Best Approximate Integration Formulas and Best Error Bounds

By Don Secrest

1. Introduction. Let $f(x)$ be a member of the class of functions

$$
\begin{aligned}
(1.1)\qquad & F_n[x_1, x_m] \\
& = \{f(x) \mid f \in C^{n-1}[x_1, x_m], f^{(n-1)} \text{ absolutely continuous}, f^{(n)} \in L^2(x_1, x_m)\}.
\end{aligned}
$$

Further, let $f(x_i) = f_i$, $i = 1, \cdots, m$. We shall refer to the points, (x_i, f_i), as the *fixed points*. We wish to find an optimal approximation to the integral

$$(1.2)\qquad F(f) = \int_{x_1}^{x_m} f(x)\, dx.$$

We shall assume a bound M on the nth derivative of f of the form,

$$(1.3)\qquad \int_{x_1}^{x_m} [f^{(n)}(x)]^2\, dx \leqq M.$$

This is a pseudonorm which may be derived from the bilinear form

$$(1.4)\qquad [f, g] = \int_{x_1}^{x_m} f^{(n)}(x) g^{(n)}(x)\, dx.$$

Following Golomb and Weinberger [1], we introduce a new bilinear form

$$(1.5)\qquad (f, g) = [f, g] + \sum_{i=1}^{n} f(x_i) g(x_i).$$

In this way we obtain a true norm since the quadratic form, (f, f), is positive definite if $m \geqq n$. If m is not greater than or equal to n we cannot form a norm in this way. Now we may write

$$(1.6)\qquad (f, f) \leqq r^2 \equiv M + \sum_{i=1}^{n} f_i^2.$$

We may now express any function f which passes through the *fixed points* as

$$(1.7)\qquad f = \bar{u} + \frac{F(f) - F(\bar{u})}{F(\bar{y})}\, \bar{y} + w,$$

where $\bar{u}$ is the function of smallest norm through the *fixed points*, $\bar{y}$ is the function such that $(\bar{y}, \bar{y}) = 1$ and $y(x_i) = 0$, $i = 1, \cdots, m$,

$$(1.8)\qquad F(\bar{y}) = \sup\{|F(v)| \mid (v, v) = 1; v(x_i) = 0, i = 1, \cdots, m\},$$

and w is the remainder. Golomb and Weinberger [1] have shown that $(\bar{u}, \bar{y}) = 0$, $(\bar{u}, w) = 0$ and $(\bar{y}, w) = 0$. Thus

$$(1.9)\qquad r^2 \geqq (f, f) \geqq (\bar{u}, \bar{u}) + \left(\frac{F(f) - F(\bar{u})}{F(\bar{y})}\right)^2$$

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or

$$(1.10)\quad F(\bar{u}) - F(\bar{y})(r^2 - (\bar{u}, \bar{u}))^{1/2} \leqq F(f) \leqq F(\bar{u}) + F(\bar{y})(r^2 - (\bar{u}, \bar{u}))^{1/2}.$$

Thus the optimal approximation to f is $\bar{u}$. This does not depend on the particular linear functional, F, we wish to approximate.

2. Determination of $\bar{u}$ and $\bar{y}$. The function, $\bar{u}$, which minimizes

$$(2.1)\qquad (f, f) = \int_{x_1}^{x_m} [f^{(n)}(x)]^2\, dx + \sum_{i=1}^{n} f^2(x_i)$$

and passes through the *fixed points* is the function which minimizes the integral in (2.1) as the sum is a constant for any such function. This problem was solved in [2] for the case $n = 2$ and later in [3] for any n. They show that $\bar{u}$ is the spline function of order $2n - 1$. A spline function is defined as follows:

(a) The spline of order r, S_r, is a polynomial of degree r in the intervals

$$(-\infty, x_1), [x_1, x_2), \cdots, [x_m, \infty).$$

(b) S_r has continuous derivatives through the $(r - 1)$st. Thus for any f in $F_n[x_1, x_m]$ passing through the *fixed points* the spline function S_{2n-1} is the optimal approximant for computing the values of linear functionals. The best approximation to the integral (1.2) is the integral of S_{2n-1}. It is shown in [4] that this integral is the "best integral" of Sard [5], [6], [7].

The function $\bar{y}$ has the properties $(\bar{y}, \bar{y}) = 1$ and $\bar{y}(x_i) = 0$, $i = 1, \cdots, m$. Of all functions y with these properties,

$$(2.2)\qquad F(\bar{y}) \geqq |F(y)|.$$

This problem was solved by Sard [5]. For the best integration formulas,

$$(2.3)\qquad \left| \int_{x_1}^{x_m} f(x)\, dx - \sum_{i=1}^{m} A_i f(x_i) \right| \leqq M^{1/2} \left[\int_{x_1}^{x_m} K^2\, dx \right]^{1/2},$$

where K is the Peano kernel. Thus

$$(2.4)\qquad \int_{x_1}^{x_m} \bar{y}\, dx = \left[\int_{x_1}^{x_m} K^2\, dx \right]^{1/2} = \sqrt{K_2}.$$

For the functions y, $M = 1$ and $y(x_i) = 0$. Thus the maximum value $F(y)$ can take on is $\sqrt{K_2}$. The kernel K^2 was shown [8], [4] to be identical with the monospline whose roots are its knots $x_1, \cdots, x_m$ and for which x_1 and x_m are roots of order $2n$. The monospline for this problem is

$$(2.5)\qquad \bar{y}\sqrt{K_2} = \frac{1}{(2n-1)!} \left[\frac{(x - x_1)^{2n}}{2n} + S_{2n-1}(x) \right].$$

Note that

$$(2.6)\qquad F(\bar{y}) = \sqrt{K_2}.$$

Both $\bar{u}$ and $\bar{y}$ contain $m + n - 1$ unknown coefficients. These may be determined by the m relations $\bar{u}(x_i) = f_i$ and $\bar{y}(x_i) = 0$ and the $n - 1$ relations

$$\bar{u}^{(i)}(x_m) = y^{(i)}(x_m) = 0, \qquad i = n, \cdots, 2n - 2.$$

3. Results. We may compute the coefficients of the spline function $\bar{u}$ by solving a system of linear equations. Let us define a matrix,

$$\mathbf{C} = \begin{bmatrix} \mathbf{D} & \mathbf{L} \\ \mathbf{H}^{\mathsf{T}} & \mathbf{0} \end{bmatrix}, \tag{3.1}$$

where the superscript T denotes transposition. $\mathbf{D}$ is an $(m - 1)$-by-$(m - 1)$ order matrix with

$$D_{ij} = (x_{m+1-i} - x_j)_+^{2n-1}, \tag{3.2}$$

where the subscript $+$ is defined as follows:

$$(y)_+ = \begin{cases} y & y > 0, \\ 0 & y \leqq 0, \end{cases} \tag{3.3}$$

$$L_{ij} = (x_{m+1-i} - x_1)^{n-j}, \tag{3.4}$$

and

$$H_{ij} = (x_m - x_i)^{n-j},$$

and $\mathbf{0}$ is an $(n - 1)$-by-$(n - 1)$ order null matrix. Let us further define vectors

$$\mathbf{F}_L = \begin{bmatrix} \mathbf{f}_L \\ \mathbf{0} \end{bmatrix}, \qquad \mathbf{F}_H = \begin{bmatrix} \mathbf{f}_H \\ \mathbf{0} \end{bmatrix}, \tag{3.6}$$

$$\mathbf{T}_L = \begin{bmatrix} \mathbf{P}_L \\ \mathbf{d} \end{bmatrix}, \qquad \mathbf{T}_H = \begin{bmatrix} \mathbf{P}_H \\ \mathbf{d} \end{bmatrix}, \tag{3.7}$$

where

$$\mathbf{f}_L = \begin{bmatrix} f_m - f_1 \\ \vdots \\ f_2 - f_1 \end{bmatrix}, \qquad \mathbf{f}_H = \begin{bmatrix} f_m - f_1 \\ \vdots \\ f_m - f_{m-1} \end{bmatrix}, \tag{3.8}$$

$$\mathbf{P}_L = \begin{bmatrix} (x_m - x_1)^{2n}/2n \\ \vdots \\ (x_2 - x_1)^{2n}/2n \end{bmatrix}, \qquad \mathbf{P}_H = \begin{bmatrix} (x_m - x_1)^{2n}/2n \\ \vdots \\ (x_m - x_{m-1})^{2n}/2n \end{bmatrix}, \tag{3.9}$$

and

$$\mathbf{d} = \begin{bmatrix} (x_m - x_1)^n/n \\ \vdots \\ (x_m - x_1)^2/2 \end{bmatrix}. \tag{3.10}$$

In terms of these quantities the coefficients in $\bar{u}$ are

$$a_i = [\mathbf{C}^{-1}\cdot\mathbf{F}_L]_i, \qquad i = 1, \cdots, n + m - 2, \tag{3.11}$$

where a_i is the coefficient of the term $(x - x_i)_+^{2n-1}$ in $\bar{u}$ when $i < m$, and it is the coefficient of the term $(x - x_1)^{m+n-i-1}$ for $i \geqq m$. Thus the best integral of f is

$$F(\bar{u}) = \mathbf{T}_H{}^{\mathsf{T}}\cdot\mathbf{C}^{-1}\cdot\mathbf{F}_L + (x_m - x_1)f_1 \tag{3.12}$$

or, by symmetry,

$$F(\bar{u}) = \mathbf{F}_H{}^{\mathsf{T}}\cdot\mathbf{C}^{\mathsf{T}-1}\cdot\mathbf{T}_L + (x_m - x_1)f_m\,. \tag{3.13}$$

The maximum error bound for this integral is, by (1.10), (1.5) and (1.6),

$$(3.14)\qquad \begin{aligned} E_{\text{best}} &= F(\bar{y})(r^2 - (\bar{u}, \bar{u}))^{1/2} \\ &= ((M - [\bar{u}, \bar{u}])K_2)^{1/2}. \end{aligned}$$

We may compute $[\bar{u}, \bar{u}]$ by integration by parts:

$$(3.15)\qquad \begin{aligned} [\bar{u}, \bar{u}] &= \int_{x_1}^{x_m} \bar{u}^{(n)}\bar{u}^{(n)}\, dx \\ &= (-1)^{n-1} \int_{x_1}^{x_m} \bar{u}^{(2n-1)}\bar{u}'\, dx \\ &= (-1)^{n-1}(2n-1)! \sum_{i=1}^{m-1} a_i(f_m - f_i) \\ &= (-1)^{n-1}(2n-1)!\, \mathbf{F}_H{}^{\mathsf{T}}\cdot \mathbf{C}^{-1}\cdot \mathbf{F}_L . \end{aligned}$$

Since $\bar{y}$ is a monospline with the same knots as the spline $\bar{u}$ we may compute its coefficients in terms of the matrix $\mathbf{C}$ also. From (2.5) and the fact that $\bar{y}(x_i) = 0$ and x_1 and x_m are zeros of multiplicity $2n$, we may compute the coefficients in S_{2n-1} of (2.5). Then upon integrating $\bar{y}$ we obtain

$$(3.16)\qquad F(\bar{y}) = \frac{(-1)^n}{[(2n-1)!]}\left[\frac{(x_m - x_1)^{2n+1}}{2n(2n+1)} - \mathbf{T}_H{}^{\mathsf{T}}\cdot \mathbf{C}^{-1}\cdot \mathbf{T}_L\right]\frac{1}{K_2^{1/2}} = K_2^{1/2}.$$

4. Discussion. We may obtain the coefficients for the best integration formulas by noticing that the functional values enter (3.12) linearly. Thus we may write

$$(4.1)\qquad F(\bar{u}) = \sum_{i=1}^{m} W_i f_i ,$$

where

$$(4.2)\qquad W_{m+1-i} = (\mathbf{T}_H{}^{\mathsf{T}}\cdot \mathbf{C}^{-1})_i , \qquad i = 1, \cdots , m-1,$$

and

$$(4.3)\qquad W_1 = x_m - x_1 - \sum_{i=2}^{m} W_i .$$

Similar relations follow from (3.13).

When $m = n$, the best integration formulas are the same as those obtained by integrating the Lagrange interpolation coefficient. In this case $[\bar{u}, \bar{u}] = 0$ and so the error bound is just the usual bound obtained from the Peano kernel. When $[\bar{u}, \bar{u}] \neq 0$ the error bound (3.14) is better than the bound used by Sard [5], [6], [7], for these formulas.

In this paper we have discussed the error bound for integration. The spline function $\bar{u}$ is the optimal approximation for any function in $F_n[x_1 , x_m]$ which passes through the *fixed points* and may be used for evaluating any linear functional. To find the optimal error bound it is only necessary to compute the corresponding $\bar{y}$. In this way we may find optimal error bounds for interpolation and differentiation. This will be discussed further in a future paper.

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