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Optimal Approximation and Error Bounds in Spaces of Bivariate Functions*

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1. INTRODUCTION

In this paper we consider the problem of finding the optimal approximation to a linear functional F in terms of a given set of other functionals, $F_1, \ldots, F_n$. We shall assume that these functionals are defined on a class of real-valued functions of two real variables having properties similar to the space of functions $B_{p,q}(\alpha, \beta)$ discussed by Sard [21, Chap. 4]. We shall call this class of functions $T^{p,q}(\alpha, \beta)$. In Section 4, we give a precise definition of $T^{p,q}(\alpha, \beta)$ and introduce an inner product which makes f a member of a Hilbert space with a reproducing kernel. We shall only consider linear functionals which are bounded with respect to the norm on the Hilbert space and for which Sard's kernel theorem [21, p. 175] holds. By the optimal approximation we shall mean the linear combination of the F_i which minimizes the norm of the error functional R.

As we shall show in Section 2, the optimal approximation and error bounds can be found if the representers of the functionals involved are known. The representers can be determined if one knows the reproducing kernel for the space. The principal result of this paper is the construction of the reproducing kernel for a Hilbert space of functions in $T^{p,q}(\alpha, \beta)$. We then apply this result to the problem of finding the optimal approximation to a definite integral by a cubature sum. In Section 6 some numerical examples related to approximate multiple integration are given.

The results of this paper are related to the theory of bivariate spline

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functions in that the optimal approximations are splines, i.e., they are piecewise polynomials. These splines differ from the bivariate splines of Ahlberg, Nilson, and Walsh [1, 3] in that the points of interpolation are not restricted to a rectangular grid. Also the splines in this paper are of total degree $2m - 1$ rather than being of odd degree in each variable.

For functions of one variable, the problem of optimal approximation has been studied extensively. References are given below. Let $F^{(k)}[a, b] = \{f \mid f^{(k-1)} \text{ abs cont}, f^{(k)} \in L^2[a, b]\}$. If the functionals F_i, $i = 1,..., n$ have the property that k of them are linearly independent over π_{k-1}, the set of polynomials of degree less than or equal to $k - 1$, $F^{(k)}[a, b]$ is a Hilbert space with respect to the norm

$$\| v \|^2 = \int_a^b [v^{(k)}(x)]^2 \, dx + \sum_{i=1}^{k} [F_i(v)]^2.$$

de Boor and Lynch [12] and Golomb and Weinberger [15] have calculated the reproducing kernel for $F^{(k)}[a, b]$ with respect to this norm. If $F_i(f) = f(x_i)$, $i = 1,..., n$, the optimal approximation is the natural polynomial spline (type II′ spline in the terminology of Ahlberg, Nilson, and Walsh) of degree $2k - 1$ which interpolates f at the points x_i, $i = 1,..., n$. The connection between splines and the optimal approximation of functionals was first pointed out by Schoenberg [23]. Related results have been obtained by Secrest [27–29], who pointed out the connection between splines and the optimal approximations of Golomb and Weinberger [15], and by Ahlberg and Nilson [2] and Schoenberg [25].

2. Representers in Hilbert Space and the Optimal Approximation of Linear Functionals

Let H be a real Hilbert space. Let F be a bounded linear functional on H. We wish to approximate F by a sum $\sum_{i=1}^{n} A_i F_i$ where the F_i are a given set of bounded linear functionals with representers ϕ_i. Golomb and Weinberger [15] and de Boor and Lynch [12] show that the optimal approximation $\bar{F}(f)$ to F at f equals $F(\bar{u})$ where $\bar{u}$ is the element of the Hilbert space of minimum norm among all elements interpolating f with respect to the F_i, $i = 1,..., n$. Then $\bar{u}$ can also be characterized [12] as the element of the subspace $S = \langle \phi_i, i = 1,..., n \rangle$ which interpolates f with respect to the F_i, $i = 1,..., n$.

Optimal error bounds can be obtained from the hypercircle inequality

$$| F(f) - F(\bar{u})| \leqslant \| \bar{R} \| \, [r^2 - (\bar{u}, \bar{u})]^{1/2}, \tag{2.1}$$

where $\bar{R}$ is the optimal error functional and $r^2 \geqslant \| f \|^2$. Let ϕ be the representer of the functional F. Then $\| \bar{R} \| = \| \phi - \sum_{i=1}^{n} A_i^* \phi_i \|$ where the A_i^* are the optimal weights. Let $\bar{\phi} = \phi - \sum_{i=1}^{n} A_i^* \phi_i$. It is shown in [12] that $F_i(\bar{\phi}) = 0$, $i = 1,..., n$. Thus

$$\| \bar{R} \|^2 = (\bar{\phi}, \bar{\phi}) = \bar{R}(\bar{\phi}) = F(\bar{\phi}). \tag{2.2}$$

Therefore the optimal approximation and error bounds can be calculated if the functions $\bar{\phi}$ and $\bar{u}$ can be found. Assume H has the reproducing kernel $K(X, Y)$. If L is a bounded linear functional and h is its representer then $h(X) = L_Y K(X, Y)$, where the subscript Y means that L operates on $K(X, Y)$ as a function of Y. Thus $\bar{\phi}$ and $\bar{u}$ can be calculated directly from the reproducing kernel.

3. Construction of the Reproducing Kernel for the Hilbert space $T_{(\alpha,\beta)}^{p,q}$

For $p \geqslant 1$, let $F^{(p)}[a, b] = \{g \mid g^{(p-1)} \text{abs cont}, g^{(p)} \in L^2[a, b]\}$. Let α be an arbitrary point in $[a, b]$ and let P_i be the linear projection defined by

$$P_i g = g^{(i)}(\alpha) \frac{(x-\alpha)^i}{i!}. \tag{3.1}$$

Then $\bar{P}_i = \sum_{j<i} P_j$ is also a linear projection, $i = 0, 1, 2,...$.
For all functions $g \in F^{(p)}[a, b]$ we have the Taylor series representation

$$\begin{aligned} g(x) &= \sum_{i=0}^{p-1} \frac{(x-\alpha)^i}{i!} g^{(i)}(\alpha) + \int_a^b \frac{(x-t)^{p-1}}{(p-1)!} \psi(\alpha, t, x)\, g^{(p)}(t)\, dt \\ &= \bar{P}_p g(x) + (I - \bar{P}_p)\, g(x), \end{aligned} \tag{3.2}$$

where

$$\psi(\alpha, t, x) = \begin{cases} 1 & \text{if } \alpha \leqslant t < x, \\ -1 & \text{if } x \leqslant t < \alpha, \\ 0 & \text{otherwise.} \end{cases}$$

Likewise for $q \geqslant 1$ and β an arbitrary point in $[c, d]$ let Q_j be the linear projection on $F^{(q)}[c, d]$ defined by

$$Q_j h = h^{(j)}(\beta) \frac{(y-\beta)^j}{j!}. \tag{3.3}$$

Then $\bar{Q}_j = \sum_{i<j} Q_i$ is also a linear projection, $j = 0, 1, 2,...$. For all functions $h \in F^{(q)}[c, d]$ we have the Taylor series representation

$$\begin{aligned} h(y) &= \sum_{j=0}^{q-1} \frac{(y-\beta)^j}{j!} h^{(j)}(\beta) + \int_c^d \frac{(y-u)^{q-1}}{(q-1)!} \psi(\beta, u, y)\, h^{(q)}(u)\, du \\ &= \bar{Q}_q h(y) + (I - \bar{Q}_q)\, h(y). \end{aligned} \tag{3.4}$$

Let D be the rectangle $[a, b] \times [c, d]$. We now wish to construct a Taylor series expansion for real-valued functions defined on D. We initially assume that $f \in F^{(m)}[a, b] \otimes F^{(m)}[c, d]$, where $m = p + q$. We expand the identity operator as follows:

$$\begin{aligned} I = I \otimes I &= \bar{P}_p \otimes \bar{Q}_q + \bar{P}_p \otimes (I - \bar{Q}_q) + (I - \bar{P}_p) \otimes \bar{Q}_q \\ &\quad + (I - \bar{P}_p) \otimes (I - \bar{Q}_q) \\ &= \sum_{i<p} \sum_{j<q} P_i \otimes Q_j + \sum_{i<p} P_i \otimes (I - \bar{Q}_q) + (I - \bar{P}_p) \otimes \sum_{j<q} Q_j \\ &\quad + (I - \bar{P}_p) \otimes (I - \bar{Q}_q). \end{aligned} \tag{3.4}$$

We can write $(I - \bar{Q}_q)$ as $(I - \bar{Q}_{m-i}) + \sum_{q \leqslant j < m-i} Q_j$. Likewise

$$(I - \bar{P}_p) = (I - \bar{P}_{m-j}) + \sum_{p \leqslant i < m-j} P_i .$$

Therefore,

$$\sum_{i<p} P_i \otimes (I - \bar{Q}_q) = \sum_{i<p} \sum_{q \leqslant j < m-i} P_i \otimes Q_j + \sum_{i<p} [P_i \otimes (I - \bar{Q}_{m-i})],$$

and

$$(I - \bar{P}_p) \otimes \sum_{j<q} Q_j = \sum_{j<q} \sum_{p \leqslant i < m-j} P_i \otimes Q_j + \sum_{j<q} [(I - \bar{P}_{m-j}) \otimes Q_j].$$

Thus

$$\begin{aligned} I = \sum_{i+j<m} P_i \otimes Q_j + \sum_{j<q} [(I - \bar{P}_{m-j}) \otimes Q_j] + \sum_{i<p} [P_i \otimes (I - \bar{Q}_{m-i})] \\ + (I - \bar{P}_p) \otimes (I - \bar{Q}_q). \end{aligned} \tag{3.5}$$

This implies that $f(x, y) \in F^{(m)}[a, b] \otimes F^{(m)}[c, d]$ has the representation

$$\begin{aligned} f(x, y) &= \sum_{i+j<m} \frac{(x-\alpha)^i}{i!} \frac{(y-\beta)^j}{j!} f_{i,j}(\alpha, \beta) \\ &\quad + \sum_{j=0}^{q-1} \frac{(y-\beta)^j}{j!} \int_a^b \frac{(x-t)^{m-j-1}}{(m-j-1)!} \psi(\alpha, t, x) f_{m-j,j}(t, \beta)\, dt \\ &\quad + \sum_{i=0}^{p-1} \frac{(x-\alpha)^i}{i!} \int_c^d \frac{(y-u)^{m-i-1}}{(m-i-1)!} \psi(\beta, u, y) f_{i,m-i}(\alpha, u)\, du \\ &\quad + \int_a^b \int_c^d \frac{(x-t)^{p-1}}{(p-1)!} \frac{(y-u)^{q-1}}{(q-1)!} \psi(\alpha, t, x)\, \psi(\beta, u, y) f_{p,q}(t, u)\, dt\, du, \end{aligned}$$

where we use the notation $f_{i,j}$ to denote partial derivatives. This is just the representation obtained by Sard [21, p. 163].

(3.5) gives a decomposition of $F^{(m)}[a, b] \otimes F^{(m)}[c, d]$ into a direct sum of subspaces.

$$\begin{aligned}(f,f)_* &= \int_a^b \int_c^d [f_{p,q}(x, y)]^2\, dx\, dy + \sum_{j<q} \int_a^b [f_{m-j,j}(x, \beta)]^2\, dx \\ &\quad + \sum_{i<p} \int_c^d [f_{i,m-i}(\alpha, y)]^2\, dy + \sum_{i+j<m} [f_{i,j}(\alpha, \beta)]^2 \qquad (3.7) \\ &= [f,f] + \sum_{i+j<m} [f_{i,j}(\alpha, \beta)]^2\end{aligned}$$

is an inner product on $F^{(m)}[a, b] \otimes F^{(m)}[c, d]$. We note that $[f, f]$ is a seminorm with null-space $\mathcal{Q}$ equal to the set of polynomials of degree less than or equal to $m - 1$. The dimension of $\mathcal{Q}$ is $k = m(m + 1)/2$.

It can easily be seen that $F^{(m)}[a, b] \otimes F^{(m)}[c, d]$ is not the largest class of functions for which (3.6) holds. Equivalently, $F^{(m)}[a, b] \otimes F^{(m)}[c, d]$ is not complete under this norm. We complete this space by completing each subspace. The completion of $(I - \bar{P}_{m-j})\, F^{(m)}[a, b]$ is $(I - \bar{P}_{m-j})\, F^{(m-j)}[a, b]$, $j = 0,\ldots, q - 1$, and the completion of $(I - \bar{Q}_{m-i})\, F^{(m)}[c, d]$ is $(I - \bar{Q}_{m-i})\, F^{(m-i)}[c, d]$, $i = 0,\ldots, p - 1$. This makes all of the tensor product spaces in the summations complete. We claim that the completion of $(I - \bar{P}_p)\, F^{(p)}[a, b] \otimes (I - \bar{Q}_q)\, F^{(q)}[c, d]$ is the set χ of all functions with the property that

$$\begin{aligned}&f_{i,j}(x, y) \in C[D],\ i < p, j < q, \\ &f_{p-1,q-1}(x, y) \text{ is abs cont}, f_{p,q} \in L^2[D] \qquad (3.8) \\ &\bar{P}_p f = \bar{Q}_q f = 0.\end{aligned}$$

(For a definition of absolute continuity as applied to functions of two variables see Sard [21, p. 534].) To prove this let $\{f^\mu\}$ be a Cauchy sequence in χ. Then $\{f^\mu_{p,q}\}$ is a Cauchy sequence in $L^2[D]$ which converges to an element $e \in L^2[D]$. We must show that there exists an element $f \in \chi$ with the property $f_{p,q} = e$.

Let

$$f = \int_\alpha^x \int_\beta^y \frac{(x - t)^{p-1}}{(p - 1)!} \frac{(y - u)^{q-1}}{(q - 1)!}\, e(t, u)\, dt\, du.$$

Then $f_{p,q} = e$. We now show that $f \in \chi$. There exist constants M, N such that

$$\left| \frac{(x - t)^{p-1-i}}{(p - 1 - i)!} \right| < M, \qquad 0 \leqslant i \leqslant p - 1,$$

$$\left| \frac{(y - u)^{q-1-j}}{(q - 1 - j)!} \right| < N, \qquad 0 \leqslant j \leqslant q - 1.$$

Since $e \in L^2[D]$, there exists a sequence $\{e^\mu\}$ of continuous functions defined on D such that

$$\| e - e^\mu \|_{L^2} \to 0 \text{ as } \mu \to \infty.$$

We let

$$s^\mu = \int_\alpha^x \int_\beta^y \frac{(x-t)^{p-1}}{(p-1)!} \frac{(y-u)^{q-1}}{(q-1)!} e^\mu(t, u)\, dt\, du, \qquad \mu = 1, 2, \ldots.$$

Then for $i < p, j < q$

$$\begin{aligned} &|f_{i,j}(x, y) - s^\mu_{i,j}(x, y)| \\ &\quad = \left| \int_\alpha^x \int_\beta^y \frac{(x-t)^{p-1-i}}{(p-1-i)!} \frac{(y-u)^{q-1-j}}{(q-1-j)!} [e(t, u) - e^\mu(t, u)]\, dt\, du \right| \\ &\quad \leqslant \left(\int_\alpha^x \int_\beta^y \left| \frac{(x-t)^{p-1-i}}{(p-1-i)!} \frac{(y-u)^{q-1-j}}{(q-1-j)!} \right|^2 dt\, du \right)^{1/2} \| e - e^\mu \|_{L^2} \\ &\quad \leqslant (b-a)(d-c)\, MN \| e - e^\mu \|_{L^2} \to 0 \end{aligned}$$

uniformly as $\mu \to \infty$. Therefore $f_{i,j}$, $i < p, j < q$, are continuous since they are the uniform limits of continuous functions. The function $f_{p-1,q-1}(x, y) = \int_\alpha^x \int_\beta^y e(t, u)\, dt\, du$ is absolutely continuous since $f_{p,q}(x, y) = e(x, y)$ is in $L^2[D]$ and thus is defined a.e. and is integrable on D. Clearly f satisfies the last property in (3.8). Thus we have a space which is the direct sum of complete spaces and therefore is complete. We call this space $T^{p,q}(\alpha, \beta)$. It has the properties

$$\begin{aligned} &f_{i,j} \in C[D],\ i < p, j < q, \\ &f_{m-j-1,j}(x, \beta) \text{ abs cont}, f_{m-j,j}(x, \beta) \in L^2[a, b],\ j = 0, \ldots, q-1, \\ &f_{i,m-i-1}(\alpha, y) \text{ abs cont}, f_{i,m-i}(\alpha, y) \in L^2[c, d],\ i = 0, \ldots, p-1, \\ &f_{p-1,q-1}(x, y) \text{ abs cont}, f_{p,q} \in L^2[D]. \end{aligned} \tag{3.9}$$

Since the derivatives $f_{p+i,j}(x, y)$, $i = 0, \ldots, q-j$, $j = 0, \ldots, q-1$, need only exist along the line $y = \beta$, all partials with respect to y must be taken before any partials with respect to x of order greater than p are taken. A similar condition holds for $f_{i,q+j}(x, y)$, $j = 0, \ldots, p-i$, $i = 0, \ldots, p-1$.

We now construct the reproducing kernel for $T^{p,q}(\alpha, \beta)$ with norm (3.7). Let $G_1, \ldots, G_k$, be the functionals defined by

$$G_\mu(f) = f_{i,j}(\alpha, \beta), \qquad \mu = 1, \ldots, k,$$

and let $q_1, \ldots, q_k$ be elements of $\mathscr{H}$ with the property

$$G_i(q_j) = \delta_{ij},\ 1 \leqslant i, j \leqslant k.$$

Note that the $q_1, \ldots, q_k$ are just the functions $(x-\alpha)^i/i!\,(y-\beta)^j/j!$, $i+j<m$. We also let X be the point (x, y) and let $Y=(\xi, \eta)$.

THEOREM 1. *The reproducing kernel* $K^*(X, Y)$ *for the space* $T^{p,q}(\alpha, \beta)$ *with norm given by* (3.7) *is*

$$K^*(X, Y) = \theta^{2p-1}(x, \xi)\,\theta^{2q-1}(y, \eta) + \sum_{j=0}^{q-1} \frac{(\eta-\beta)^j}{j!}\frac{(y-\beta)^j}{j!}\,\theta^{2(m-j)-1}(x, \xi)$$
$$+ \sum_{i=0}^{p-1} \frac{(x-\alpha)^i}{i!}\frac{(\xi-\alpha)^i}{i!}\,\theta^{2(m-i)-1}(y, \eta) + \sum_{i=1}^{k} q_i(X)\,q_i(Y) \tag{3.10}$$

where

$$\theta^{2p-1}(x, \xi) = (-1)^p \left\{ \frac{(x-\xi)^{2p-1}}{(2p-1)!} - \sum_{i=0}^{p-1} \left[\frac{(\alpha-\xi)_+^{2p-1-i}}{(2p-1-i)!}\frac{(x-\alpha)^i}{i!} + (-1)^i \frac{(x-\alpha)_+^{2p-1-i}}{(2p-1-i)!}\frac{(\xi-\alpha)^i}{i!} \right] \right\}$$

and $\theta^{2q-1}(y, \eta)$ *is defined similarly.*

Proof. The proof is based on the fact that $T^{p,q}(\alpha, \beta)$ is the direct sum of tensor products of single-variable spaces for which the reproducing kernels are known. Let $K_i(X, Y)$ be the reproducing kernel of the i-th element in the direct sum. Then $(f, \sum_i K_i)_{(Y)} = \sum_i (f_i, K_i)_{i(Y)} = \sum_i f_i(X) = f(X)$, where f_i is the projection of f onto the i-th subspace. Thus $K^*(X, Y) = \sum_i K_i(X, Y)$. Each subspace is the tensor product of two single-variable spaces. It can easily be seen that the norms on each of these subspaces have the property that $(f, g)_i = ((f, g_1)_i', g_2)_i''$, where g is the product of elements g_1 and g_2 in the component spaces and the primes are used to indicate the inner products on these spaces. Thus each $K_i(X, Y)$ is the product of the reproducing kernels on the respective single-variable spaces.

de Boor and Lynch [12] have calculated the reproducing kernel for the space $F^{(p)}[a, b]$ with norm given by

$$(f, f) = \sum_{i=0}^{p-1} [f^{(i)}(\alpha)]^2 + \int_a^b [f^{(p)}(x)]^2\,dx. \tag{3.11}$$

It is

$$\sum_{i=0}^{p-1} \frac{(x-\alpha)^i}{i!}\frac{(\xi-\alpha)^i}{i!} + \int_a^b g^p(x, t)\,g^p(\xi, t)\,dt, \tag{3.12}$$

where $g^p(x, t) = (x-t)^{p-1}/(p-1)!\;\psi(\alpha, t, x)$.

Thus

$$K^*(X, Y)$$

$$= \sum_{i=1}^{k} q_i(X)\, q_i(Y) + \sum_{j=0}^{q-1} \frac{(y-\beta)^j}{j!} \frac{(\eta-\beta)^j}{j!} \int_a^b g^{m-j}(x, t)\, g^{m-j}(\xi, t)\, dt$$

$$+ \sum_{i=0}^{p-1} \frac{(x-\alpha)^i}{i!} \frac{(\xi-\alpha)^i}{i!} \int_c^d g^{m-i}(y, u)\, g^{m-i}(\eta, u)\, du$$

$$+ \left[\int_a^b g^p(x, t)\, g^p(\xi, t)\, dt\right]\left[\int_c^d g^q(y, u)\, g^q(\eta, u)\, du\right]. \tag{3.13}$$

Evaluation of the integrals in (3.13) gives (3.10), which concludes the proof.

4. Construction of the Reproducing Kernel for the Hilbert Space H

In de Boor and Lynch [12] it was shown that the optimal approximation $\bar{F}(f)$ to F at f is exact for the n-dimensional subspace spanned by the representers of the F_i, $i = 1,..., n$. We would like to have this approximation also be exact for functions in $\mathcal{Q}$, i.e., polynomials of degree less than or equal to $m - 1$. We do this by considering a norm similar to (3.7) but involving the approximating functionals $F_1,..., F_n$, rather than the G_i, $i = 1,..., k$. This will force $\mathcal{Q}$ to be contained in the subspace $S = \langle \phi_1,..., \phi_n \rangle$ where ϕ_i is the representer of F_i, $i = 1,..., n$.

We shall assume that $F, F_1,..., F_n$ are linearly independent and are of the form

$$Lf = \sum_{\substack{i<p\\ j<q}} \iint f_{i,j}(x, y)\, d\mu^{i,j}(x, y)$$
$$+ \sum_{\substack{i+j<m\\ i\geqslant p}} \int f_{i,j}(x, \beta)\, d\mu^{i,j}(x) + \sum_{\substack{i+j<m\\ j\geqslant q}} \int f_{i,j}(\alpha, y)\, d\mu^{i,j}(y) \tag{4.1}$$

where the functions $\mu^{i,j}$ are of bounded variation. We also assume that the functionals $F_1,..., F_n$, have the property that there exists a set of weights A_i, $i = 1,..., n$ such that $F(f) - \sum_{i=1}^{n} A_i F_i(f) = 0$ for all $f \in \mathcal{Q}$, the null space of $[f, f]$. Let $F_1,..., F_l$ be a subset of the F_i which is maximally linearly independent over $\mathcal{Q}$. If $l = k$, then

$$(f, f) = \sum_{i=1}^{k} [F_i f]^2 + [f, f] \tag{4.2}$$

defines a norm on $T^{p,q}(\alpha, \beta)$. If $l < k$, then there exists a subspace V_0 of dimension $k - l$ with the property that $F_1(f) = \cdots = F_n(f) = 0$ for all f in V_0. By our assumption, $F(f) = 0$ for all $f \in V_0$. Let $\Phi_1, ..., \Phi_{k-l}$ be $k - l$ of the functionals G_i, $i = 1,..., k$, chosen so that $F_1, ..., F_l, \Phi_1, ..., \Phi_{k-l}$, are linearly independent over $\mathcal{Q}$. Let P be the linear projection defined by

$$Pf(X) = \sum_{i=1}^{k-l} \Phi_i(f)\, p_i(X),$$

where $p_1, ..., p_{k-l}$ are elements of V_0 with the property that

$$\Phi_i(p_j) = \delta_{ij}, \; 1 \leqslant i, j \leqslant k - l.$$

Note that the p_i are a subset of the q_i, $i = 1,..., k$. Our approximation problem is not affected if we consider the problem on $H = (I - P)\, T^{p,q}(\alpha, \beta)$. H is a Hilbert space with respect to the norm

$$(f, f) = [f, f] + \sum_{i=1}^{l} [F_i(f)]^2. \tag{4.3}$$

In many applications it will happen that $k = l$. As an example of when this is not the case consider $T^{3,3}(0, 0)$ with $n = 7$, $F(f) = \int_{-1}^{1} \int_{-1}^{1} f(x, y)\, dx\, dy$, $F_i(f) = f(x_i, y_i)$, $i = 1,..., 7$, where the (x_i, y_i) are the points of the Radon 7-point, fifth-degree cubature formula. (See Stroud [31].) In this case $k = 21$. This formula is exact for all elements in $\mathcal{Q}$, the set of polynomials of degree less than or equal to five, and thus we can construct a Hilbert space in the manner described above.

We now construct the reproducing kernel function for the Hilbert Space H. Let

$$P_{(X)}P_{(Y)}K^*(X, Y) = K_1^*(X, Y) = \sum_{i=1}^{k-l} p_i(X)\, p_i(Y),$$

and

$$(I - P)_{(X)}\, (I - P)_{(Y)}\, K_1^*(X, Y) = \bar{f}(X, Y) = K^*(X, Y) - \sum_{i=1}^{k-l} p_i(X)\, p_i(Y). \tag{4.4}$$

Let $f \in T^{p,q}(\alpha, \beta)$. Then

$$(I - P) f(Y) = (f, K^*(X, Y) - K_1^*(X, Y))* = (f, \bar{f}) = (f, \bar{f})_* - \sum_{i=1}^{k-l} \Phi_i(f)\, \Phi_i(\bar{f}).$$

Therefore we have shown

LEMMA 1. *The reproducing kernel function for the Hilbert space H with norm given by*

$$(f,f) = [f,f] + \sum_{i=1}^{k} [G_i f]^2 \qquad G_i \notin \{\Phi_1, \ldots, \Phi_{k-l}\}$$

is $\bar{f}(X, Y)$.

Let $\bar{P}$ be the projection operator from H onto $(I - P)\mathcal{Q}$ defined by

$$\bar{P}f(X) = \sum_{i=1}^{l} F_i(f)\, \phi_i(X)$$

where the ϕ_i, $i = 1,\ldots, l$ are defined by $\phi_i \in (I - P)\mathcal{Q}$ and

$$F_i(\phi_j) = \delta_{ij} \qquad 1 \leqslant i, j \leqslant l.$$

THEOREM 2. *The reproducing kernel $K(X, Y)$ for the Hilbert space H with norm given by* (4.3) *is*

$$(I - \bar{P})_X (I - \bar{P})_Y \bar{f}(X, Y) + \sum_{i=1}^{l} \phi_i(X)\, \phi_i(Y).$$

Proof. Let $v \in H$.

$$\bar{P}v(Y) = \left(v, \sum_{i=1}^{l} \phi_i(X)\, \phi_i(Y)\right).$$

We now must show that

$$(I - \bar{P})v\,(Y) = (v, (I - \bar{P})_X (I - \bar{P})_Y \bar{f}(X, Y))_X.$$

$$\begin{aligned}(v, (I - \bar{P})_X (I - \bar{P})_Y \bar{f}(X, Y))_X &= [v, (I - \bar{P})_X (I - \bar{P})_Y \bar{f}(X, Y)]_X \\ &= [v, (I - \bar{P})_Y \bar{f}(X, Y)] \\ &= (I - \bar{P})_Y\, [v, \bar{f}(X, Y)],\end{aligned}$$

where the interchange of integration and the operator $\bar{P}$ is justified by Sard's kernel theorem [21, p. 175]. But $[v, \bar{f}(X, Y)]_X = (I - \tilde{P})_Y\, v(Y)$ where $\tilde{P}$ is the projection from H onto $(I - P)\mathcal{Q}$ defined by

$$\tilde{P}f(X) = \sum_{i=1}^{k} G_i(f)\, q_i(X) \qquad G_i \notin \{\Phi_1, \ldots, \Phi_{k-l}\}.$$

Then $(I - \bar{P})_Y (I - \tilde{P})_Y v = (I - \bar{P})_Y v$, which completes the proof.

Remark 1. The proof of the preceding theorem is largely independent of the particular Hilbert space $\mathscr{H}$. It in fact holds for any real Hilbert space $\mathscr{H}$ whose norm is obtained by adding a finite sum of squares of linear functionals to a semi-norm $[\cdot, \cdot]$ with a finite dimensional null space η of dimension l. Assume that the reproducing kernel $K^*(X, Y)$ can be found for a particular norm

$$(v, v)_* = [v, v] + \sum_{i=1}^{l} [G_i v]^2.$$

where $G_1, ..., G_l$, are any set of "sufficiently smooth" linear functionals, i.e., functionals which are bounded and for which the identity

$$(G_i)_Y [v, K^*(X, Y)]_{(X)} = [v, (G_i)_Y K^*(X, Y)]_{(X)}$$

holds, which are linearly independent over η. Let $L_1, ..., L_l$ be any other set of "sufficiently smooth" linear functionals which are also linearly independent over η and let $\bar{P}$ be the projection operator from $\mathscr{H}$ onto η defined by

$$\bar{P}v = \sum_{i=1}^{l} L_i v q_i ,$$

where $q_1, ..., q_l$ are elements of η with the property

$$L_i(q_j) = \delta_{ij} \qquad 1 \leqslant i, j \leqslant l.$$

Then proceeding in the same way as in the proof of *Theorem* 2, it can be shown that the reproducing kernel for $\mathscr{H}$ with norm given by

$$(v, v) = [v, v] + \sum_{i=1}^{l} [L_i v]^2$$

is

$$K(X, Y) = (I - \bar{P})_X (I - \bar{P})_Y K^*(X, Y) + \sum_{i=1}^{l} q_i(X) q_i(Y).$$

Remark 2. The functions ϕ_i, $i = 1, ..., l$, in the reproducing kernel $K(X, Y)$ are the representers of the functionals $F_1, ..., F_l$. To see this let $v \in H$. Then

$$(v, \phi_i) = [v, \phi_i] + \sum_{j=1}^{l} F_j(v) F_j(\phi_i) = F_i(v).$$

Thus the optimal approximation $\bar{F}$ is exact for functions in $(I - P)\mathscr{Q}$. Since $\bar{F}$ is obviously exact for functions in V_0, it is exact for all functions in $\mathscr{Q}$.

5. Application to Cubature

In this section we apply the results of the preceding section to obtain formulas for the optimal approximation and error bounds for the approximation of the functional $F(f) = \int_a^b \int_c^d f(x, y)\, dx\, dy$ by a cubature sum $\sum_{i=1}^n A_i F_i(f) = \sum_{i=1}^n A_i f(x_i, y_i)$. We shall also assume that the maximal number of the functionals F_i, $i = 1,..., n$ which are linearly independent over $\mathscr{Q}$, the set of polynomials of degree less than or equal to $m - 1$, is k, the dimension of $\mathscr{Q}$. For this case the reproducing kernel is

$$K(X, Y) = \bar{f} - \sum_{i=1}^{k} (\bar{f}(X_i, Y)\, \phi_i(X) + \bar{f}(X, X_i)\, \phi_i(Y) - \phi_i(X)\, \phi_i(Y)) + \sum_{i=1}^{k} \sum_{j=1}^{k} \bar{f}(X_i, X_j)\, \phi_i(X)\, \phi_j(Y), \qquad X_i = (x_i, y_i). \tag{5.1}$$

Since $\bar{u}$ is a linear combination of the representers ϕ_i, $i = 1,..., n$, we find that $\bar{u}$ has the form

$$\bar{u}(x, y) = p(x, y) + \sum_{i=1}^{n} \lambda_i \bar{f}(X, X_i) \qquad p(x, y) \in \mathscr{Q}. \tag{5.2}$$

If the set of interpolation points includes the point (α, β), (5.2) becomes

$$\bar{u}(x, y) = p(x, y) + \sum_{\substack{i=1 \\ i \neq \mu}}^{n} \lambda_i \bar{f}(X, X_i), \tag{5.3}$$

where $X_\mu = (\alpha, \beta)$. This simplification results from the fact that $\theta^{2p-1}(x, \alpha) \equiv \theta^{2q-1}(y, \beta) \equiv 0$ and thus $\bar{f}(X, X_\mu) \equiv 0$. We first assume that (α, β) is not one of the interpolation points. We shall determine the $n + k$ coefficients in (5.2) by solving a linear system of equations. We obtain n of these equations from the interpolation conditions. We obtain the remaining equations from the fact that $\bar{u} \perp v$ for all $v \in \mathscr{F} = \{v \in H \mid F_i(v) = 0, i = 1,..., n\}$. In Lemma 2 we proved that $\bar{f}$ has the property that for any $v \in H$

$$[\bar{f}, v]_X = v(\xi, \eta) - \sum_{i=1}^{k} G_i(v)\, G_i(\bar{f}) = v(\xi, \eta) - \sum_{i+j<m} (-1)^{i+j} \frac{(\alpha - \xi)^i}{i!} \frac{(\beta - \eta)^j}{j!} v_{i,j}(\alpha, \beta).$$

This implies that for all functions $v \in \mathscr{F}$

$$(\bar{f}, v)_X = v(\xi, \eta) - \sum_{i+j<m} (-1)^{i+j} \frac{(\alpha - \xi)^i}{i!} \frac{(\beta - \eta)^j}{j!} v_{i,j}(\alpha, \beta).$$

Thus

$$(\bar{u}, v) = ((p(x, y) + \sum_{l=1}^{n} \lambda_l \bar{f}(X, X_l)), v) = \sum_{l=1}^{n} \lambda_l (\bar{f}(X, X_l), v)$$

$$= \sum_{l=1}^{n} \lambda_l \left[v(x_l, y_l) - \sum_{i+j<m} (-1)^{i+j} \frac{(\alpha - x_l)^i}{i!} \frac{(\beta - y_l)^j}{j!} v_{i,j}(\alpha, \beta) \right]$$

$$= \sum_{l=1}^{n} \lambda_l v(x_l, y_l) \tag{5.4}$$

$$- \sum_{i+j<m} (-1)^{i+j} v_{i,j}(\alpha, \beta) \sum_{l=1}^{n} \lambda_l \frac{(\alpha - x_l)^i}{i!} \frac{(\beta - y_l)^j}{j!} = 0.$$

Since $v \in \mathscr{F}$, the first sum in (5.4) is zero. The second sum will be zero for all $v \in \mathscr{F}$ if and only if

$$\sum_{l=1}^{n} \lambda_l (\alpha - x_l)^i (\beta - y_l)^j = 0 \qquad i + j < m. \tag{5.5}$$

These $n + k$ equations are linearly independent since the only function which satisfies both (5.5) and the homogeneous interpolatory conditions is the zero function.

We determine the $n + k - 1$ coefficients in (5.3) in the same way. We obtain n of the equations from the interpolatory conditions. Instead of (5.4) we obtain

$$\sum_{\substack{l=1 \\ l \neq \mu}}^{n} \lambda_l v(x_l, y_l) - \sum_{i+j<m} (-1)^{i+j} v_{i,j}(\alpha, \beta) \sum_{\substack{l=1 \\ l \neq \mu}}^{n} \lambda_l \frac{(\alpha - x_l)^i}{i!} \frac{(\beta - y_l)^j}{j!} = 0. \tag{5.6}$$

If (α, β) is one of the interpolation points, $v(\alpha, \beta) = 0$ since $v \in \mathscr{F}$. Thus (5.6) will be zero for all $v \in \mathscr{F}$ if and only if

$$\sum_{\substack{l=1 \\ l \neq \mu}}^{n} \lambda_l (\alpha - x_l)^i (\beta - y_l)^j = 0 \qquad 0 < i + j < m. \tag{5.7}$$

Thus (5.7) provides the remaining $k - 1$ equations to determine the coefficients of (5.3).

It would be desirable to find other representations for certain configurations of points since the systems of equations we have obtained are ill-conditioned and therefore their use may result in inaccurate results if n is very large. The use of the representations (5.2) and (5.3), however, does not require that the representers $\phi_1, \ldots, \phi_l$, be explicitly known. In most cases it appears that these functions would be quite difficult to find.

The function $\bar{\phi}(x, y)$ equals $\bar{R}_Y(K(X, Y))$. We recall that $\bar{R} = F - \sum_{i=1}^{n} \bar{A}_i F_i$, where the $\bar{A}_i$ are the optimal weights. Also $\bar{R}(v) = 0$ for all $v \in \mathscr{Q}$. Therefore

$$\bar{\phi}(x, y) = \bar{R}_Y \bar{f} - \bar{R}_Y \left(\sum_{i=1}^{k} \phi_i(X) \bar{f}(X_i, Y) \right)$$

$$= F_Y \bar{f} - \sum_{i=1}^{n} \bar{A}_i \bar{f}(X, X_i) - q(x, y), \tag{5.8}$$

where $q(x, y) \in \mathscr{Q}$. If (α, β) is one of the interpolation points, say X_μ, we obtain

$$\bar{\phi}(x, y) = F_Y \bar{f} - \sum_{\substack{i=1 \\ i \neq \mu}}^{n} \bar{A}_i \bar{f}(X, X_i) - q(x, y). \tag{5.9}$$

We shall determine the $n + k$ coefficients of (5.8), the $\bar{A}_i$, $i = 1, \ldots, n$, and the k coefficients of the polynomial $q(x, y)$, by solving a linear system of equations. We obtain n of these equations from the fact that $\bar{\phi} \in \mathscr{F}$. Thus

$$\bar{\phi}(x_i, y_i) = 0 \qquad i = 1, \ldots, n. \tag{5.10}$$

We get the remaining equations from the fact that $\bar{R}(v) = 0$ for all $v \in \mathscr{Q}$ and thus $\bar{R}((\alpha - x)^i (\beta - y)^j) = 0$, $i + j < m$. This implies that

$$\sum_{l=1}^{n} \bar{A}_l (\alpha - x_l)^i (\beta - y_l)^j = \left(\frac{(\alpha - a)^{i+1} - (\alpha - b)^{i+1}}{i + 1} \right) \left(\frac{(\beta - c)^{j+1} - (\beta - d)^{j+1}}{j + 1} \right) \quad i + j < m. \tag{5.11}$$

If (α, β) is one of the interpolation points, we replace (5.11) by

$$\sum_{\substack{l=1 \\ l \neq \mu}}^{n} \bar{A}_l (\alpha - x_l)^i (\beta - y_l)^j = \left(\frac{(\alpha - a)^{i+1} - (\alpha - b)^{i+1}}{i + 1} \right) \left(\frac{(\beta - c)^{j+1} - (\beta - d)^{j+1}}{j + 1} \right) \quad 0 < i + j < m. \tag{5.12}$$

Eqs. (5.10) and (5.11), and (5.10) and (5.12) are linearly independent since the corresponding coefficient matrices are the same as those used to find the coefficients in the formula for $\bar{u}$.

The calculation of $F_Y(\bar{f}) = \int_a^b \int_c^d \bar{f}(X, Y)\, d\xi\, dn$ is straightforward.

$$F(\bar{u}) = \sum_{i=1}^{n} \bar{A}_i f(x_i, y_i). \tag{5.13}$$

If (α, β) is not one of the interpolation points, all of the weights, $\bar{A}$, $i = 1,..., n$, were obtained in the calculation of $\bar{\phi}$. If $(\alpha, \beta) = X_\mu$, one of the interpolation points, all of the weights except $\bar{A}_\mu$ were obtained in the calculation of $\bar{\phi}$. $\bar{A}_\mu$ can be determined from the fact that $\bar{R}(1) = 0$. Thus

$$\sum_{l=1}^{n} \bar{A}_l = (b - a)(d - c),$$

or

$$\bar{A}_\mu = (b - a)(d - c) - \sum_{\substack{l=1 \\ l \neq \mu}}^{n} \bar{A}_l\,. \tag{5.14}$$

The calculation of $F(\bar{\phi}) = \int_a^b \int_c^d \bar{\phi}(x, y)\, dx\, dy$ is straightforward. Assume $\| f \| = r$ and $[f, f] = M^2$. Since the function $\bar{u}$ has the property that $F_i(\bar{u}) = F_i(f)$, $i = 1,..., n$, we can rewrite the hypercircle inequality (2.1) to get

$$| F(f) - F(\bar{u})| \leqslant \| \bar{R} \| \, [M^2 - [\bar{u}, \bar{u}]].^{1/2} \tag{5.15}$$

If (α, β) is not one of the interpolation points,

$$\begin{aligned}
[\bar{u}, \bar{u}] &= \Big[\bar{u}, \Big(p(x, y) + \sum_{i=1}^{n} \lambda_i \bar{f}(X, X_i)\Big)\Big] = \Big[\bar{u}, \sum_{i=1}^{n} \lambda_i \bar{f}(X, X_i)\Big] \\
&= \sum_{i=1}^{n} \lambda_i \bar{u}(x_i, y_i) \\
&\quad - \sum_{i+j<m} (-1)^{i+j}\, \bar{u}_{i,j}(\alpha, \beta) \Big\{ \sum_{l=1}^{n} \lambda_l \frac{(\alpha - x_l)^i}{i!} \frac{(\beta - y_l)^j}{j!} \Big\} \\
&= \sum_{i=1}^{n} \lambda_i \bar{u}(x_i, y_i) = \sum_{i=1}^{n} \lambda_i f(x_i, y_i)
\end{aligned} \tag{5.16}$$

using (5.5). If $(\alpha, \beta) = X_\mu$, one of the interpolation points, instead of (5.16), we obtain

$$[\bar{u}, \bar{u}] = \sum_{\substack{i=1 \\ i \neq \mu}}^{n} \lambda_i f(x_i, y_i) - f(\alpha, \beta) \sum_{\substack{i=1 \\ i \neq \mu}}^{n} \lambda_i . \tag{5.17}$$

The function $\bar{u}$ can be considered to be a bivariate spline function in that it minimizes a pseudo-norm, namely, $[\cdot, \cdot]$, subject to the constraint that it interpolate the function f at the points X_i, $i = 1,..., n$. $\bar{u}$ is a piecewise polynomial function of degree $2m - 1$. If the point (α, β) is in the interior of the rectangle D, all partial derivatives of order p in x have a jump at the line $x = \alpha$, and all partial derivatives of order q in y have a jump at the line $y = \beta$. Regardless of where the point (α, β) is in the rectangle D, the partial derivatives of order $2p - 1$ in x have jumps at the lines $x = x_i$, $i = 1,..., n$, and the partial derivatives of order $2q - 1$ in y have jumps at the lines $y = y_i$, $i = 1,..., n$.

6. Numerical Examples

In this section we give several examples related to approximate multiple integration on a rectangle. We choose as the functional $F(f)$ to be approximated, the integral $\int_{-1}^{1} \int_{-1}^{1} dy\, dx/x + y + 4$. Since $f(x, y) = 1/(x + y + 4)$ is infinitely differentiable on $D = [-1, 1] \times [-1, 1]$, it is a member of $T^{p,q}(\alpha, \beta)$ for all p and q and all (α, β) in D. We choose several values of p and q and two different points (α, β) and compute the corresponding optimal approximations and error bounds. We use the two sets of points

$$E_1 = \{(0, 0), (1, 1), (-1, 1), (1, -1), (-1, 1)\},$$

and

$$E_2 = \{(0, 0), (-1, 0), (1, 0), (-1/2, 1/2), (1/2, 1/2), (1/2, -1/2), (-1/2, -1/2), (-1, -1), (0, -1), (1, -1), (-1, 1), (0, 1), (1, 1)\}.$$

In the first example we consider $f(x, y)$ to be a member of the class of functions $T^{1,1}(\alpha, \beta)$ in the Hilbert space H. We carry out the calculations for two different points (α, β). In each case (α, β) is one of the points of the cubature sum. Therefore to calculate $\bar{u}$ we use the equations $\bar{u}(x_i, y_i) = f(x_i, y_i)$, $i = 1,..., n$, and (5.7). To calculate $\bar{\phi}$ we use equations (5.10) and (5.12). We solve the linear systems of equations by inversion of the coefficient matrices using a maximal pivot method. Since the coefficient matrices for the calculation of both $\bar{u}$ and ϕ are the same, only one matrix inversion is necessary.

TABLE 1

$(\alpha, \beta) = (0, 0)$

Set of points	E_1	E_2
$F(\bar{u})$	0.105357(01)	0.104628(01)
$\Vert \bar{R} \Vert^2$	0.280159	0.120729
M^2	0.171642(−01)	0.171642(−01)
$[\bar{u}, \bar{u}]$	0.992063(−02)	0.137910(−01)
B	0.450482(−01)	0.201802(−01)
$F(f) - F(\bar{u})$	−0.707544(−02)	0.220431(−03)

TABLE 2

$(\alpha, \beta) = (1, 1)$

Set of points	E_1	E_2
$F(\bar{u})$	0.108654(01)	0.105251(01)
$\Vert \bar{R} \Vert^2$	0.123803(01)	0.238149
M^2	0.124486(−01)	0.124486(−01)
$[\bar{u}, \bar{u}]$	0.854701(−02)	0.107326(−01)
B	0.695000(−01)	0.202149(−01)
$F(f) - F(\bar{u})$	−0.400425(−01)	−0.601050(−02)

To calculate the optimal approximation, $F(\bar{u})$, we use Eq. (5.13) where the weights $\bar{A}_i$ are obtained as coefficients in the formula for $\bar{\phi}$ (5.9). To calculate $\Vert \bar{R} \Vert$, the function-independent part of the error bound

$$| F(f) - F(\bar{u})| \leqslant \Vert \bar{R} \Vert \, [M^2 - [\bar{u}, \bar{u}]]^{1/2},$$

we integrate $\bar{\phi}$. In practice the calculation of M^2, the square of the pseudonorm $[f, f]$, is quite difficult. An upper bound for M^2 can always be found, however, by replacing each integral by the product of the maximum of the square of the appropriate derivative times the measure of the domain of integration. The pseudo-norm $[\bar{u}, \bar{u}]$ is calculated by (5.17) where the λ_i are coefficients in the formula for $\bar{u}$. Table 1 lists the optimal approximation and error bounds obtained when we let $(\alpha, \beta) = (0, 0)$. Table 2 lists the optimal approximation and error bounds when $(\alpha, \beta) = (1, 1)$. The numbers in parentheses indicate the exponents and B denotes the error bound, $\Vert \bar{R} \Vert \, [M^2 - [\bar{u}, \bar{u}]]^{1/2}$.

TABLE 3

$(\alpha, \beta) = (0, 0)$

Set of points	E_2
$F(\bar{u})$	0.104190(01)
$\|\bar{R}\|^2$	0.284981(−02)
M^2	0.420252(−01)
$[\bar{u}, \bar{u}]$	0.122915(−01)
B	0.920517(−02)
$F(f) - F(\bar{u})$	0.459631(−02)

TABLE 4

$(\alpha, \beta) = (1, 1)$

Set of points	E_2
$F(\bar{u})$	0.104731(01)
$\|\bar{R}\|^2$	0.106450(−02)
M^2	0.293879(−01)
$[\bar{u}, \bar{u}]$	0.359353(−02)
B	0.524005(−02)
$F(f) - F(\bar{u})$	−0.810142(−03)

In the second example we consider $f(x, y) = 1/(x + y + 4)$ to be a member of $T^{2,2}(\alpha, \beta)$. Table 3 lists the optimal approximation and error bounds obtained when $(\alpha, \beta) = (0, 0)$. Table 4 lists the optimal approximation and error bounds when $(\alpha, \beta) = (1. 1)$.

All of the preceding calculations were carried out in double precision floating point arithmetic on the Univac 1108 Computer at the University of Utah Computer Center.

Much of the work on error analysis of cubature formulas has dealt with cross-product formulas in contrast to the results of this paper. References can be found in Stroud and Secrest [32]. If two single variable formulas are used, one of which is exact for polynomials of degree $\leqslant p - 1$, and the other is exact for polynomials of degree $\leqslant q - 1$, the cross-product formula obtained from them is exact for polynomials in two variables of degree less than or equal to $p - 1$ in one variable and less than or equal to $q - 1$ in the other. Thus the optimal cubature formulas discussed in this paper differ from cross-product formulas even if a cross-product set of points is used since the optimal formulas are exact for all polynomials of total degree less than or equal to $m - 1$, where $m = p + q$.

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