ON HANDLING SINGULARITIES IN FINITE ELEMENTS*

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ABSTRACT. In the practice of the Boundary Element Method, a basic task involves the quadrature over a quadrilateral or triangle of an integrand function which has a singularity of known form at a vertex. A not uncommon situation is that this quadrature has already been studied in depth for the standard triangle or the square, and all that is now necessary is to apply the known results in the context of a different triangle or parallelogram, one that has been obtained from the standard region by an affine transformation.

It can be surprising to someone who has not done it himself, how difficult this task can be.

This article provides an account of how easy it is to be misled in this area. Besides describing an apparently cost effective approach which turns out to be a disaster, I discuss some of the advantages and disadvantages of using rules based on extrapolation either as an alternative to, or in conjunction with Gaussian rules. This article is anecdotal in character.

1. Introduction

In books and research articles, the seeker after knowledge will find plenty of information about how to integrate regular or ''well behaved'' integrand functions over various standard regions. These will include in great detail, a standard square, such as $H:[0,1)^2$ and possibly in less detail, a standard triangle, usually an isosceles right-angled one

$$T_2:\ x \ge 0;\ \ y \ge 0;\ \ x+y < 1$$

and, of course, higher-dimensional analogues of these.

If our knowledge seeker is interested in implementing a finite element program, he will want more than this. He has to deal with large number of elements. Many will be similar to one another. The majority will involve integrating regular integrand functions over nonstandard triangles and quadrilaterals. This is not particularly difficult. But there will be a small but significant proportion which are more difficult, having one or another of the features mentioned below. He may have regions which only approximate to triangles or squares. He may have, for example, a plane curvilinear triangle, such as a quadrant of a circle, or a more general curvilinear triangle such as the surface of an octant of a sphere. These boundaries and surfaces may be specified either in a convenient form, or in some inconvenient possibly highly implicit form. His integrand function may have singularities. These are usually quite simple singularities and the user is usually well aware of their nature and location. But,

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while the singularity may be simple in structure, integrating over it may be tedious. In any single problem, it is most unlikely that a single element will have all these inconvenient features, but one might.

This article is about some of the problems encountered by such a user. My feeling is that a user spends nearly all of the time which he devotes to numerical quadrature to attempting to adapt the results given in textbooks for standard regions and regular integrands to his problem. He finds, to his dismay, that this topic is not discussed in textbooks, and he turns for help to his local quadrature expert. All too often he finds the quadrature expert, while sympathetic and ready to help, to be of little use. This is because the quadrature expert has not previously encountered this sort of problem in detail. His attempts to help may be hampered by misconceptions. Sometimes he imagines that all these problems can be handled by scaling, and tries to prove this incorrect hypothesis. Other times he thinks that nothing can be scaled which may also be wrong. Either misconception can lead to seemingly endless discussion and unnecessarily inefficient programs.

My hope is that this article, which is written for the quadrature expert and which is anecdotal in nature, may be helpful in directing attention to some of the pitfalls in this area.

It is worth stating at the outset that in a one-dimensional context these problems are very rare, and when one is encountered, there is usually a quick remedy that only works in one dimension. This problem is essentially multidimensional.

In this article, we shall treat principally two quadrature methods. These are Gaussian Quadrature, and Linear Extrapolation Quadrature of which Romberg Integration is a special case. We shall look at the effect of Affine Transformations of the coordinate system on these integration procedures. We shall discuss briefly the Duffy transformation (of a triangle into a square).

2. Extrapolation Quadrature

It is well known that polynomials are basic to Gaussian Quadrature. A corresponding role in the theory underlying Extrapolation Quadrature is played by Homogeneous functions. As a preliminary, we remind the reader of the definition and simple properties of these functions.

A function $f(x,y)$ is said to be homogeneous (about the origin) of degree α if

$$f(\lambda x, \lambda y) = \lambda^{\alpha} f(x,y) \quad \text{for all } \lambda > 0 \,.$$

We shall often denote such a function by $f_{\alpha}(x,y)$.

A monomial $x^p y^q$ is homogeneous of degree $p+q$, and many properties relating to the polynomial degree of functions of monomials have direct analogues in the context of homogeneous degree. Thus, $(f_{\alpha})^{\beta}$ and $f_{\alpha} f_{\beta}$ are of degree $\alpha\beta$ and $\alpha+\beta$, respectively, and $f_{\alpha}(M\mathbf{x})$ when $|M| \neq 0$ is also of degree α; $\partial^s f_{\alpha} / \partial x^s$ is of degree $\alpha - s$.

In more than one dimension, many more interesting functions are homogeneous. For example, $r = (x^2+y^2)^{1/2}$ is homogeneous of degree 1, and $\theta = \arctan y/x$ is homogeneous of degree zero, as is any function $\Phi(\theta)$.

Extrapolation Quadrature, abbreviated here to EQ, is a natural development of Richardson's deferred approach to the limit. It is a technique designed for integration over hypercubes or simplices. Romberg integration is a special and important one-dimensional example of Extrapolation Quadrature. In this section, we shall restrict the discussion to integration over the square $[0,1)^2$. However, all results below are valid for the triangle T_2 also. See Lyness (1991) for a brief elaboration of this remark.

In this paper we adopt the following convention for the polynomial degree of a quadrature rule. A rule of degree d is one which integrates all polynomials of degree d exactly. A rule of *strict* degree d is one of degree d but not of degree $d+1$.

In this paper we treat only degree zero quadrature rules. These are rules which integrate the constant function correctly. We denote by Q any degree zero quadrature rule for $[0,1)^2$;

that is,

$$Qf = \sum w_j f(x_j, y_j) \qquad \text{with } \sum w_j = 1 , \tag{2.1}$$

and we define its m-copy $Q^{(m)}f$ in the standard way as the approximation to the exact integral, If, obtained by subdividing the square into m^2 squares each of side $1/m$ and applying a properly scaled version of Q to each. In our context it is usually advantageous to use either the mid-rectangle rule or the vertex trapezoidal rule for Q. The theory allows any rule which integrates the constant function correctly.

In general, one would expect the rule $Q^{(m)}f$ with a large value of m to be a better approximation to If than the rule with a small value of m. A measure of this effect would be provided by an asymptotic expansion of the error functional $E^{(m)}f = Q^{(m)}f - If$ in inverse powers of m or other suitable expansion functions. We can justify the use of Extrapolation Quadrature if such an expansion exists and its form is known. Whether or not there is one available depends on the nature of $f(\mathbf{x})$.

Briefly, these error functional expansions are built up from two basic asymptotic expansions given in the following two theorems.

THEOREM 2.2. *When $f(\mathbf{x})$ together with its partial derivatives of order p or less are integrable over H, and Q is a degree zero quadrature rule for H, then*

$$Q^{(m)}f - If = \frac{B_1}{m} + \frac{B_2}{m^2} + \cdots + \frac{B_{p-1}}{m^{p-1}} + O(m^{-p}) , \tag{2.2}$$

where $B_s = B_s(H;Q;f)$ are independent of m.

This is a straightforward generalization of the classical Euler Maclaurin formula.

THEOREM 2.3. *When $f(\mathbf{x})$ is homogeneous of degree α and has no singularity in H except possibly at the origin, and Q is a degree zero quadrature rule for H, then*

$$Q^{(m)}f - If = \frac{A_{2+\alpha}}{m^{2+\alpha}} + \frac{C_{2+\alpha}\ln m}{m^{2+\alpha}} \tag{2.3}$$

$$+ \frac{B_1}{m} + \frac{B_2}{m^2} + \cdots + \frac{B_{p-1}}{m^{p-1}} + O(m^{-p}),$$

where the coefficients A, B, and C are independent of m, and $C_{2+\alpha} = 0$ unless α is an integer.

A detailed proof of this is given in Lyness (1976i).

We may construct an expansion for any function which is a linear sum of any number of component functions, so long as each component satisfies the hypotheses of one or the other of these theorems. This is easy to do when

$$f(x,y) = f_\alpha(x,y)g(x,y) , \tag{2.4}$$

where g is regular. Here we may expand $g(x,y)$ in a Taylor expansion about the origin retaining only monomial terms of degree $p-1$ or less and deferring the rest to the remainder term. This gives rise to an expression for $f(x,y)$ of the form

$$f_\alpha(x,y)g(x,y) = g(0,0)f_\alpha(x,y) + f_{\alpha+1}(x,y) + \ldots + f_{\alpha+p-1}(x,y) + g_{\alpha+p}(x,y) . \tag{2.5}$$

The final term g is not a homogeneous function but satisfies the hypothesis of Theorem 2.2 above. All the other terms in this expansion are homogeneous of the indicated degree and so satisfy the hypotheses of Theorem 2.3 above. Thus, (2.5) may be used to establish error functional expansions valid for classes of familiar functions. For example, in Lyness (1976i) the approach outlined above is used to show the following theorem.

THEOREM 2.7. *Let $F(x,y)$ be of the form*

$$F(x,y) = r^{\alpha}\Phi(\theta)h(r)g(x,y)\ , \tag{2.6}$$

where (r,θ) are the polar coordinates of (x,y) and Φ, h, and g are analytic functions; and let Q be a degree zero quadrature rule for H. Then

$$Q^{(m)}F - IF \ \ -wig \ \sum_{t=0} \frac{A_{2+\alpha+t}}{m^{2+\alpha+t}} + \sum_{s=1} \frac{B_s}{m^s} \qquad \alpha \neq \text{integer} \tag{2.7}$$

$$-wig \ \sum_{s=1} \frac{A_s + B_s + C_s \ \ln m}{m^s} \qquad \alpha = \text{integer}\ .$$

Some logarithmic singularities can also be treated. The corresponding expansions are obtained by differentiating already-available expansions with respect to some incidental parameter, such as α. We may exploit the identity

$$\frac{\partial}{\partial\alpha}(r^{\alpha}g(x,y)) = r^{\alpha}\ \ln r\ \ g(x,y) \tag{2.8}$$

to obtain an expansion like (2.7) but having additional terms $\log m/m^s$ and, when these are already present, terms $(\ln m)^2/m^s$. For more detailed information about these and other expansions, the reader may refer to Lyness (1976ii). However, this is a continuing research area; other expansions have been discovered since then and more may remain to be discovered. See Sidi (1983).

The user of Linear Extrapolation Quadrature need not concern himself about the derivation of the expansion. Once he has satisfied himself that it exists and knows its form, he can proceed to apply extrapolation. This is done by constructing linear sums of values of $Q^{(m)}f$ in such a way as to eliminate the early terms of the relevant expansion. The Neville algorithm can be used when the expansion is a simple one, like the one in Theorem 2.2 above. But, in general, all that one has to do is to solve a set of linear equations.

We close this section by stating the corresponding results for Gaussian Quadrature. It is convenient to present the following definition as a theorem.

THEOREM 2.9. *When $f(x,y)$ is a polynomial of degree d and Q is a degree d quadrature rule, with respect to a specified region R and a specified weight function $w(x,y)$, then*

$$Qf - I(R)f \ = 0\ , \tag{2.9}$$

where $I(R)f \ = \int_R w(x,y)f(x,y)dxdy$.

Note that, in Gaussian Quadrature, the singularity enters through a weight function, and in general, no m-copy rule is treated. The user of Gaussian Quadrature improves his accuracy by using a sequence of different rules of successively higher degree. On the other hand, the user of Extrapolation Quadrature achieves the same end using the same basic rule with a sequence of successively higher mesh ratios m.

Again, the user need not concern himself about where the weights and abscissas came from. If they are available, he simply has to use them in a straightforward rule evaluation program.

3. Affine Transformation

As mentioned in the introduction, Quadrature rules and theory is conventionally discussed in the literature in the context of standard regions. In this article, we are particularly interested in nonstandard regions of the same general character. To this end we employ the Affine Transformation (represented by a nonsingular $N \times N$ constant matrix A). The mapping

$$\mathbf{x} = A\mathbf{x}' \tag{3.1}$$

takes any parallelogram (or triangle) R into another parallelogram (or triangle) R'. To be specific, when R is defined by inequalities involving the components of $\mathbf{x}$, the region R' is defined by the same set of inequalities, but with each component of $\mathbf{x}$ replaced by the corresponding component of $A\mathbf{x}$. It is readily established that, given any triangle R' having one vertex at the origin, there exists an Affine transformation A which takes the standard triangle R into R'. This remark is valid when R' is any parallelogram and R the standard square. But one cannot obtain a general quadrilateral in this way. Besides transforming regions, an Affine transformation transforms associated Quadrature rules.

DEFINITION 3.2. *The affine transform of the rule*

$$Qf = \sum w_j f(\mathbf{x}_j)$$

with respect to A is

$$Q'f = \sum W_j f(\mathbf{X}_j)\ , \tag{3.3}$$

where $W_j = w_j / |\det A|$ and $\mathbf{X}_j = A^{-1}\mathbf{x}_j$.

The abscissas of the new rule are in precisely the same positions relative to the region R' as the abscissas of Q are relative to R. The weights have been scaled uniformly to account for a possibly different area. It is readily verified that the Affine transform of a degree zero quadrature rule is also a degree zero quadrature rule. (See Theorem 3.8 below.) We now relate the error functionals of these two rules.

Lemma 3.4. *Let A be an affine transformation that takes R into R'; let $Q'f$ be the affine transform of Qf, and let the respective error functionals be*

$$Ef = Qf - \int_R w(\mathbf{x}) f(\mathbf{x}) d^N x\ , \tag{3.4}$$

$$E'\phi = Q'\phi - \int_{R'} W(\mathbf{x})\phi(\mathbf{x}) d^N x\ , \tag{3.5}$$

where $W(\mathbf{x}) = w(A\mathbf{x})$. Then, when

$$\phi(\mathbf{x}) = f(A\mathbf{x})\ , \tag{3.6}$$

it follows that

$$Ef = |\det A| E'\phi. \tag{3.7}$$

Proof. This is a matter of elementary algebraic substitution.

Note that R may be a general region but we only use it for triangles or squares. The important part of this result is that it states that two numbers are equal. It is not a result about form. That comes later.

This lemma can be used to establish results about Extrapolation Quadrature. But, as a preliminary, we use it to confirm a well known result.

THEOREM 3.8. *When Q is a rule of polynomial degree d for a region R with weight function $w(\mathbf{x})$, then its Affine transform Q' is a rule of the same polynomial degree for the region R' with weight function $w(A\mathbf{x})$.*

Proof. Let $\phi \varepsilon \Pi_d$. It follows immediately from (3.6) that $f \varepsilon \Pi_d$. Since by hypothesis Q is of polynomial degree d, it follows that Ef given by (3.4) is zero; and then, from (3.7) that $E'\phi = 0$. Consequently $E'\phi = 0$ for all $\phi \varepsilon \Pi_d$ and this establishes the theorem.

We may now use the same approach to derive the less trivial analogues about extrapolation.

THEOREM 3.9. *Theorem 2.2 above is valid precisely as written when H is replaced by R, a general parallelogram.*

We restate Theorem 3.9 in a notation which allows us to derive it from Theorem 2.2.

THEOREM 3.9′. *Let R' be a parallelogram and Q' be a degree zero quadrature rule for R'. Then when $\phi(x)$, together with its partial derivatives of order p or less, are integrable over R',*

$$Q'^{(m)}\phi - I(R')\phi = \frac{B_1}{m} + \frac{B_2}{m^2} + \ldots + \frac{B_{p-1}}{m^{p-1}} + O(m^{-p}) \ , \tag{3.9}$$

where $B_s = B_s(R';Q';\phi)$ are independent of m.

Proof. Let $\phi(x)$ satisfy the hypothesis in the theorem. It follows immediately that $f(x)$ given by (3.6) satisfies the same hypothesis with respect to R. Thus Theorem 2.2 may be applied to $f(x)$ establishing that Ef has expansion (2.2). However, from (3.7) it follows that the same expansion applies to $E'\phi|\det A|$. This is precisely the statement in (3.9) above, with

$$B_s(R';Q';\phi) = B_s(r;Q;f)/|\det A| \ , \tag{3.10}$$

which establishes the theorem.

The key to the proofs of the last two theorems is that $f(x)$ and $\phi(x)$ share some property. In the first theorem, this property is that they are both polynomials of the same degree. In the previous theorem, both have continuous partial derivatives of order p. However, in the present context the really important shared property is the following.

LEMMA 3.11. *Let $\phi(x) = f(Ax)$ with $\det A \neq 0$. Then if one of f or ϕ is homogeneous of degree α, so is the other, and if one has no singularity except at the origin, the same is true about the other.*

The proof is trivial. This is displayed as a lemma simply because of its importance.

THEOREM 3.12. *Theorem 2.3 is valid precisely as written when H is replaced by R, a general parallelogram.*

The proof is logically similar to that of the previous theorem, the property shared by f and ϕ being the one described in the lemma.

However, this approach to handling the parallelograms and triangles denoted by R' is not general. One may be interested in a singularity of the sort encountered in Theorem 2.7, whose principal component is r^a. When one applies Lemma 3.4 directly, one finds in just the same way that the error functional asymptotic expansion (2.7) applies when $F(x,y)$ has a singularity whose principal component is of the form $(Ax^2 + 2Hxy + By^2)^{\alpha/2}$, this being the particular homogeneous function into which r^a is transformed by the transformation which takes R into R'. The geometrically inclined reader can visualize a plot of R containing the circular contours of r^{-1}. It is this whole picture which is transformed into a plot of R'; the circular contours become elliptical. Nevertheless, we have the following theorem.

THEOREM 3.13. *Theorem 2.7 is valid, precisely as written when H is replaced by R, a general parallelogram.*

Proof. We recall that Theorem 2.7 was derived from Theorems 2.2 and 2.3 by means of expansion (2.5), which developed $F(x,y)$ as a series of homogeneous functions, to which Theorem 2.3 was applied, together with a remainder term, to which Theorem 2.2 was applied. We need only employ the same expansion, but apply Theorems 3.11 and 3.12 to the respective terms instead. This gives the result in the theorem.

Theorem 3.9 is technically new and I believe Theorem 3.13 is new. The author has attempted to establish these results before by transforming each term in the expansion separately. In the simpler case, it is possible but very tedious to do this. In the singular case, the integral representations of the coefficients are too formidable. The proofs given above avoid this by not providing direct formulas for the coefficients. This is no real hardship as, in the practice of Linear Extrapolation Quadrature, one needs only the form of the error functional expansion and details about the coefficients are not required.

Theorems 3.9, 3.12, and 3.13 illustrate a major convenience of using Extrapolation Quadrature. This is that the effect of the singularity is taken care of by using the proper expansion. For the same singularity, this is the same for all triangles and for all parallelograms. Once this expansion is known, one may go ahead and carry out extrapolation using a linear equation solver. On the other hand, Theorem 3.8 confirms that in Gaussian Quadrature the situation is quite different. The affine transform rule Q' applies to a different weight function $w(Ax)$ and not to $w(x)$. Unless these two weight functions happen to be closely related, one will need a completely new set of Gaussian rules for each new triangle. In the familiar case in which $w(x) = 1$, clearly $w(Ax) = w(x)$ and one can use the affine transformed rule. There are other special cases described in the next section. But, in general, one cannot expect a relationship, so, when there is a singularity, separate sets of rules are needed for separate triangles.

4. Gaussian Quadrature with Singularities

It is conventional wisdom that, whether singularities are present or not, the proper use of Gaussian Quadrature is generally more cost effective than the proper use of Extrapolation Quadrature by a factor of about two or even more in the number of function values needed to attain a particular accuracy. So one's natural inclination is to prefer to use Gaussian Quadrature. In the regular case, in which no nontrivial weight function is involved, it is straightforward to obtain weights and abscissas from standard texts such as Stroud (1971) or Davis and Rabinowitz (1984). And, as mentioned above, an affine transformed rule can be used when the region is an affine transform of a standard region.

The term "proper use" in the first sentence above is vital. This implies that in the singular case, the appropriate weight function is identified, and Gaussian Quadrature is carried out using the weights and abscissas corresponding to that weight function; or in the EQ case extrapolation is based on the correct error functional expansion. Improper use of these techniques usually has the effect of utterly compromising the accuracy or reducing the rate of convergence to a snails pace. As usual, one would find that the accuracy increases with the number of function values used, however unwisely the abscissas and weights are chosen. The symptom of misuse here is not lack of convergence, but extremely slow convergence.

The identification of the appropriate weight function in the context of finite element methods is usually no problem whatever. However, finding lists of weights and abscissas is a different matter. The common experience seems to be that one cannot locate lists of weights and abscissas for Gaussian Quadrature rules having genuine two dimensional singular weight functions.

To proceed, there are several possibilities. The two most attractive are the following.

(a) Look for some analytic transformation that may reduce the present numerical problem into another less intractable or more familiar numerical problem. The Duffy transformation described in Section 5 is an example.

(b) If an error functional expansion is available, use Extrapolation Quadrature.

A looming disaster overhangs the following approach.

(c) Try to get by using a different Gaussian rule, perhaps one pertaining to a nearby weight function for which weights and abscissas are available. The lurking dangers here are discussed in detail in Section 6.

We pursue a somewhat obvious approach in the rest of this section, which we could also characterize as being both self serving and altruistic. If these rules are not listed and we need them, surely others will need them from time to time. What we ought do is to calculate them ourselves, use them in our problem, and also publish them for others to use later. Naturally, this is a not insignificant task. To do this calculation one needs accurate numerical values of the moments, one needs to design a quadrature rule structure, and, if one wants an optimal rule, one will almost certainly have to solve systems of nonlinear equations. If we take short cuts to simplify the calculation, the resulting rules will be less cost effective, possibly leaving EQ a more attractive choice. Let us suppose that all these problems have been successfully tackled, and we now have a Gaussian type quadrature rule for a standard triangle R and a weight function $w(x)$.

The trouble is that one can use this rule only for integration over this triangle R. If one wants to integrate over a different triangle R', we have already noted that the affine transformation that changes R into R' also changes the weight function to $w(Ax)$. In general, if one wants the same weight function $w(x)$, but for a different region R', one has to calculate a new set of quadrature rules. The immediate answer to the suggestion that we publish this list of rules is that this list is not general enough. A triangle with a fixed vertex at the origin requires four parameters to specify it. Our list treats only a single choice of these parameters. To be useful, the list should cover a relatively general problem and not one extremely special case.

This is the general situation, but there are exceptions. In fact, so many familiar weight functions are exceptional in some way, that the user has to be forgiven for imagining that all are. The critical point is to note whether $w(Ax)$ and $w(x)$ are closely related. This depends on $w(x)$ and A. Specifically, if for some k we have

$$w(x) = kw(Ax) \ ,$$

then one can obtain one set of rules directly from the other set. One case in which this happens is when $w(x)$, reexpressed as a function of r and θ, turns out to be independent of θ, and in addition the transformation A is a rotation about the origin. A second case occurs when $w(x)$ is homogeneous (about the origin of degree α) and A is a uniform magnification. In either case, to obtain the second set one takes the affine transform of each rule of the first set (which incorporates the factor det A into each weight) and then multiplies each weight by $k^{2+\alpha}$.

Examples of the first case include $1/r$ and $\ln r/r$. Examples of the second case include $1/r$ and $1/(\lambda x+\mu y)$. Thus, if one has available a rule of polynomial degree d for $w(x) = r^{\alpha}$ for the standard triangle T_2, one may rotate the triangle and rotate each abscissa by the same angle, keeping the weights constant; then one may magnify the triangle by a linear factor k, moving the abscissas accordingly, but also multiplying the weights by $k^{2+\alpha}$. In this very favorable case one has reduced to two the number of parameters needed for the list of rules. However, this particular example can be handled more elegantly using the Duffy transformation.

5. The Duffy Transformation

If one has a "product" singularity which fits conveniently into the integration region, for example

$$x^{\alpha}y^{\beta}g(x,y) \tag{5.1}$$

for the unit square $[0,1)^2$, then one can handle the problem using cartesian product formulas involving one-dimensional weight functions, such as the Gauss Jacobi Quadrature Rules. This suggests that it may be useful to look for a transformation that takes an apparently intransigent "singularity-region" pair into an easier one, like the one above.

A somewhat sophisticated example of this is the Duffy transformation technique for the triangle. In 1982, apropos of nothing, Duffy published a paper about integrating over triangles and tetrahedra. He suggested the following transformation.

$$\int_0^1 dx \int_0^x dy \;\; f(x,y) = \int_0^1 dx \int_0^1 dt \;\; x f(x,tx) \ . \tag{5.2}$$

For example, instead of integrating

$$f(x,y) = (x^2+y^2)^{\alpha/2} g(x,y) \tag{5.3}$$

over the triangle

$$\tilde{T}\!: \quad x < 1; \;\; y > 0; \;\; x-y > 0 \ , \tag{5.4}$$

one might prefer to integrate

$$x f(x,tx) = x^{1+\alpha}(1+t^2)^{\alpha/2} g(x,tx) \tag{5.5}$$

over the rectangle $[0,1)^2$.

The vertex singularity has been smeared out to make a more conventional line singularity. When $\alpha = -1$, what was originally a weak singularity has disappeared, leaving an analytic function, which can be handled using a product Gauss Legendre quadrature rule. For general noninteger α, a product of a Gauss Jacobi rule with a Gauss Legendre rule is appropriate.

In fact, this transformation is much more powerful and more useful than was at first realized, particularly as a tool for use in the Boundary Element Method.

Given a rectangle and a function that is singular at the origin, one can always divide it into two triangles and apply the Duffy transformation to each. In some cases one may be lucky. For example, suppose for $\tilde{T}$

$$f(x,y) = x^{\lambda} y^{\mu} f_{\alpha}(x,y) g(x,y) , \tag{5.6}$$

where $f_{\alpha}(x,y)$ is homogeneous of degree α and $g(x,y)$ is regular. Applying the transformation leads to the problem of integrating over a rectangle the function

$$xf(x,tx) = x^{1+\lambda+\mu+\alpha} t^{\mu} f_{\alpha}(1,t) g(x,tx) . \tag{5.7}$$

If the only singularity of $f_{\alpha}(x,y)$ is at the origin, then $f_{\alpha}(1,t)$ is regular and one can use here the cartesian product of a pair of Gauss Jacobi rules.

Duffy's method for integrating over a square is to subdivide it into two triangles and then use the transformation above to transform each into a square. In some cases it is useful to iterate the whole procedure.

The same technique is available in any number of dimensions. In three dimensions one first splits the cube into three square-based pyramids and separately transform each pyramid back into a cube using the three-dimensional Duffy transformation.

6. A Misuse of Gaussian Quadrature

In view of the difficulty in finding lists of Gaussian rules for singular weight functions, it is very tempting to use weights and abscissas for a nearby weight function $W(x)$ instead, particularly when these are available and the ones for $w(x)$ are not. We suppose that Gaussian rules are available for a triangle R with weight function $w(x)$, singular at a vertex $x=0$ of R; but, unfortunately, we are evaluating an integral whose integrand has the singular behavior described by $w(x)$ over R'. The regions R and R', although close to each other, are related by an affine transformation. There is a mismatch here. Since

$$\int_R w(x) g(x) dx = |\det A| \int_{R'} w(Ax) g(Ax) dx , \tag{6.1}$$

we have Gaussian rules available for R with $w(x)$ or for R' with $w(Ax)$ but not for R' with $w(x)$. The quantity we want to evaluate may be reexpressed as

$$\int_{R'} w(x) f(x) dx = \int_{R'} w(Ax) \left(\frac{w(x)}{w(Ax)} f(Ax) \right) dx . \tag{6.2}$$

An initially promising but in fact deceptive approach is to use the available Gaussian rule on the right-hand member of (6.2). $f(Ax)$ like $f(x)$ is regular, so whether it is worth using this rule depends on the smoothness of $w(x)/w(Ax)$. We pursue this example by taking $w(x) = r^{\alpha}$. Then $W(Ax)$ has the form $(Ax^2+2Hxy+By^2)^{\alpha/2}$. The function

$$w(x)/w(Ax) = \left[\frac{x^2+y^2}{Ax^2+2Hxy+By^2} \right]^{\alpha/2} \qquad \textbf{(6.3)}$$

is somewhat deceptive. It can be expressed as a function of y/x and so is constant along any radius vector. But these constants are different for different radius vectors. For example, on the x-axis, $w/W = A^{-\alpha/2}$, while on the y-axis, $w/W = B^{-\alpha/2}$. Technically, this means that the function is not Hölder continuous at the origin. But one needs only minimal intuition to see that such a function is simply not readily approximated by a polynomial or entire function and so Gaussian Quadrature with this component in the integrand seems pointless.

If a user remains to be convinced that this misuse of Gaussian Quadrature is expensive, he should be invited to carry out minor numerical experiments. To do this he does not need to attempt his problem for which presumably results are not available. At issue is how well a Gaussian Rule integrates a function with this sort of behavior at the origin. A numerical example is given in Section 8.

There are two further points to be made en passant. It might have happened that, in the example above, the various limits of w/W as x approached the origin were identical. In the particular example, this would happen if A were orthogonal. Such cases are precisely those discussed toward the end of Section 4 in which one may, in any case, construct a Gaussian Rule for R' from one for R.

The other point is that w/W is, in fact, a homogeneous function of degree zero. Unless it is constant, such a function causes trouble in Gaussian Quadrature. But Extrapolation Quadrature handles these with no trouble at all. (See Subsection 7.2 below.)

7. Further Remarks about Extrapolation Quadrature

Up to this point in this article, I have taken the view that most users, given the choice, would prefer Gaussian Quadrature to Extrapolation Quadrature. The first reason for believing this is that most users have never heard of EQ. However, the ones that know anything about it know that Gaussian Quadrature is generally more cost effective. My belief is that this attitude will change as more and more users find how easy it is to handle EQ. In this section we look at some problems in which even the most intrepid Gaussian Integrator would concede that a role exists for EQ.

7.1. MIXED SINGULARITIES

One can envisage all sorts of really complicated singular behavior of an integrand function at a point. In this subsection we consider a singularity only one stage removed in difficulty from a standard singularity. Let us suppose that the integrand has a double singularity form, such as

$$f(x,y) = r^{-1}g_1(x,y) + r^{-1/2}g_2(x,y)$$

or

$$f(x,y) = r^{-1}g_1(x,y) + r^{-1}\ln r \; g_2(x,y)$$

or

$$f(x,y) = r^{-1}g_1(x,y) + g_2(x,y) \ ,$$

where g_1 and g_2 are both regular. It is necessary to distinguish between the case in which function values of g_1 and of g_2 are both available and the case in which function values of f are available, f is known to be of this form, but function values of g_1 and g_2 are not available separately. In the former case, the problem is straightforward. One can simply evaluate the two parts of the integral separately. Two applications of Gaussian Quadrature instead of one may increase the cost sufficiently to make Extrapolation Quadrature competitive. In the latter case one requires a double type Gaussian rule, that is, one that preserves the integrity of two components of a singularity. There is presently no developed theory for constructing this type of quadrature rule, though some individual one-dimensional rules of this type are known. However, in either case, EQ may be used simply based on the concatenation of the two error functional expansions. In the second and third example, this concatenation coincides with one of the component expansions.

7.2. HOMOGENEOUS SINGULARITIES

EQ handles some functions of low Hölder continuity quite well. Typical of these is $\Phi(\theta)$, a nontrivial homogeneous function of degree zero. For example, let A, B, C, and D be positive. The function

$$\Phi(\theta) = (Ax+By)/(Cx+Dy)$$

is regular in $[0,1]^2$ except at the origin, where one finds a singularity which occurs because the limit as (x,y) approaches the origin depends on the angle of approach. In spite of the fact that it is bounded wherever defined, it cannot be ignored for Gaussian Quadrature. However, since it is homogeneous (of degree zero), EQ handles this integrand function with no difficulty. A function of this type was mentioned in an example in Section 6.

Much more sophisticated singularities in which this sort of singularity is a component can be handled in a simple manner using EQ, but are virtually out of reach of Gaussian Quadrature. Take, for example, the result given in Theorem 2.7 about the integrand function being of the form

$$F(x,y) = r^{\alpha}\Phi(\theta)h(r)g(x,y) \ . \tag{7.1}$$

A Gaussian rule having weight r^{α} will handle $r^{\alpha}p_1(x,y)$. A double-type Gaussian rule will handle $r^{\alpha}p_1(x,y) + r^{\alpha+1}p_2(x,y)$ which covers these functions in (7.1) when $\Phi(\theta)$ is constant. However, when $\Phi(\theta)$ is not specified individually, but is known to be non trivial, one is led to the conclusion that Gaussian Quadrature cannot be applied and EQ is the obvious choice.

7.3. ROLE IN CONSTRUCTING GAUSSIAN RULES

Towards the end of Section 4, we considered very briefly the possibility of constructing ones own set of Gaussian Rules. We mentioned that to do this one requires accurate numerical values of the moments. If the weight function is one for which no convenient analytic form for the moments is available, one may have to calculate these numerically for oneself. In one dimension, one thinks in terms of a sledgehammer approach to get the moments used to construct the elegant rule.

In two or more dimensions, the sledgehammer approach can be unexpectedly expensive. If EQ is available, it can be effectively used in this subsidiary role.

8. A Numerical Example

The following example deals with approximations to

$$If = \int_0^1 \int_0^1 \cos\theta \, dxdy = \frac{1}{2}\left[\log(\sqrt{2}+1) + \sqrt{2} - 1\right],$$

where $\cos\theta = x/r$ and (r,θ) are standard polar coordinates. In this contrived and stylized example of a Hölder discontinuous function, we use principally the product midpoint trapezoidal rule $Qf = f(1/2, 1/2)$ and its m-copy version.

The first task when using Extrapolation Quadrature is to be absolutely assured that one is using the correct expansion. Since $\cos\theta$ is a homogeneous function of degree zero, expansion (2.3) with $\alpha = 0$ is appropriate. Only even powers are needed since the rule is symmetric. Nevertheless, Table 1 illustrates some expensive numerical tests one might make if one wanted to convince oneself — or someone else. The convention used here about expansion exponents is that they represent negative exponents of m, they are in order of magnitude, and if two (or more) are equal, corresponding log (or log power) terms occur in the expansion. Since the exact result is available, we have presented in these tables the error, $Qf - If$. The reader will agree that at a cost of about 21,000 function values, Table 1 presents prima facie numerical evidence that the second sequence treated may be the most appropriate.

TABLE 1

EXPENSIVE NUMERICAL EXPERIMENT TO VERIFY THE CORRECT EXPANSION

THE BASIC PRODUCT TRAPEZOIDAL RULE RESULTS

mesh	Rf	If	Rf - If
mesh = 1	Rf = 0.7071	If = 0.6478	Rf - If = 0.5931D-01
mesh = 2	Rf = 0.6698	If = 0.6478	Rf - If = 0.2199D-01
mesh = 4	Rf = 0.6551	If = 0.6478	Rf - If = 0.7296D-02
mesh = 8	Rf = 0.6501	If = 0.6478	Rf - If = 0.2275D-02
mesh = 16	Rf = 0.6485	If = 0.6478	Rf - If = 0.6815D-03
mesh = 32	Rf = 0.6480	If = 0.6478	Rf - If = 0.1986D-03
mesh = 64	Rf = 0.6479	If = 0.6478	Rf - If = 0.5669D-04
mesh =128	Rf = 0.6478	If = 0.6478	Rf - If = 0.1594D-04

THE EXTRAPOLATION TABLE; expansion exponents are; 2 4 6 8 10

k	m	(k,1,1)	(k,2,1)	(k,3,1)	(k,4,1)	(k,5,1)	(k,6,1)
1	1	0.059313	0.9546D-02	0.1922D-02	0.4584D-03	0.1133D-03	0.2823D-04
2	2	0.021988	0.2399D-02	0.4813D-03	0.1146D-03	0.2831D-04	0.7058D-05
3	4	0.007296	0.6011D-03	0.1203D-03	0.2865D-04	0.7079D-05	0.1764D-05
4	8	0.002275	0.1504D-03	0.3008D-04	0.7163D-05	0.1770D-05	0.0000D+00
5	16	0.000681	0.3760D-04	0.7521D-05	0.1791D-05	0.0000D+00	0.0000D+00
6	32	0.000199	0.9401D-05	0.1880D-05	0.0000D+00	0.0000D+00	0.0000D+00
7	64	0.000057	0.2350D-05	0.0000D+00	0.0000D+00	0.0000D+00	

```
0.0000D+00
 8128    0.000016   0.0000D+00   0.0000D+00   0.0000D+00   0.0000D+00
0.0000D+00

 THE EXTRAPOLATION TABLE; expansion exponents are;  2  2  4  6  8

 k  m   (k,1,1)  (k,2,1)    (k,3,1)    (k,4,1)    (k,5,1)    (k,6,1)
 1  1  0.059313 0.5931D-01 0.1621D-04 0.9690D-06 0.1579D-07-0.5428D-
10
 2  2  0.021988-0.7396D-02 0.1922D-05 0.3069D-07 0.7634D-11 0.5071D-
13
 3  4  0.007296-0.7379D-03 0.1489D-06 0.4870D-09 0.8034D-13 0.8663D-
16
 4   8    0.002275-0.1152D-03   0.9761D-08   0.7689D-11   0.3996D-15
0.0000D+00
 5  16    0.000681-0.2093D-04   0.6173D-09   0.1205D-12   0.0000D+00
0.0000D+00
 6  32    0.000199-0.4111D-05   0.3869D-10   0.0000D+00   0.0000D+00
0.0000D+00
 7  64    0.000057-0.8463D-06   0.0000D+00   0.0000D+00   0.0000D+00
0.0000D+00
 8128    0.000016   0.0000D+00   0.0000D+00   0.0000D+00   0.0000D+00
0.0000D+00

 THE EXTRAPOLATION TABLE; expansion exponents are;  2  2  4  4  6

 k  m   (k,1,1)  (k,2,1)    (k,3,1)    (k,4,1)    (k,5,1)    (k,6,1)
 1  1  0.059313 0.5931D-01 0.1621D-04 0.2354D-05-0.3187D-07-0.1045D-
08
 2  2  0.021988-0.7396D-02 0.1922D-05-0.4420D-06-0.1526D-08-0.4233D-
12
 3  4  0.007296-0.7379D-03 0.1489D-06-0.7322D-08-0.2427D-10-0.4930D-
14
 4    8    0.002275-0.1152D-03    0.9761D-08-0.2792D-09-0.3840D-12
0.0000D+00
 5   16    0.000681-0.2093D-04    0.6173D-09-0.1247D-10    0.0000D+00
0.0000D+00
 6  32    0.000199-0.4111D-05   0.3869D-10   0.0000D+00   0.0000D+00
0.0000D+00
 7  64    0.000057-0.8463D-06   0.0000D+00   0.0000D+00   0.0000D+00
0.0000D+00
 8128    0.000016   0.0000D+00   0.0000D+00   0.0000D+00   0.0000D+00
0.0000D+00
```

In Table 2, three approaches which are realistic are illustrated. Extrapolation Quadrature based on both an appropriate and an inappropriate error functional expansion are given. These cost 204 function values. For the comparison, some product Gauss-Legendre approximations using up to 400 function values are given. These results speak for themselves as to the effect of the proper use of Gaussian and Extrapolation Quadrature.

TABLE 2

THE BASIC PRODUCT TRAPEZOIDAL RULE RESULTS

mesh	Rf	If	Rf - If
1	0.7071	0.6478	0.5931D-01
2	0.6698	0.6478	0.2199D-01
3	0.6594	0.6478	0.1164D-01
4	0.6551	0.6478	0.7296D-02
5	0.6528	0.6478	0.5041D-02
6	0.6515	0.6478	0.3711D-02
7	0.6507	0.6478	0.2858D-02
8	0.6501	0.6478	0.2275D-02

THE EXTRAPOLATION TABLE; expansion exponents are; 2 2 4 6 8

k	m	(k,1,1)	(k,2,1)	(k,3,1)	(k,4,1)	(k,5,1)	(k,6,1)
1	1	0.059313	0.5931D-01	0.2242D-04	0.3222D-05	0.4052D-06	-0.2092D-07
2	2	0.021988	-0.1302D-01	0.6228D-05	0.6401D-06	0.6766D-09	0.1642D-09
3	3	0.011642	-0.3333D-02	0.2285D-05	0.1211D-06	0.2305D-09	0.7314D-10
4	4	0.007296	-0.1480D-02	0.9798D-06	0.3381D-07	0.1052D-09	0.0000D+00
5	5	0.005041	-0.8186D-03	0.4824D-06	0.1196D-07	0.0000D+00	0.0000D+00
6	6	0.003711	-0.5126D-03	0.2633D-06	0.0000D+00	0.0000D+00	0.0000D+00
7	7	0.002858	-0.3478D-03	0.0000D+00	0.0000D+00	0.0000D+00	0.0000D+00
8	8	0.002275	0.0000D+00	0.0000D+00	0.0000D+00	0.0000D+00	0.0000D+00

THE EXTRAPOLATION TABLE; expansion exponents are; 2 4 6 8 10

k	m	(k,1,1)	(k,2,1)	(k,3,1)	(k,4,1)	(k,5,1)	(k,6,1)
1	1	0.059313	0.9546D-02	0.2592D-02	0.1060D-02	0.5335D-03	0.3052D-03
2	2	0.021988	0.3365D-02	0.1156D-02	0.5546D-03	0.3115D-03	0.1930D-03
3	3	0.011642	0.1708D-02	0.6508D-03	0.3385D-03	0.2027D-03	0.1320D-03
4	4	0.007296	0.1032D-02	0.4166D-03	0.2276D-03	0.1420D-03	0.0000D+00
5	5	0.005041	0.6899D-03	0.2893D-03	0.1634D-03	0.0000D+00	0.0000D+00
6	6	0.003711	0.4937D-03	0.2126D-03	0.0000D+00	0.0000D+00	0.0000D+00
7	7	0.002858	0.3707D-03	0.0000D+00	0.0000D+00	0.0000D+00	0.0000D+00
8	8	0.002275	0.0000D+00	0.0000D+00	0.0000D+00	0.0000D+00	0.0000D+00

PRODUCT GAUSS-LEGENDRE RESULTS

```
npg = 4   Gf =  0.6489  If =  0.6478 Gf - If =  0.1130D-02
npg = 8   Gf =  0.6479  If =  0.6478 Gf - If =  0.9276D-04
npg =12   Gf =  0.6478  If =  0.6478 Gf - If =  0.2008D-04
npg =16   Gf =  0.6478  If =  0.6478 Gf - If =  0.6646D-05
npg =20   Gf =  0.6478  If =  0.6478 Gf - If =  0.2796D-05
```

In fact, example (8.1) is one which Duffy's transformation renders trivial. Dividing the square into two equal triangles, and then using Duffy's transformation on both, leads to

$$If = \int_0^1 \int_0^1 \frac{x(1+t)}{\sqrt{(1+t^2)}} dx \; dt \;,$$

which is too straightforward to pursue numerically.

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