

On the Numerical Evaluation of a Particular Singular Two-Dimensional Integral

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Abstract. We investigate the possibility of using two-dimensional Romberg integration to approximate integrals, over the square $0 \leq x, y \leq 1$, of integrand functions of the form $g(x, y)/(x - y)$ where $g(x, y)$ is, for example, analytic in x and y .

We show that Romberg integration may be properly justified so long as it is based on a diagonally symmetric rule and function values on the singular diagonal, if required, are defined in a particular way. We also investigate the consequences of ignoring these function values (i.e. setting them to zero) in the context of such a calculation.

We also derive the asymptotic expansion on which extrapolation methods can be based when $g(x, y)$ has a point singularity of a specified nature at the origin.

1. The calculation of the aerodynamic load on a lifting body occasionally requires the calculation of a two-dimensional Cauchy principal value integral of the type

$$\int_0^1 \int_0^1 \frac{g(x, y)}{x - y} dx dy.$$

(See, for example, Bisplinghoff, Ashley and Halfman [1].) One approach to the evaluation of such integrals has been described by Song [5]. In this paper we show that, with some minor provisos, a straightforward application of two-dimensional Romberg integration may be used in this problem.

The two-dimensional integral

$$(1.1) \quad If = \int_0^1 \int_0^1 f(x, y) dx dy$$

may be approximated numerically using a two-dimensional quadrature rule Q defined by

$$(1.2) \quad Qf = \sum_{j=1}^{\nu} w_j f(x_j, y_j), \quad \sum_{j=1}^{\nu} w_j = 1.$$

This rule has *polynomial degree* $d(Q)$ when

$$(1.3) \quad Qf = If \quad \text{for all } f \in \pi_d,$$

where π_d is the set of polynomials of degree d or less.

Definition 1.4. A *symmetric rule* Q is one for which

$$(1.4) \quad Qf = \tilde{Q}\tilde{f} \quad \text{for all } \tilde{f}(1 - x, 1 - y) = f(x, y).$$

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The m^2 -copy of the rule Q is defined by

$$(1.5) \quad Q^{(m)}f = \sum_{k_1=0}^{m-1} \sum_{k_2=0}^{m-1} \sum_{j=1}^{\nu} \frac{w_j}{m^2} f\left(\frac{x_j + k_1}{m}, \frac{y_j + k_2}{m}\right).$$

This is a weighted sum of function values obtained by subdividing the unit square into m^2 equal squares of side $1/m$ and applying a properly scaled version of Q to each. $Q^{(m)}$ has the same polynomial degree $d(Q)$ and is symmetric when Q is symmetric.

THEOREM 1.6. *Let Qf and $Q^{(m)}f$ be defined as above. Let $f(x, y)$ be a function, all of whose derivatives $f^{(r, s)}(x, y)$ whose total order satisfies $r + s \leq p$ are integrable over the unit square. Then*

$$(1.6) \quad Q^{(m)}f - If = \sum_{s=1}^{l-1} \frac{B_s(Q; f)}{m^s} + O(m^{-l}), \quad 2 \leq l \leq p,$$

where

$$(1.7) \quad B_s(Q; f) = \sum_{s_1=0}^s C_{s_1, s-s_1}(Q) \int_0^1 \int_0^1 f^{(s_1, s-s_1)}(x, y) dx dy$$

are coefficients which are independent of m . When $f(x, y)$ is a polynomial of degree $d(f)$ or less

$$(1.8) \quad B_s(Q; f) = 0 \quad \forall s > d(f).$$

Moreover, when Q is a symmetric rule

$$(1.9) \quad B_s(Q; f) = 0 \quad \forall s \text{ odd}$$

and when Q is a rule of polynomial degree $d(Q)$

$$(1.10) \quad B_s(Q; f) = 0, \quad s = 1, 2, \dots, d(Q).$$

The foregoing definitions and results are well known (see, e.g. Lyness [3]). However, Theorem 1.6, on which the theory of Romberg integration is based, requires that, unlike the integrands we treat in this paper, the integrand $f(x, y)$ and its partial derivatives be integrable over the unit square.

In this paper, we are interested in modifying and extending these results so that an extrapolation method may be used to approximate the two-dimensional principal value integrals mentioned above. We treat an integrand function

$$(1.11a) \quad f(x, y) = \frac{g(x, y)}{x - y}, \quad x \neq y,$$

where $g(x, y)$ and all its partial derivatives up to a total order $p + 1$ are integrable over the unit square.

The function $f(x, y)$ is not defined at points along the diagonal. In the subsequent analysis it is convenient to extend the definition as follows:

$$(1.11b) \quad f(x, y) = \frac{1}{2} \left[\frac{\partial g}{\partial x} - \frac{\partial g}{\partial y} \right], \quad x = y.$$

In our approach, we restrict ourselves to quadrature rules which are symmetric about the diagonal.

Definition 1.12. A *diagonally symmetric rule* Q is one for which

$$(1.12) \quad Qf = \tilde{Q}\tilde{f} \quad \text{for all } \tilde{f}(x, y) = f(y, x).$$

Based on this symmetry we split both $f(x, y)$ and $g(x, y)$ into symmetric and antisymmetric parts. Thus, we define

$$(1.13) \quad g_+(x, y) = \frac{1}{2} [g(x, y) + g(y, x)], \quad g_-(x, y) = \frac{1}{2} [g(x, y) - g(y, x)],$$

and

$$(1.14) \quad f(x, y) = f_-(x, y) + f_+(x, y),$$

where

$$(1.15a) \quad f_-(x, y) = \frac{g_+(x, y)}{x - y}, \quad x \neq y,$$

$$(1.15b) \quad = 0, \quad x = y,$$

$$(1.16a) \quad f_+(x, y) = \frac{g_-(x, y)}{x - y}, \quad x \neq y,$$

$$(1.16b) \quad = \frac{1}{2} \left[\frac{\partial g}{\partial x} - \frac{\partial g}{\partial y} \right], \quad x = y.$$

The reason for definition (1.11b) is now apparent. While not altering the nature of the problem, it makes the symmetric part of $f(x, y)$ differentiable. Since $f_-(x, y)$ is antisymmetric about the diagonal it follows that when Q is a diagonally symmetric quadrature rule

$$(1.17) \quad Qf_- = Q^{(m)}f_- = If_- = 0$$

and so

$$(1.18) \quad Q^{(m)}f - If = Q^{(m)}f_+ - If_+.$$

Moreover, when $g(x, y)$ is a polynomial of degree $d(g)$, it follows that $f_+(x, y)$ is a polynomial of degree $d(g) - 1$.

We may now obtain an analogue of Theorem 1.6, relating to function (1.11) by using (1.18) and applying Theorem 1.6 to the function $f_+(x, y)$. This gives

THEOREM 1.19. *Let Q be a diagonally symmetric rule (Definition 1.12). Let $f(x, y) = g(x, y)/(x - y)$, where $g(x, y)$ and all its derivatives of total order $p + 1$ or less are integrable over the unit square; and let $f(x, x)$ be defined according to (1.11b). Then*

$$(1.19) \quad Q^{(m)}f - If = \sum_{s=1}^{l-1} \frac{B_s(Q; f_+)}{m^s} + O(m^{-l}), \quad 2 \leq l \leq p,$$

where the coefficients $B_s(Q; f_+)$ are defined in (1.7) and satisfy properties (1.8), (1.9) and (1.10).

In terms of $g(x, y)$ the first condition for the vanishing of terms in this expansion is simply that, when $g(x, y)$ is a polynomial of degree $d(g)$,

$$(1.20) \quad B_s(Q; f_+) = 0 \quad \forall s > d(g) - 1.$$

In practice then, one may apply Romberg integration in any of its many forms to this problem using any set of mesh ratios $m_0 < m_1 < m_2 \cdots$ so long as it is based on a diagonally symmetric rule Q . Most standard rules Q are diagonally symmetric. For example, the midpoint or the vertex rules

$$(1.21) \quad Qf = f(\frac{1}{2}, \frac{1}{2}),$$

$$(1.22) \quad Qf = \frac{1}{4}(f(0, 0) + f(1, 0) + f(0, 1) + f(1, 1))$$

can be used. These happen also to be symmetric in the sense of Definition 1.4 and so the error functional has an even expansion. Thus, Romberg integration takes precisely the same form as in the conventional case, though it is necessary to replace the indeterminate function values on the diagonal by $f(x, x) = (\partial g/\partial x - \partial g/\partial y)/2$.

In some applications, the values of $\partial g/\partial x$ and $\partial g/\partial y$ on the diagonal may not be available, or may be inconvenient to obtain. In Section 2 we discuss briefly the effect on the theory if these are simply ignored (or set to zero). This is not recommended, but it is permissible at the expense of replacing an even expansion by a full expansion. In the rest of this section we pursue, in a practical context, the obvious alternative of avoiding the problem by using a rule which does not require such evaluations. This is also accomplished only at additional expense.

Thus, we require a rule Q satisfying the following properties:

- (a) Q is diagonally symmetric (so the theory is applicable).
- (b) None of the m^2 -copy rules $Q^{(m)}$ require function values on the diagonal (so as to avoid evaluations of $\partial g/\partial x$ and $\partial g/\partial y$).
- (c) Q is symmetric (so the error functional expansion (1.19) is even in character).

Even with these restrictions there is an almost limitless choice of rule Q . And, as in Romberg integration, it is an open question as to which choice of Q , together with which mesh ratio sequence $m_0 < m_1 < m_2 < \cdots$ is most appropriate. We shall confine ourselves to drawing attention to some of the simplest rules. Of interest are particularly the degree of $d(Q)$ and the number of function values $\nu(Q^{(m)})$ required by the m^2 -copy.

Undoubtedly, the simplest such rules satisfying these conditions are those of the form

$$(1.23a) \quad Qf = \frac{1}{2}(f(\alpha, 1 - \alpha) + f(1 - \alpha, \alpha)), \quad 0 < \alpha < \frac{1}{2}.$$

For these rules

$$(1.23b) \quad d(Q) = 1; \quad \nu(Q^{(m)}) = 2m^2.$$

The choice $\alpha = 1/4$ gives an aesthetically pleasing pattern of points. Slightly more sophisticated rules have been suggested by Squire [6]. These are of the form

$$(1.24a) \quad Qf = \frac{1}{4}(f(\beta, \frac{1}{2}) + f(1 - \beta, \frac{1}{2}) + f(\frac{1}{2}, \beta) + f(\frac{1}{2}, 1 - \beta)), \quad 0 \leq \beta < \frac{1}{2}.$$

For these, in general

$$(1.24b) \quad d(Q) = 1; \quad \nu(Q^{(m)}) = 4m^2, \quad \beta \neq 0.$$

Two special cases are of interest. When $\beta = \frac{1}{2} - \sqrt{1/6}$, this rule is of degree $d(Q) = 3$. When $\beta = 0$, this rule reduces to a symmetrized version of the cartesian product of the midpoint and the endpoint trapezoidal rules, namely

$$(1.25a) \quad Qf = \frac{1}{4}(f(0, \frac{1}{2}) + f(1, \frac{1}{2}) + f(\frac{1}{2}, 0) + f(\frac{1}{2}, 1))$$

and

$$(1.25b) \quad d(Q) = 1; \quad \nu(Q^{(m)}) = 2m(m + 1), \quad \beta = 0,$$

as points lie on the edge of the square and are shared between neighboring squares.

When the rule is of degree 1, the application of Romberg integration is standard. One chooses a mesh sequence $0 < m_0 < m_1 < m_2 < \dots$. One defines the initial column of the Romberg table by

$$(1.26) \quad T_0^k = Q^{(m_k)}f$$

and calculates elements of the Romberg table in the usual way

$$(1.27) \quad T_p^k = \frac{m_k^2 T_{p-1}^k - m_{k+p}^2 T_{p-1}^{k+1}}{m_k^2 - m_{k+p}^2}.$$

The elements T_p^k of the p th column are exact whenever $g(x, y)$ is a polynomial of degree $2p$ or less.

A word of caution about the choice of mesh sequence is in order. In the classical version of one-dimensional Romberg integration, the geometric sequence

$$(1.28) \quad m_j = 2^j, \quad j = 0, 1, 2, \dots,$$

is suggested, partly because of the possibility of reusing function values. In higher dimensions the relative gain arising from the reuse of function values diminishes while the cost of using high mesh ratios may become prohibitive. For example, if one uses the rule (1.25) or (1.23) with $\alpha = \frac{1}{4}$ the situation is that the set of points required by $Q^{(m)}f$ includes those required by $Q^{(n)}f$, $n < m$, only if m/n is an odd integer. Thus, at best, only approximately one ninth of the function values required by $Q^{(m)}$ are likely to have been calculated previously. Incidentally, by using the sequence (1.28) one ensures that there is no reuse of function values. The argument in favor of sequence (1.28) simply has no validity in this context.

A sequence which in general seems to balance the requirements of numerical stability and economy is the familiar

$$(1.29) \quad m_j = 1, 2, 3, 4, 6, 8, 12, 16, \dots$$

but, as in the classical Romberg integration case, a convincing theory in this area is lacking.

2. In this section, we examine the effect of using a rule which involves function values on the diagonal, but ignoring the singular values of $f(x, y)$, i.e. setting $f(x, x) = 0$.

We write the quadrature rule in a form which displays the points on the diagonal; thus

$$(2.1) \quad Qf = \sum_{j=1}^{\nu_1} w_j f(x_j, y_j) + \sum_{j=1}^{\nu_2} W_j f(t_j, t_j), \quad x_j \neq y_j.$$

We define the first summation on the right as $\tilde{Q}^{[1]}f$. In general, $\tilde{Q}^{[m]}f$ is a rule which coincides with $Q^{(m)}f$ except that the function values on $x = y$ are omitted. Specifically,

Definition 2.2.

$$(2.2) \quad \tilde{Q}^{[m]}f = Q^{(m)}f - \sum_{k=0}^{m-1} \sum_{j=1}^{\nu_2} \frac{W_j}{m^2} f\left(\frac{t_j + k}{m}, \frac{t_j + k}{m}\right).$$

We define

$$(2.3) \quad q(x) = f(x, x)$$

and the one-dimensional operator R by

$$(2.4) \quad Rq = \sum_{j=1}^{\nu_2} W_j q(t_j),$$

in which case it follows that

$$(2.5) \quad Q^{(m)}f - \tilde{Q}^{[m]}f = \frac{1}{m} R^{(m)}q.$$

Should $\sum W_j = 1$, R is a quadrature rule operator. Otherwise, R has many properties in common with quadrature rule operators. If $\sum W_j \neq 0$, it is simply a scaled version of a quadrature rule. When $\sum W_j = 0$, it is a null rule defined in Lyness [2]. In all cases, a one-dimensional version of Theorem 1.6 provides an expansion for $R^{(m)}q$, namely

$$(2.6) \quad R^{(m)}q = b_0 + \frac{b_1}{m} + \dots + \frac{b_{l-1}}{m^{l-1}} + O(m^{-l}), \quad 1 \leq l \leq p,$$

where

$$(2.7) \quad b_0 = c_0(R) \int_0^1 q(x) dx; \quad b_j = c_j(R) \int_0^1 q^{(j)}(x) dx.$$

The coefficients $c_k(R)$ are simply the numbers obtained by applying the operator R to $B_k(x)/k!$, where $B_k(x)$ is the Bernoulli polynomial of degree k . This may be written in the form

$$(2.8) \quad c_k(R) = R_x(B_k(x)/k!).$$

When R is symmetric $b_j = 0$ for odd j and when R is of polynomial degree $d(R)$, $b_1 = b_2 = \dots = b_{d(R)} = 0$. When q is a polynomial of degree $d(q) - 1$, $b_j = 0 \forall j > d(q) - 1$. Using these results together with those of Theorem 1.19, it follows that

THEOREM 2.9.

$$(2.9) \quad \tilde{Q}^{[m]}f - If = \sum_{s=1}^{l-1} \frac{C_s}{m^s} + O(m^{-l}),$$

where

$$(2.10) \quad C_s = B_s(Q; f_+) - b_{s-1}.$$

Thus, one may ignore the singularity and still employ an extrapolation method. However, the structure of these coefficients shows that there is no obvious way to choose a rule Q so that an even expansion is obtained. When Q is symmetric R is also symmetric. In this case we have $B_s = b_s = 0$ for odd s , but this does not imply that any of the coefficients C_s are zero.

Thus, one is forced to use a version of Romberg integration based on a full expansion. An examination of the number of function values required to obtain a result of specified polynomial degree in $g(x, y)$ shows that it would be usually advantageous to use a rule like (1.25) above (which does not require singular points and which has an even error functional expansion) than to use say (1.21) above and ignore the singularity.

The conditions required to make some of the coefficients vanish are noted here, but these are of mainly academic interest. If $g(x, y)$ is a polynomial of degree $d(g)$, then

$$(2.11) \quad C_s = 0, \quad s > d(g).$$

If Q is symmetric and of degree $d(Q)$, then

$$(2.12) \quad C_s = 0, \quad s = 2, 4, \dots, d(Q) - 1.$$

If Q is of degree $d(Q)$ and R is a rule, or a scaled rule of degree $d(R)$, then

$$(2.13) \quad C_s = 0, \quad s = 2, 3, \dots, \min(d(Q), d(R)).$$

If, in addition, R is a null rule of degree $d(R)$, $C_1 = 0$. (A null rule of degree d is one which integrates (incorrectly) all polynomials of degree d or less to zero. See Lyness [2].)

For practical purposes, construction of a rule Q having properties such as these is not worthwhile. However, it is interesting to note that if Q is the product of two identical one-dimensional rules of degree $d(Q)$ which assign equal weights to each abscissa, i.e.

$$(2.14) \quad Qf = \frac{1}{\nu^2} \sum_{i=1}^{\nu} \sum_{j=1}^{\nu} f(x_i, x_j),$$

then

$$(2.15) \quad Rq = \frac{1}{\nu^2} \sum_{i=1}^{\nu} q(x_i)$$

is a scaled version of a rule of degree $d(Q)$ and in view of (2.13) the expansion contains terms $m^{-1}, m^{-d-1}, m^{-d-2} \dots$.

3. In the two previous sections we treated an integrand function $g(x, y)/(x - y)$, where $g(x, y)$ together with its derivatives of order up to $p + 1$ are integrable over the unit square. This restriction on $g(x, y)$ allowed us to apply Theorem 1.6 to the function $f_+(x, y)$, a fundamental step in constructing the theory.

In this section we extend the previous theory to cover cases in which $g(x, y)$ has an integrable point singularity of a type specified below at the origin. This extension is based on Theorem 3.1 below which is a generalization of Theorem 1.6.

In the sequel, (r, θ) is the polar coordinate representation of (x, y) . The functions $h(r), \phi(\theta)$ and $G(x, y)$ are analytic in $0 \leq r \leq \sqrt{2}; 0 \leq \theta \leq \pi/2$ and $0 \leq x, y \leq 1$, respectively.

THEOREM 3.1 (LYNESS [3, THEOREM 5.14]). *Let*

$$(3.1) \quad F(x, y) = r^\alpha \phi(\theta) h(r) G(x, y).$$

Then

$$(3.2a) \quad Q^{(m)}F - IF \sim \sum_{t=0} A_{\alpha+2+t}(Q; F) \frac{1}{m^{\alpha+2+t}} + \sum_{s=1} B_s(Q; F) \frac{1}{m^s}, \quad \alpha \neq \text{integer},$$

$$(3.2b) \quad Q^{(m)}F - IF \sim \sum_{s=1} \frac{A_s(Q; F) + B_s(Q; F)}{m^s} + \sum_{s=1} \frac{C_s(Q; F) \ln m}{m^s}, \quad \alpha = \text{integer}.$$

We now treat the same problem as treated in Sections 1 and 2 but with an integrand function given by

$$(3.3) \quad f(x, y) = \frac{g(x, y)}{x - y} = \frac{r^\alpha \phi(\theta) h(r) G(x, y)}{x - y}.$$

The functions $f_-(x, y)$ and $f_+(x, y)$ are defined precisely as in Eqs. (1.13)–(1.16) above and satisfy (1.17) and (1.18). The function $f_+(x, y)$ is of the same form as $F(x, y)$ in (3.1), and so we may apply Theorem 3.1 to $f_+(x, y)$ to obtain the following result.

THEOREM 3.4. *Let $f(x, y)$ be given by (3.3) and Q be diagonally symmetric. Then the error functional $Q^{(m)}f - If$ has an asymptotic expansion of form (3.2), the arguments $(Q; f)$ in the coefficients on the right being replaced by $(Q; f_+)$.*

Note that a function evaluation at the origin, if required by Q , may be ignored at the expense of introducing at most one additional term into the expansion (see [3, Theorem 5.17]).

An expansion of the type described in Theorem 3.4 may be used as the basis of an extrapolation procedure to estimate an integral whose integrand is of form (3.3). An example (of a form treated in [6]) is

$$(3.5) \quad \int_0^1 \int_0^1 \frac{G(x, y)}{x^2 - y^2} dx dy.$$

Expressing the integrand in the form

$$(3.6) \quad f(x, y) = r^{-1} \frac{1}{\cos \theta + \sin \theta} \frac{G(x, y)}{x - y},$$

we may apply Theorem 3.4 directly to obtain

$$(3.7) \quad Q^{(m)}f - If \sim \sum_{s=1} \frac{D_s(Q; f_+)}{m^s} + \frac{C_s(Q; f_+)}{m^s} \ln m$$

so long as Q is diagonally symmetric. If in addition Q is symmetric, the terms C_s with s odd are zero and may be omitted. (See Lyness [3, Equation (4.19)].)

Nearly all the expansions given in [3] may be generalized in this way to produce corresponding expansions for the case in which the additional $(x - y)^{-1}$ is present and the rule Q is diagonally symmetric.

For example, when $g(x, y)$ has the form $r^\alpha (\ln r)^q \phi(\theta) h(r) G(x, y)$ where q is any nonnegative integer, the appropriate expansion for the error functional may be derived in an equally straightforward manner from one of those described in Sections 6 and 7 of [3]. Moreover, when $g(x, y)$ has singularities of the type $x^\alpha y^\beta (\ln x)^q$ where $\alpha, \beta > -1$ and q is any nonnegative integer, a suitable expansion exists, being based trivially on one-dimensional expansions given in [4].

A prospective user of these expansions should be aware that in many cases a significant proportion of the coefficients displayed in expansion (3.2) may be zero. Including nonexistent terms in an extrapolation process is not harmful but results in an unnecessarily expensive calculation. Some of the cases in which some coefficients are zero are given in [3].

4. We have shown, in Section 1, that when $g(x, y)$ is analytic, one may employ any of the many variants of two-dimensional Romberg integration to evaluate integrals of the form

$$(4.1) \quad \int_0^1 \int_0^1 \frac{g(x, y)}{x - y} dx dy,$$

and most of the standard properties associated with Romberg integration are valid. There are, however, two provisos. These are that a diagonally symmetric rule Q should be used and that the function values on the diagonal if required should be calculated using (1.11b). As is usually the case, when the rule Q is symmetric, the expansion on which Romberg integration is based is an even expansion in inverse powers of m .

We have also shown that if one uses a rule which requires function values on the diagonal but ignores these function values, then one may still use Romberg integration in the same way, but the expansion required is a full expansion in inverse powers of m .

In Section 3 we have generalized the theory of Section 1 to cover cases in which $g(x, y)$ has a point singularity of a specified nature at the origin.

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