f\| \leq \max_{|z| \leq 1} |f(z)|$$

which is obvious from (7) may be sufficient for most purposes. For instance, in

$$I = \int_0^1 e^{x^4+x} \frac{dx}{\sqrt{x^3+7}}$$

we have clearly

$$\left| e^{z^4+z} \frac{1}{\sqrt{7+z^3}} \right| \leq \frac{e^2}{\sqrt{6}} \qquad (|z| \leq 1)$$

and so the error would be less than $W_n^{\frac{1}{2}} e^2 6^{-\frac{1}{2}}$ in this case.

Next the estimate (8) will be unfavorable compared to estimates from, say, Gauss-Quadrature in the case of a function with slowly growing derivatives. A function like e^x on $(0, 1)$ is an example of this kind. In the other direction, we may get considerably more favorable estimates from the present method if the integrand is very large or infinite near the right hand end-point of integration. An extreme example of this kind is

$$I = \int_0^1 \log\frac{1}{1-x}\,\frac{dx}{x} = \frac{\pi^2}{6}$$

in which no error estimate is available at all from the usual Gauss-quadrature formulae whereas (8) tells us that the error is surely less than $\frac{\pi^2}{6} W_n^{\frac{1}{2}}$ with the present method. For a less extreme case, consider $f(x) = e^{\lambda x}$. For fixed n we would get a Gaussian error estimate of the form $C_n \lambda^{2n} e^{\lambda}$. With the present method our estimate is

$$W_n^{\frac{1}{2}} \left\{ \sum_{k=0}^{\infty} \frac{\lambda^{2k}}{k!^2} \right\}^{\frac{1}{2}} \sim W_n^{\frac{1}{2}} \frac{e^{\lambda}}{(4\pi\lambda)^{\frac{1}{4}}} \qquad (\lambda \to \infty).$$

Evidently if n is fixed then for large enough λ the latter will be superior.

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