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A Prototype Four-Dimensional Galerkin-Type Integral

By

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Abstract

An error functional expansion is constructed for a four-dimensional integral over $[0,1]^4$ whose integrand function has a singularity structure of a type that occurs in integrals in the Galerkin boundary element method. We show with an example how extrapolation may be used to evaluate this integral.

§1. Introduction

In applications of the boundary element method, one needs to evaluate many four-dimensional integrals. In a wide class of problems, these integrals are each of the form

$$\int_{\mathcal{R}_1}\int_{\mathcal{R}_2} |\mathbf{x}_1-\mathbf{x}_2|^{\gamma} h(\mathbf{x}_1,\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2. \tag{1.1}$$

Here γ is typically a negative integer, and $\mathcal{R}_1$ and $\mathcal{R}_2$ are each a specified two-dimensional planar region. The function h is usually innocuous, often simply a multinomial. The more interesting of these integrals are those in which the regions $\mathcal{R}_1$ and $\mathcal{R}_2$ intersect, either at a single point or along a common edge. In the example treated here, these regions coincide.

A significant proportion of the extensive literature on Galerkin methods is devoted to the numerical evaluation of these somewhat intractable integrals. See, for example, [ScWe92] and [SaLa00]. However, the possibility of using

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extrapolation methods (generalizations of Romberg Integration) has received little consideration. In this note, we investigate in detail a single prototype example to see whether a proper underlying error expansion for extrapolation exists; and to provide a springboard for a more thorough investigation.

§2. Prototype Example

Our prototype example is one of the simplest examples of (1.1). Here we set $h = 1$, $\mathcal{R}_1 = \mathcal{R}_2 = [0,1]^2$ and $\gamma = -1$. This leaves

$$I_4 f = \int_{[0,1]^4} \left\{(x_1 - x_2)^2 + (y_1 - y_2)^2\right\}^{-1/2} dx_1 dy_1 dx_2 dy_2. \tag{2.1}$$

This four-dimensional integrand function is singular in the two-dimensional manifold

$$\{(x_1 - x_2) = 0\} \cap \{(y_1 - y_2) = 0\}. \tag{2.2}$$

In spite of this singularity, the integral (2.1) converges; we show in the Appendix that

$$I_4 f = 4\log(1+\sqrt{2}) - \frac{4}{3}(\sqrt{2}-1) \cong 2 \cdot 97. \tag{2.3}$$

However, we seek a numerical method for evaluating integrals similar to this, and we treat this one (our prototype) with a view to generalizing the theory later. In this paper, we confine ourselves to extrapolation based on the following set of cubature rules.

Definition 2.1. For positive integer m, the four-dimensional *product m-panel midpoint trapezoidal rule* for the region $[0,1]^4$ is

(2.4)
$$Q_4^{[m;0,0,0,0]} f = \frac{1}{m^4} \sum_{j_1=1}^{m} \sum_{j_2=1}^{m} \sum_{j_3=1}^{m} \sum_{j_4=1}^{m} f^* \left(\frac{2j_1 - 1}{2m}, \frac{2j_2 - 1}{2m}, \frac{2j_3 - 1}{2m}, \frac{2j_4 - 1}{2m} \right).$$

Here f^* is identical with f except that any point for which f is indeterminate is "ignored", that is, replaced by zero. In our example, points for which both $j_1 = j_3$ and $j_2 = j_4$ have to be ignored. There are m^2 of these points out of a total of m^4 points. The four zeros in the superscript simply indicate that the midpoint trapezoidal rule is used in each dimension.

The principal purpose of this paper is to show that, for our prototype integrand function $f = |r_{12}|^{-1}$, the error functional has an asymptotic expansion of the form

$$Q_4^{[m;0,0,0,0]} f - If \sim \frac{A_1}{m} + \frac{C_2 \log m}{m^2} + \frac{A_2}{m^2} + \frac{A_3}{m^3} + \sum_{s=2} \frac{B_{2s}}{m^{2s}}, \tag{2.5}$$

where the coefficients A_i, B_i and C_i are independent of m.

After doing so, we give a numerical example to illustrate how this expansion may be applied in extrapolation quadrature.

§3. Some N-Dimensional Error Expansions

Two familiar integration rules for $[0,1]^N$ are the *product midpoint trapezoidal rule*

$$Q_N^{[m;0,0,\ldots,0]}\psi = \frac{1}{m^N} \sum_{j_1=1}^{m} \sum_{j_2=1}^{m} \cdots \sum_{j_N=1}^{m} \psi\left(\frac{2j_1-1}{2m}, \frac{2j_2-1}{2m}, \ldots, \frac{2j_N-1}{2m}\right). \tag{3.1}$$

and the *product endpoint trapezoidal rule*,

$$Q_N^{[m;\pm1,\pm1,\ldots,\pm1]}\psi = \frac{1}{m^N} \sum_{k_1=0}^{m}{}'' \sum_{k_2=0}^{m}{}'' \cdots \sum_{k_N=0}^{m}{}'' \psi\left(\frac{k_1}{m}, \frac{k_2}{m}, \ldots, \frac{k_N}{m}\right). \tag{3.2}$$

As is conventional, the double prime on the summation symbol indicates that a factor (1/2) is to be applied to the first and last element in the summation. In the rest of this paper, $Q_N^{[m]}$ may stand for either (3.2) or (3.1).

Theorem 3.2. *When $\psi(\mathbf{x})$ and its derivatives of order $2p$ and less are integrable over $[0,1]^N$,*

$$Q_N^{[m]}\psi = I\psi + \sum_{s=1}^{p} \frac{B_{2s}}{m^{2s}} + O(m^{-2p-1}). \tag{3.3}$$

This is an N-dimensional version of the standard Euler-Maclaurin expansion. Simple integral representations are known for the coefficients B_s, which depend on ψ and on Q_N but are independent of m.

When the integrand function ψ has a singularity in $[0,1]^N$, (3.3) is generally not valid. However, an expansion is known for integrand functions that are homogeneous of specified degree about the origin and $C^\infty[0,1]^N \setminus (\mathbf{0})$.

Definition 3.3. $f(\mathbf{x})$ is homogeneous about the origin of degree λ if $f(k\mathbf{x}) = k^\lambda f(\mathbf{x})$ for all $k > 0$ and $|\mathbf{x}| > 0$.

Examples of these include $(x^2y)^{\lambda/3}$, $(x^2+y^2)^{\lambda/2}$, and, with $\lambda = -1$, our prototype integrand function in (2.1).

Theorem 3.4 [Ly76]. *Let $\gamma > -N$; let $\psi_\gamma(\mathbf{x})$ denote an N-dimensional homogeneous function of degree $\gamma > -N$, which is $C^\infty[0,1]^N \setminus (\mathbf{0})$. Then*

$$Q_N^{[m]}\psi_N^* \sim I\psi_N + \frac{A_{\gamma+N}}{m^{\gamma+N}} + \frac{C_{\gamma+N}\log m}{m^{\gamma+N}} + \sum_{\substack{s=1 \\ 2s\neq\gamma+N}}^{\ell-1} \frac{B_{2s}}{m^{2s}}, \tag{3.4}$$

where $C_{\gamma+N} = 0$ unless $\gamma + N$ is an even integer.

As before, the asterisk indicates that indeterminate function values are to be ignored. In this paper, we require this theorem with $N = 2$ only.

We note that the prototype integrand in (2.1) is homogeneous of degree -1 about the origin. Were it not for the singularities in $[0,1]^4$ (mentioned in (2.2)), the expansion we seek would be (3.4) with $N = 4$ and $\gamma = -1$; the leading terms would then be $O(1/m^3)$. In view of the singularities, this expansion is invalid. In this paper we establish the correct expansion (2.5), where the leading term is $O(1/m)$.

§4. Error Functional Expansion for the Prototype Example

In this section we establish the asymptotic expansion (2.5) above.

Theorem 4.5. *Let $t_1 = x_1 - x_2$ and $t_2 = y_1 - y_2$, and let the four-argument function $f(x_1, y_1; x_2, y_2)$ be expressible as follows:*

$$f(x_1, y_1, x_2, y_2) = \phi(t_1, t_2), \tag{4.1}$$

where the two-argument function ϕ is symmetric in t_1 and in t_2. Then, for all positive integer m,

$$Q_4^{[m;0,0,0,0]} f = Q_2^{[m;\pm1,\pm1]}\psi, \tag{4.2}$$

where

$$\psi(t_1, t_2) = 4\phi(t_1, t_2)(1 - t_1)(1 - t_2). \tag{4.3}$$

The rules Q were defined in Section 3. The theorem involves only finite sums and its proof is straightforward. Note that the prototype function $f = |r_{12}|^{-1}$ satisfies the conditions of this theorem with $\phi(t_1, t_2) = (t_1^2 + t_2^2)^{-1/2}$.

Proof. Applying (4.1) in (2.4) gives immediately

$$Q_4^{[m;0,0,0,0]} f = \frac{1}{m^4} \sum_{j_1=1}^{m} \sum_{j_2=1}^{m} \sum_{j_3=1}^{m} \sum_{j_4=1}^{m} \phi\left(\frac{j_1 - j_3}{m}, \frac{j_2 - j_4}{m}\right). \tag{4.4}$$

This can be reduced to a double summation by noting that for any function Φ,

$$\sum_{j_1=1}^{m}\sum_{j_3=1}^{m}\Phi(j_1-j_3)\equiv\sum_{k_1=-m}^{m}\Phi(k_1)(m-|k_1|). \tag{4.5}$$

(In the sum on the left, there are m elements (j_1, j_3) for which $j_1 - j_3 = 0$; more generally, there are $m - |k_1|$ elements (j_1, j_3) for which $j_1 - j_3 = k_1$. The terms in the sum on the right for which $k_1 = |m|$ vanish, but it is helpful at this stage to leave them in.) Applying (4.5) twice, one may reduce the quadruple sum (4.4) to

$$Q_4^{[m;0,0,0,0]}f=\frac{1}{m^2}\sum_{k_1=-m}^{m}\sum_{k_2=-m}^{m}\phi\left(\frac{k_1}{m},\frac{k_2}{m}\right)\left(1-\left|\frac{k_1}{m}\right|\right)\left(1-\left|\frac{k_2}{m}\right|\right). \tag{4.6}$$

Since $\phi(t_1, t_2)$ is symmetric under sign reversal of t_1 and of t_2, this summation may be partitioned into four identical summations, giving

$$Q_4^{[m;0,0,0,0]}f=\frac{4}{m^2}\sum_{k_1=0}^{m}{}''\sum_{k_2=0}^{m}{}''\phi\left(\frac{k_1}{m},\frac{k_2}{m}\right)\left(1-\left|\frac{k_1}{m}\right|\right)\left(1-\left|\frac{k_2}{m}\right|\right). \tag{4.7}$$

Here, as before, the double prime indicates that a factor $\frac{1}{2}$ is to be applied to initial and final terms in the sum. The reader may verify that, when $k_i = m$, the term involved is zero; when $k_i = 0$, the factor $\frac{1}{2}$ is necessary because this contribution in (4.6) has to be shared between two different elements in (4.7).

This expression is clearly a discretization of a two-dimensional integral

$$I_2\psi=\int_0^1\int_0^1\psi(x_1,x_2)dx_1dx_2,$$

where ψ is given by (4.3) above. In fact, reference to (3.2) confirms that this discretization is specifically

$$Q_2^{[m;\pm1,\pm1]}\psi=\frac{1}{m^2}\sum_{k_1=0}^{m}{}''\sum_{k_2=0}^{m}{}''\psi\left(\frac{k_1}{m},\frac{k_2}{m}\right). \tag{4.8}$$

This establishes the theorem. □

Note that, at this stage, we have used only the circumstances that $f(x_1, y_1; x_2, y_2)$ may be expressed as $\phi(x_1 - x_2, y_1 - y_2)$ and that ϕ is symmetric. No other property of f has been used.

The following corollary is a simple consequence of this theorem.

Corollary 4.6.

$$I_4 f = I_2 \psi. \tag{4.9}$$

Since both integrands are Riemann integrable, this is simply a matter of setting $h = 1/m$ in (4.2) and taking the limit.

We now apply Theorem 4.5 to our prototype integrand function

$$f(x_1, y_1; x_2, y_2) = \left\{(x_1 - x_2)^2 + (y_1 - y_2)^2\right\}^{-1/2}.$$

This reduces $Q_4^{[m,0,0,0,0]} f$ to $Q_2^{[m,\pm 1,\pm 1]} \psi$ with

$$\begin{aligned} \psi(t_1, t_2) &= 4(t_1^2 + t_2^2)^{-1/2}(1 - t_1)(1 - t_2) \\ &= g^{(-1)}(t_1, t_2) + g^{(0)}(t_1, t_2) + g^{(1)}(t_1, t_2), \end{aligned}$$

where

$$\begin{aligned} g^{(-1)}(t_1, t_2) &= 4(t_1^2 + t_2^2)^{-1/2} \\ g^{(0)}(t_1, t_2) &= -4(t_1^2 + t_2^2)^{-1/2}(t_1 + t_2) \\ g^{(1)}(t_1, t_2) &= 4(t_1^2 + t_2^2)^{-1/2} t_1 t_2 \end{aligned}$$

are homogeneous functions of degrees -1, 0, and 1, respectively; since none of these has a singularity in $[0, 1]^2$ except at the origin, we may apply Theorem 3.4 with $N = 2$ to each, giving

$$Q_2^{[m;\pm 1,\pm 1]} g^{(i)} \sim I_2 g^{(i)} + \frac{A_{i+2}^i}{m^{i+2}} + \frac{C_{i+2}^i \log m}{m^{i+2}} + \sum_{s=1} \frac{B_{2s}^i}{m^{2s}} \qquad i = -1, 0, 1. \tag{4.10}$$

Adding these three asymptotic expansions gives

$$Q_2^{[m;\pm 1,\pm 1]} \psi \sim I_2 \psi + \frac{A_1^{-1}}{m} + \frac{A_2^0}{m^2} + \frac{A_3^1}{m^3} + \frac{C_2^0 \log m}{m^2} + \sum_{s=1} \frac{B_{2s}^{-1} + B_{2s}^0 + B_{2s}^1}{m^{2s}}. \tag{4.11}$$

Note that in accordance with Theorem 3.4, we have omitted C_{i+2}^i when $i + 2$ is odd. Using (4.2) and (4.9), we may reduce (4.11) to

$$Q_4^{[m;0,0,0,0]} f - I_4 f \sim \frac{A_1}{m} + \frac{C_2 \log m}{m^2} + \frac{A_2}{m^2} + \frac{A_3}{m^3} + \sum_{s=2} \frac{B_{2s}}{m^{2s}}, \tag{4.12}$$

as stated in Section 2.

§5. Numerical Application of Extrapolation

This asymptotic expansion may be used to provide the basis for four-dimensional extrapolation quadrature in the following way. One may obtain a sequence of approximation $Q^{[m_i]}f = Q^{[m_i;0,0,0,0]}f$, each requiring m_i^4 function values. Having available, say p, of these approximations for $m = m_1, m_2, \ldots, m_p$, respectively, one discards all but the p most significant terms from the asymptotic expansion and, using perhaps a linear equation solver, finds a solution $\tilde{I}f$ to the set of p linear equations

$$(5.1)\quad \tilde{I}f + \frac{\tilde{A}_1}{m_i} + \frac{\tilde{C}_2 \log m_i}{m_i^2} + \frac{\tilde{A}_2}{m_i^2} + \frac{\tilde{A}_3}{m_i^3} + \sum_{s=2}^{p-3} \frac{\tilde{B}_{2s}}{m_i^{2s}} = Q^{[m_i]}f \qquad i = 1, 2, \ldots, p.$$

For illustration, with $p = 4$, these equations may be written as follows.

$$\begin{pmatrix} 1, & \frac{1}{m_1}, & \frac{\log m_1}{m_1^2}, & \frac{1}{m_1^2} \\ 1, & \frac{1}{m_2}, & \frac{\log m_2}{m_2^2}, & \frac{1}{m_2^2} \\ 1, & \frac{1}{m_3}, & \frac{\log m_3}{m_3^2}, & \frac{1}{m_3^2} \\ 1, & \frac{1}{m_4}, & \frac{\log m_4}{m_4^2}, & \frac{1}{m_4^2} \end{pmatrix} \begin{pmatrix} \tilde{I}f \\ \tilde{A}_1 \\ \tilde{C}_2 \\ \tilde{A}_2 \end{pmatrix} = \begin{pmatrix} Q^{[m_1]}f \\ Q^{[m_2]}f \\ Q^{[m_3]}f \\ Q^{[m_4]}f \end{pmatrix}$$

Table 1 displays some of the results obtained using this technique to evaluate our prototype integral. In the m-th row we show the approximation $Q^{[m;0,0,0,0]}f$ and the extrapolate $\tilde{I}f$ calculated using (5.1) with $p = m$ and

Table 1. Numerical Results for Prototype Example

m	ν	$Q^{[m;0,0,0,0]}f$	$\Sigma\nu$	$\tilde{I}f$	$\tilde{I}f - If$	$\bar{I}f - If$
1	1	0	1	0		
2	16	0.1354E+01	17	0.2707106781E+01	−.27E-0	−.27E-0
3	81	0.1848E+01	98	0.2843194763E+01	−.13E-0	−.74E-1
4	256	0.2108E+01	354	0.2967272235E+01	−.59E-2	−.20E-1
5	625	0.2269E+01	979	0.2973125627E+01	−.84E-4	−.70E-2
6	1296	0.2379E+01	2275	0.2973229910E+01	.20E-4	−.31E-2
7	2401	0.2459E+01	4676	0.2973212687E+01	.31E-5	−.15E-2
8	4096	0.2520E+01	8772	0.2973209845E+01	.25E-6	−.86E-3
9	6561	0.2568E+01	15333	0.2973209614E+01	.15E-7	−.52E-3
10	10000	0.2607E+01	25333	0.2973209600E+01	.13E-8	−.37E-3
Exact		0.2973E+01	Exact	0.2973209598E+01		
Condition Number of Final Entry				6.59×10^4		

$m_i = 1, 2, .., m$. One can see clearly how slowly the trapezoidal rule approximations $Q^{[m;0,0,0,0]}f$ converge. In fact, the $m = 48$ approximation using 5.3 million function values is 0.2893E+1 (roughly 3% accuracy). However, using the first ten of these approximations, each of which is individually extraordinarily inaccurate, we obtain an extrapolate $\tilde{I}f$ having eight-figure accuracy at a cost of fewer than 26,000 function values.

It is important in the practice of extrapolation that the appropriate expansion, in this case (5.1), is used. A few extra unnecessary terms causes only minor deterioration in the result. However, if a term is missing, major inaccuracy may follow. The final two columns in Table 1 illustrate this. In the penultimate column, we list the truncation error $\tilde{I}f - If$. In the final column, we list the truncation error $\bar{I}f - If$ in the approximations $\bar{I}f$ (not shown) obtained using a modification of (5.1) which omits the $C_2 \log m/m^2$ term. The same process leads to a final approximation having only three-figure accuracy rather than eight-figure accuracy.

Note that one would expect results based on transformations to a smooth integrand followed by the use of an appropriate Gaussian rule to be as good as or better than the ones above.

In this application, one is interested only in the first element, $\tilde{I}f$, of the solution vector of the set of linear equations (5.1) and not in the other elements such as $\tilde{A}_i$. The condition number given in the table refers to the condition of this single element $\tilde{I}f$. This is different from and significantly smaller than condition numbers associated with the *full* solution vector.

§6. Concluding Remarks

This prototype example is useful because an exact integral is available, the derivation of the error expansion is relatively straightforward, and the numerical results are encouraging. Unfortunately, it is far from general. When one replaces the square $[0, 1]^2$ by a rectangle or a triangle, the derivations given here cannot be readily modified. Nevertheless, preliminary results, both numerical and theoretical, indicate that expansions of this general type are valid in a much wider context.

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Appendix (The Exact Integral)

In this appendix, we evaluate our prototype integral $I_4 f$ given in (2.1) analytically. Using standard procedure, or simply applying the corollary 4.6, ($I_4 f = I_2 \psi$) we find

$$\begin{aligned} I_4 f &= \int_{[0,1]^4} \left\{(x_1 - x_2)^2 + (y_1 - y_2)^2\right\}^{-1/2} dx_1 dy_1 dx_2 dy_2 \\ &= \int_0^1 \int_0^1 \frac{(1-t_1)(1-t_2)}{(t_1^2 + t_2^2)^{1/2}} dt_1 dt_2. \end{aligned} \tag{6.1}$$

The region $t_1, t_2 \in [0,1]^2$ may be partitioned by the line $t_1 = t_2$ into two triangular regions; in polar coordinates, one of these is

$$\Delta_1; \quad \theta \in \left[0, \frac{\pi}{4}\right] \quad r \in [0, 1/\cos\theta]. \tag{6.2}$$

In view of the symmetry of the integrand, the integral over Δ_1 coincides with the integral over the other triangle Δ_2. We find successively

$$\begin{aligned} I_4 f &= I_2 \psi = 2I(\Delta_1)\psi \\ &= 2\int_0^{\pi/4} \left[\int_0^{1/\cos\theta} \left[\frac{(1 - r\cos\theta)(1 - r\sin\theta)}{r} r dr\right] d\theta\right] \\ &= 2\int_0^{\pi/4} \left(r - \frac{r^2}{2}(\cos\theta + \sin\theta) + \frac{r^3}{3}\cos\theta\sin\theta\right)\Big|_{r=0}^{r=1/\cos\theta} d\theta \\ &= 2\int_0^{\pi/4} \left(\frac{1}{\cos\theta}\left(1 - \frac{1}{2}\right) + \frac{\sin\theta}{\cos^2\theta}\left(-\frac{1}{2} + \frac{1}{3}\right)\right) d\theta. \end{aligned} \tag{6.3}$$

The integrals required here are simply

$$\int \frac{d\theta}{\cos\theta} = \log(\sec\theta + \tan\theta), \qquad \int \frac{\sin\theta}{\cos^2\theta} d\theta = \sec\theta; \tag{6.4}$$

and using these, we obtain the result $4\log(1 + \sqrt{2}) - \frac{4}{3}(\sqrt{2} - 1)$, as stated in (2.3) above.

References

[Ly76] Lyness, J. N., An error functional expansion for N-dimensional quadrature with an integrand function singular at a point, *Math. Comp.*, **30** (1976), 1-23.

[SaLa00] Sauter, S. A. and Lage, C., Transformation of hypersingular integrals and black-box cubature, *Math. Comp.*, **70** (2000), 223-250.

[ScWe92] Schwab, C. and Wendland, W., On numerical cubatures of singular surface integrals in boundary element methods, *Numer. Math.*, **62** (1992), 343-369.