Best Approximate Integration Formulas and Best Error Bounds

By Don Secrest

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

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

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

\[ F(f) = \int_{x_1}^{x_m} f(x) \, dx. \tag{1.2} \]

We shall assume a bound \( M \) on the \( n \)th derivative of \( f \) of the form,

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

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

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

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

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

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

\[ (f, f) \leq r^2 = M + \sum_{i=1}^{n} f_i^2. \tag{1.6} \]

We may now express any function \( f \) which passes through the fixed points as

\[ f = \bar{u} + \frac{F(f) - F(\bar{u})}{F(\bar{y})} \bar{y} + w, \tag{1.7} \]

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 \( y(x_i) = 0, i = 1, \ldots, m\),

\[ F(\bar{y}) = \sup\{|F(v)| \mid (v, v) = 1; v(x_i) = 0, i = 1, \ldots, m\}, \tag{1.8} \]

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

\[ r^2 \geq (f, f) \geq (\bar{u}, \bar{u}) + \left( \frac{F(f) - F(\bar{u})}{F(\bar{y})} \right)^2. \tag{1.9} \]

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\[(1.10) \quad F(\bar{u}) - F(\breve{y})(r^2 - (\bar{u}, \bar{u}))^{1/2} \leq F(f) \leq F(\bar{u}) + F(\breve{y})(r^2 - (\bar{u}, \bar{u}))^{1/2}.\]

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 \(\breve{y}\). The function, \(\bar{u}\), which minimizes

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

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

\[(-\infty, x_1), [x_1, x_2), \ldots, [x_m, \infty).\]

(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 \(\breve{y}\) has the properties \((\breve{y}, \breve{y}) = 1\) and \(\breve{y}(x_i) = 0, i = 1, \ldots, m\). Of all functions \(y\) with these properties,

\[(2.2) \quad F(\breve{y}) \geq |F(y)|.\]

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

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

where \(K\) is the Peano kernel. Thus

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

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 \(x_1, \ldots, x_m\) and for which \(x_1\) and \(x_m\) are roots of order \(2n\). The monospline for this problem is

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

Note that

\[(2.6) \quad F(\breve{y}) = \sqrt{K_2}.\]

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

\[\bar{u}^{(i)}(x_m) = y^{(i)}(x_m) = 0, \quad i = n, \ldots, 2n - 2.\]
3. Results. We may compute the coefficients of the spline function \( \tilde{u} \) by solving a system of linear equations. Let us define a matrix,

\[
C = \begin{bmatrix}
D & L \\
H^T & 0
\end{bmatrix},
\]

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

\[
D_{ij} = (x_{m+1-i} - x_j)^{2n-1},
\]

where the subscript \(+\) is defined as follows:

\[
(y)_+ = \begin{cases} 
  y & y > 0, \\
  0 & y \leq 0,
\end{cases}
\]

and

\[
H_{ij} = (x_m - x_i)^{n-j},
\]

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

\[
F_L = \begin{bmatrix} f_L \\
0
\end{bmatrix}, \quad F_H = \begin{bmatrix} f_H \\
0
\end{bmatrix},
\]

\[
T_L = \begin{bmatrix} P_L \\
d
\end{bmatrix}, \quad T_H = \begin{bmatrix} P_H \\
d
\end{bmatrix},
\]

where

\[
f_L = \begin{bmatrix} f_m - f_1 \\
\vdots \\
f_2 - f_1
\end{bmatrix}, \quad f_H = \begin{bmatrix} f_m - f_1 \\
\vdots \\
f_m - f_{m-1}
\end{bmatrix},
\]

\[
P_L = \begin{bmatrix} (x_m - x_1)^{2n}/2n \\
\vdots \\
(x_2 - x_1)^{2n}/2n
\end{bmatrix}, \quad P_H = \begin{bmatrix} (x_m - x_1)^{2n}/2n \\
\vdots \\
(x_m - x_{m-1})^{2n}/2n
\end{bmatrix},
\]

and

\[
d = \begin{bmatrix} (x_m - x_1)^n/n \\
\vdots \\
(x_m - x_1)^2/2
\end{bmatrix}.
\]

In terms of these quantities the coefficients in \( \tilde{u} \) are

\[
a_i = [C^{-1} \cdot F_L]_i, \quad i = 1, \ldots, n + m - 2,
\]

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

\[
F(\tilde{u}) = T_H^T \cdot C^{-1} \cdot F_L + (x_m - x_1)f_1
\]

or, by symmetry,

\[
F(\tilde{u}) = F_H^T \cdot C^{-1} \cdot T_L + (x_m - x_1)f_m.
\]
The maximum error bound for this integral is, by (1.10), (1.5) and (1.6),

\[ E_{\text{best}} = F(\tilde{y})(r^2 - (\bar{u}, \bar{u}))^{1/2} \]
\[ = ( (M - [\bar{u}, \bar{u}])K_2)^{1/2}. \]

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

\[ [\bar{u}, \bar{u}] = \int_{x_1}^{x_m} \bar{u}^{(n)}\bar{u}^{(n)} \, dx \]
\[ = (-1)^{n-1} \int_{x_1}^{x_m} \bar{u}^{(2n-1)} \, dx \]
\[ = (-1)^{n-1}(2n - 1)! \sum_{i=1}^{m-1} a_i(\bar{f}_m - \bar{f}_i) \]
\[ = (-1)^{n-1}(2n - 1)! \mathbf{F}_H^T \cdot \mathbf{C}^{-1} \cdot \mathbf{F}_L. \]

Since \(\tilde{y}\) 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 \(\tilde{y}(x_i) = 0\) 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 \(\tilde{y}\) we obtain

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

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

\[ F(\bar{u}) = \sum_{i=1}^{m} W_i f_i, \]

where

\[ W_{m+1-i} = (\mathbf{T}_H^T \cdot \mathbf{C}^{-1})_i, \quad i = 1, \ldots, m - 1, \]

and

\[ W_1 = x_m - x_1 - \sum_{i=2}^{m} W_i. \]

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 \(\tilde{y}\). 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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