Integrating Singularities using Non-uniform Subdivision and Extrapolation. [1]

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Abstract A new approach to the computation of approximations to multidimensional integrals over an n-dimensional hyper-rectangular region, when the integrand is singular, is described. This approach is based on a non-uniform subdivision of the region of integration and the technique fits well to the subdivision strategy used in many adaptive algorithms. The strategy can be applied to vertex singularities, line singularities and more general subregion singularities. The technique turns out to have good numerical stability properties.

1. Introduction

In 1976 Lyness [9] published the first paper which addresses the problem of finding the error functional expansion in multidimensional quadrature with a singular integrand function. Knowing at least the existence of such expansions is essential in order to compute such integrals effectively. Since 1976 several related papers have appeared, some giving expansions for different regions and others giving expansions for different types (or combinations) of singular behavior [3, 4, 5, 8, 10, 11, 12, 13, 14]. A common feature for these expansions is that they are based on a *uniform* subdivision of the region, applying the same rule on each subregion.

In a recent paper Espelid (1992) [7] describes a new idea applying extrapolation on a sequence of estimates produced through a *non-uniform* subdivision of the initial region. This approach can be used on problems having vertex singularities associated with homogeneous functions. The idea presented in [7] is generally applicable to any dimension and any region which can be subdivided into subregions of the same form, e. g. hypercubes, simplices, etc.. Furthermore, the technique can be applied to internal

[1]Published by: *Int. Series of Numer. Math., vol. 112, H. Brass and G. Hämmerlin (eds), 1993 (pp 77-89).*

point singularities as well. In order to apply this technique one has to know at least the position of the singular point.

In this paper we will extend this new approach to the integration of singular integrands to include problems with line singularities in 2 dimensions, line or face singularities in 3 dimensions and subregion (line, face , etc.) singularities in n-dimensions. In order to achieve this generalization we have to restrict the region of integration to an n-dimensional hyperrectangle.

This paper is organized as follows: in the next section we present the problem and develop the basic error expansion. Then we describe the new subdivision approach and finally we give some examples and concluding remarks.

2. Homogeneous functions: basic error expansion

A function $f(\mathbf{x})$, where $\mathbf{x} \in R^n$, is said to be homogeneous of degree α (about the origin) if

$$f(\lambda \mathbf{x}) = \lambda^\alpha f(\mathbf{x}) \text{ for } \forall\ \lambda > 0.$$

We will use the notation introduced by Lyness (1976), [9], and denote such a function $f_\alpha(\mathbf{x})$. Note the following simple rules: $f_\alpha f_\beta$ is of homogeneous of degree $\alpha + \beta$ and $(f_\alpha)^\beta$ is of homogeneous of degree $\alpha\beta$.

We will discuss n-dimensional integration, however we will assume that the singularity is caused by a homogeneous function about the origin which involves exactly s of the n variables, with $1 \leq s \leq n$. To simplify the presentation assume that the variables are numbered such that these s variables are $x_1, x_2, \ldots, x_s$.

Observe that we may use an affine transformation to transform the given rectangular region on to the unit n-cube. Any homogeneous function will still be homogeneous after such a transformation and its degree will be invariant. We know furthermore that any given cubature rule can be transformed as well and its polynomial degree will be invariant too. Thus, choosing the n-dimensional unit hypercube, C_n, as the region of integration represents no restriction

$$C_n : 0 \leq x_i \leq 1 \text{ for } i = 1, 2, \ldots, n.$$

Define

$$I(f) = \int_{C_n} f(\mathbf{x}) d\mathbf{x} = \int_0^1 \int_0^1 \cdots \int_0^1 f(x_1, x_2, \ldots, x_n)\ dx_1\ dx_2 \ldots dx_n. \qquad (1)$$

We will discuss how to compute numerical estimates to integration problems of type (1), where the function involved, f, is a product of a homogeneous function $f_\alpha(x_1, x_2, \ldots, x_s)$ and a function $g(\mathbf{x})$ which is regular in C_n. The function $f_\alpha(x_1, x_2, \ldots, x_s)$ is assumed to have a point singularity at the origin of C_s due to the homogeneous property. Define $\mathbf{x}_0 = (0, 0, \ldots, 0, x_{s+1}, x_{s+2}, \ldots, x_n)$ then

$$\begin{cases} f(\mathbf{x}) = f_\alpha(x_1, x_2, \ldots, x_s)\ g(\mathbf{x}), \text{with } \alpha > -s. \\ g(\mathbf{x}_0) \not\equiv 0,\ \mathbf{x}_0 \in C_n. \end{cases}$$

Furthermore we assume that the origin is the only point in C_s where f_α is non-analytic. We give a few examples to illustrate the type of singular problems we will deal with.
1) A line singularity in C_2 due to a point singularity in C_1 ($s = 1$),

$$\int_0^1 \int_0^1 x^\alpha g(x, y)\, dxdy \text{ with } \alpha > -1.$$

2) A line singularity in C_3 due to a point singularity in C_2 ($s = 2$),

$$\int_0^1 \int_0^1 \int_0^1 (x+y)^\alpha g(x, y, z)\, dxdydz \text{ with } \alpha > -2.$$

3) A face singularity in C_3 due to a point singularity in C_1 ($s = 1$),

$$\int_0^1 \int_0^1 \int_0^1 x^\alpha g(x, y, z)\, dxdydz \text{ with } \alpha > -1.$$

4) A point singularity in C_3 ($s = 3$), with $r = \sqrt{x^2 + y^2 + z^2}$,

$$\int_0^1 \int_0^1 \int_0^1 r^\alpha\, g(x, y, z)\, dxdydz \text{ with } \alpha > -3.$$

Example 4) is the only one that can be handled by the technique described in [7] directly. However, all of these problems can be dealt with by that technique after an appropriate transformation. E. g., in example 1) we may apply an inverse Duffy (1982) transformation, [6]; replacing y with t using $y = t/x$ gives

$$\int_0^1 (\int_0^x x^{\alpha-1} g(x, t/x)\, dt)\, dx \text{ with } \alpha > -1.$$

Thus integrating a function over a triangle having a vertex singularity at the origin of degree $\alpha - 1$. An additional difficulty has been introduced due to the transformation: t/x is a homogeneous function of degree 0 around the origin, however this will be handled by the described technique quite easily. It will, however, have a slightly negative effect on the performance of the method. We will give an example of such an approach in Section 5.

In order to deal with example 1) directly we may choose a product of two classical rules: a Gauss-Legendre rule in the y direction where the function is smooth and a Gauss-Jacobi rule in the other direction.

Alternatively we may subdivide the original square in m^2 equal squares and then use the same rule Q over all these squares. Denoting the compound rule $Q^{(m)}$ we get, Sidi (1983) [13] and Lyness and de Doncker-Kapenga (1987) [11],

$$Q^{(m)}(f) \sim I(f) + \sum_{\ell \geq 0} \frac{A_\ell}{m^{\alpha+2+\ell}} + \sum_{\ell \geq 0} \frac{C_\ell \log m}{m^{\alpha+2+\ell}} + \sum_{\ell \geq 1} \frac{B_\ell}{m^\ell}. \tag{2}$$

For many integrals, some of the coefficients in (2) vanish e.g., the C-coefficients vanish if α is non-integer or if a special rule Q is used; some of the B-coefficients may vanish depending on the degree of precision and symmetry of Q. Based on (2) we may now compute $Q^{(m)}$ for different values of m and then use extrapolation to improve these approximations. This last approach does not need information about where the line singularity is, while the Gauss-Legendre/Gauss-Jacobi approach is based on that information.

We will, in what follows, present an alternative approach. Just as in [7] we will base this on a *non-uniform* subdivision of the region of integration combined with extrapolation. The non-uniform aspect resembles the basic idea with the product rules: to treat the problem differently in the different directions of integration. Assume that we know (a) which variables are involved in the singularity and (b) the position of at least one vertex where the function is singular (the origin in this presentation). Cut this region into $s+1$ new subregions by dividing in two halves the region containing the singularity orthogonal to one of the s directions. Continuing this until all s directions have been divided exactly once we have: one region containing the singularity and s regions where the function is supposed to be well behaved. Considering these s subdivisions as one step we may do j such steps. The hyper-rectangle containing the singularity is now $H_n^{(s)}(h) = [0,h]^s \times [0,1]^{n-s}$, with $h = 1/2^j$. Define

$$I_{H_n^{(s)}(h)}(f) = \int_0^1 \cdots \int_0^1 (\int_0^h \cdots \int_0^h f(x_1, x_2, \ldots, x_n)\, dx_1 \ldots dx_s) dx_{s+1} \ldots dx_n. \qquad (3)$$

Suppose that both $\mathbf{x}_0$ and $\mathbf{x}$ are points in C_n. Expand $g(\mathbf{x})$ in a Taylor series around $\mathbf{x}_0$ with p basic terms and a remainder term r

$$\begin{aligned} g(\mathbf{x}) &= g(\mathbf{x}_0) + \textstyle\sum_{i=1}^s x_i \frac{\partial g}{\partial x_i}(\mathbf{x}_0) + \frac{1}{2}\sum_{i,j=1}^s x_i x_j \frac{\partial^2 g}{\partial x_i \partial x_j}(\mathbf{x}_0) + \ldots \\ &+ \textstyle\frac{1}{(p-1)!}\sum_{i_1,i_2,\ldots,i_{p-1}=1}^s x_{i_1} x_{i_2} \ldots x_{i_{p-1}} \frac{\partial^{p-1} g}{\partial x_{i_1} \partial x_{i_2} \ldots \partial x_{i_{p-1}}}(\mathbf{x}_0) + r. \end{aligned}$$

Multiply this expression by $f_\alpha(x_1, x_2, \ldots, x_s)$ and integrate over $H_n^{(s)}(h)$. Changing integration variables $x_i = h\ v_i,\ i = 1, 2, \ldots, s$, in each integration term moves all integrals to C_n and gives

$$I_{H_n^{(s)}(h)}(f_\alpha g) = c_0\ h^{\alpha+s} + \sum_{\ell=1}^{p-1} c_\ell\ h^{\alpha+s+\ell} + O(h^{\alpha+s+p}), \qquad (4)$$

with

$$\begin{cases} c_0 = \int_{C_n} f_\alpha(x_1, x_2, \ldots, x_s) g(\mathbf{x}_0) d\mathbf{x}, \\ c_\ell = \frac{1}{\ell!}\int_{C_n} f_\alpha(x_1, x_2, \ldots, x_s) \sum_{i_1,\ldots,i_\ell=1}^s x_{i_1} \cdots x_{i_\ell}\ \frac{\partial^\ell g}{\partial x_{i_1} \ldots \partial x_{i_\ell}}(\mathbf{x}_0)\ d\mathbf{x}, \\ \ell = 1, 2, \ldots p-1. \end{cases}$$

Here we have used the fact that the term ℓ involves functions which are of homogeneous degree $\alpha + \ell$ in C_s about the origin.

Suppose furthermore that we use a fixed cubature rule Q on a hyper-rectangle, H, based on L evaluation points

$$Q_H(f) = \sum_{i=1}^L w_i\ f(\mathbf{x}_i).$$

Assume that $\sum_{i=1}^{L} w_i$ equals the volume of hyperrectangle H (Q has degree of precision at least 0) and that the evaluation points $\mathbf{x}_i$ have been translated to H. Applying this rule on f over $H_n^{(s)}(h)$ then gives

$$Q_{H_n^{(s)}(h)}(f_\alpha g) = b_0\ h^{\alpha+s} + \sum_{\ell=1}^{p-1} b_\ell\ h^{\alpha+s+\ell} + O(h^{\alpha+s+p}), \tag{5}$$

where

$$\begin{cases} b_0 = Q_{C_n}(f_\alpha(x_1, x_2, \ldots, x_s)g(\mathbf{x}_0)), \\ b_\ell = \frac{1}{\ell!}Q_{C_n}(f_\alpha(x_1, x_2, \ldots, x_s)\sum_{i_1,\ldots,i_\ell=1}^{s} x_{i_1}\cdots x_{i_\ell}\ \frac{\partial^\ell g}{\partial x_{i_1}\ldots\partial x_{i_\ell}}(\mathbf{x}_0)), \\ \ell = 1, 2, \ldots p-1. \end{cases}$$

Here we have used the fact that the term ℓ involves functions which are of homogeneous degree $\alpha+\ell$ in C_s and that applying Q over $H_n(h)$ is a simple h-scaling of C_n in the first s variables. Thus the volume and the weights w_ℓ must be scaled by a h^s factor. By subtracting (4) from (5) we get the error expansion

$$E_n^{(s)}(h) = Q_{H_n^{(s)}(h)}(f_\alpha g) - I_{H_n^{(s)}(h)}(f_\alpha g) = \sum_{\ell=0}^{p-1} a_\ell\ h^{\alpha+s+\ell} + O(h^{\alpha+s+p}), \tag{6}$$

with

$$a_\ell = b_\ell - c_\ell,\ \ \ell = 0, 1, \ldots, p-1.$$

b_ℓ is the numerical estimate produced by the rule Q of the integral c_ℓ and the functions involved will become smoother with increasing values of ℓ. Therefore it is reasonable to expect $|a_\ell| >> |a_{\ell+1}|$, at least as long as $\alpha+s+\ell \leq \text{degree}(Q)$.

The extrapolation scheme will be based the error expansion (6). In fact, we assume that the error given in (6) will be the major error source in the estimate of $I(f)$. The error contribution from the rest of the original region C_n has to be kept under control and we will show how it will influence the extrapolation process and the final global estimate of $I(f)$.

3. The Series with Tail-correction Approach

We will now use the error expansion developed in the previous section combined with the series with tail-correction approach presented in [7]. Suppose that we use a strategy which repeatedly subdivides the subregion which is considered to represent the most difficult part of the integration problem (1). Each time the subregion containing the singularity needs subdivision we divide this in $s+1$ new subregions following the procedure described in the previous section. Thus, at any time, the collection of subregions will contain only one hyperrectangle containing the singularity, namely $H_n^{(s)}(h)$. At a given time we may have replaced this hyperrectangle in the collection k times. Define (with $h_i = 1/2^i$)

$$\begin{cases} I_i = I_{H_n^{(s)}(h_i)}(f_\alpha g),\ \ i = 0, 1, 2, \ldots, k, \\ U_i = I_{i-1} - I_i,\ \ i = 1, 2, \ldots, k, \\ S_k = \sum_{i=1}^{k} U_i,\ \ \hat{S}_k = \sum_{i=1}^{k} \hat{U}_i, \end{cases} \tag{7}$$

where $\hat{U}_i$ is an approximation to U_i. The elements in the sequence $U_1, U_2, \ldots$ are by definition (7) integrals over a sequence of subregions, $L_n^{(s)}(h) = [h, 2h]^s \times [0,1]^{n-s}$ for a given value of h. $L_n^{(s)}(h)$ is similar to the L-shaped regions described by Lyness (1976) [9] when $s = n$ (that is: a corner singularity in the n-cube).
We illustrate, in Figure 1, two subregion sequences in 2 dimensions:

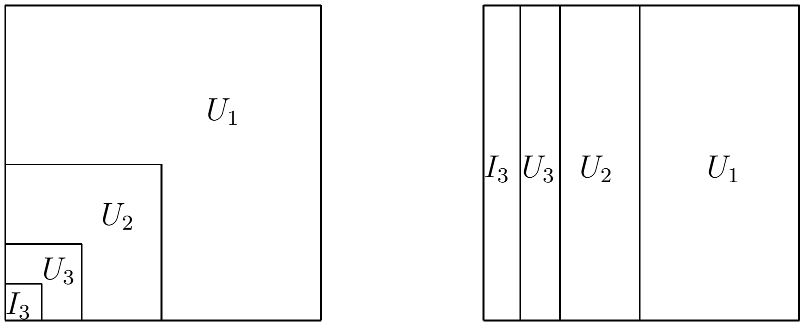

Figure 1. 2-D (a) corner and (b) line singularities: U and I-sequences.

Using the definition of U_i we get $S_k = I_0 - I_k$. Thus S_k is an approximation to I_0 with error $-I_k$. We can use the expansion for $I_{H_n^{(s)}(h)}$ with $h = h_k = 1/2^k$ given in (4)

$$S_k - I_0 = -c_0 h_k^{\alpha+s} - c_1 h_k^{\alpha+s+1} - \cdots - c_{p-1} h_k^{\alpha+s+p-1} - O(h_k^{\alpha+s+p}).$$

In practice we have to approximate U_i, e. g.: we have suggested to divide this region into s rectangles in Section 2, however we may need to subdivide further to achieve the necessary precision. $\hat{S}_k$ is an approximation to I_0 giving

$$\hat{S}_k - I_0 = \sum_{i=1}^{k} (\hat{U}_i - U_i) - c_0 h_k^{\alpha+s} - c_1 h_k^{\alpha+s+1} - \cdots - c_{p-1} h_k^{\alpha+s+p-1} - O(h_k^{\alpha+s+p}). \quad (8)$$

In [7] we discuss to use (8) as a basis for extrapolation. The conclusion is that correcting the tail of the series gives an improved approximation to a low cost and that this actually is to be preferred. Based on this we present the tail correction strategy here: using the rule Q to estimate $I_i = I_{H_n^{(s)}(h_i)}$, then $Q_i = Q_{H_n^{(s)}(h_i)}(f_\alpha g)$ is an estimate of the tail $I_i = \sum_{\ell > i} U_\ell$. Define

$$T_{i0} = Q_i + \sum_{\ell=1}^{i} \hat{U}_\ell, \; i = 0, 1, 2, \ldots, k.$$

T_{i0} is an approximation to I_0 and we have according to (6)

$$T_{i0} - I_0 = \sum_{\ell=1}^{i} E_{U_\ell} + \sum_{\ell=0}^{p-1} a_\ell h_i^{\alpha+s+\ell} + O(h_i^{\alpha+s+p}), \quad (9)$$

where $E_{U_\ell} = \hat{U}_\ell - U_\ell$. By standard linear extrapolation we may use (9) to eliminate the k first terms in the sum of h-powers. Define

$$n_1 = 2^{\alpha+s} - 1, \; n_{j+1} = 2n_j + 1, \; j = 1, 2, 3, \ldots,$$

and then

$$T_{ij} = T_{i,j-1} + (T_{i,j-1} - T_{i-1,j-1})/n_j, i = 1, 2, \ldots, k,\ j = 1, 2, 3, \ldots, i. \qquad (10)$$

We may put the T_{ij} in a standard extrapolation tableau as follows

$$\begin{array}{llll} T_{00} & & & \\ T_{10} & T_{11} & & \\ \vdots & \vdots & \ddots & \\ T_{k0} & T_{k1} & \cdots & T_{kk} \end{array}$$

This gives after j extrapolation steps in row k

$$T_{kj} = I_0 + \sum_{\ell=j}^{p-1} a_\ell^{(j)} h_k^{\alpha+s+\ell} + O(h_k^{\alpha+s+p}) + \sum_{\ell=1}^{k} (1 - \beta_{k+1-\ell,j}) E_{U_\ell}. \qquad (11)$$

We refer the reader to [7] for more details about these $\beta-$coefficients. The important point to make is that these coefficients may be computed and make it possible to keep track of the effect of not knowing each U_ℓ exactly. We may avoid that these errors ruin the extrapolation process by simply deciding that if the effect becomes disturbing, then compute a better approximation to at least one these U_ℓs.

We face two different alternatives if we are not satisfied with the global approximation: (A) Compute a better value for $\hat{U}_\ell$ and update the T-tableau. This can easily be done directly in the last row of this tableau, estimate the new errors and finally decide what to do next. (B) If we are not satisfied with the extrapolation error then increase k: put $h_{k+1} = h_k/2$, compute $\hat{U}_{k+1}$ and Q_{k+1} and create a new row in the T-tableau.

In [7] we observed that T_{kk} can be written

$$T_{kk} = \sum_{i=1}^{k} \gamma_i^{(k)} \hat{U}_i + \sum_{i=0}^{k} \delta_i^{(k)} Q_i,$$

and defined the condition number for T_{kk} as

$$\tau_s^{(k)} = (1 - \frac{1}{2^s}) \sum_{i=1}^{k} |\gamma_i^{(k)}| (\frac{1}{2^s})^{i-1} + \sum_{i=0}^{k} |\delta_i^{(k)}| (\frac{1}{2^s})^i.$$

Observe that the volumes associated with the estimates $\hat{U}_i$ and Q_i enter this expression. We can compute $\tau_s^{(k)}$ once the exponent sequence is known, ([7]):

s / k	1	2	3	4	7	10
1	5.83	6.92	6.30	4.49	1.55	1.07
2	5.83	4.28	3.13	1.80	1.02	1.00
3	5.83	2.96	2.15	1.24	1.00	1.00
4	5.83	2.30	1.81	1.09	1.00	1.00
5	5.83	1.97	1.67	1.04	1.00	1.00

Table 1 τ-table for $s + \alpha = 1/2$.

The extrapolation procedure is remarkably stable and increasing the number of extrapolation steps has a positive effect on the methods stability. $H_n^{(s)}(h)$ has volume h^s and this volume will decrease in each step with a factor $\frac{1}{2^s}$. This decrease in volume counter-effects the influence by the coefficients $\gamma_i^{(k)}$ and $\delta_i^{(k)}$ on the condition number.

4. Integrating logarithmic singularities

Now suppose that the function f is a product of a homogeneous function f_α, a logarithmic function $\ln g_\beta$ and a function $g(\mathbf{x})$ which is regular in C_n. The functions $f_\alpha(x_1, x_2, \ldots, x_s)$ and $g_\beta(x_1, x_2, \ldots, x_s)$ are both assumed to have a point singularity at the origin of C_s due to the homogeneous property.

$$f(\mathbf{x}) = f_\alpha(x_1, x_2, \ldots, x_s)\,(\ln g_\beta(x_1, x_2, \ldots, x_s))\; g(\mathbf{x}), \text{with } \alpha > -s.$$

Furthermore we assume that origin is the only point in C_s where f_α and g_β are non-analytic. Repeating the line of arguments that led to (4), (5) and (6) we get the error expansion

$$E_n^{(s)}(h) = Q_{H_n^{(s)}(h)}(f) - I_{H_n^{(s)}(h)}(f) = \sum_{\ell=0}^{p-1}(\tilde{a}_\ell + \hat{a}_\ell \ln h)\; h^{\alpha+s+\ell} + O(h^{\alpha+s+p}\ln h), \quad (12)$$

where we have

$$\begin{cases} \tilde{a}_\ell = \tilde{b}_\ell - \tilde{c}_\ell,\; \ell = 0, 1, 2, \ldots, p-1. \\ \tilde{b}_0 = Q_{C_n}(f_\alpha(\ln g_\beta) g(\mathbf{x}_0)), \\ \tilde{b}_\ell = \frac{1}{\ell!}\, Q_{C_n}(f_\alpha(\ln g_\beta)\sum_{i_1,\ldots,i_\ell=1}^{s} x_{i_1}\cdots x_{i_\ell}\, \frac{\partial^\ell g}{\partial x_{i_1}\ldots\partial x_{i_\ell}}(\mathbf{x}_0)),\; \ell = 1, 2, \ldots p-1. \\ \tilde{c}_0 = \int_{C_n} f_\alpha(\ln g_\beta) g(\mathbf{x}_0) d\mathbf{x}, \\ \tilde{c}_\ell = \frac{1}{\ell!}\int_{C_n} f_\alpha(\ln g_\beta)\sum_{i_1,\ldots,i_\ell=1}^{s} x_{i_1}\cdots x_{i_\ell}\, \frac{\partial^\ell g}{\partial x_{i_1}\ldots\partial x_{i_\ell}}(\mathbf{x}_0)\; d\mathbf{x},\; \ell = 1, 2, \ldots p-1, \end{cases}$$

and

$$\begin{cases} \hat{a}_\ell = \hat{b}_\ell - \hat{c}_\ell,\; \ell = 0, 1, 2, \ldots, p-1. \\ \hat{b}_0 = \beta\, Q_{C_n}(f_\alpha g(\mathbf{x}_0)), \\ \hat{b}_\ell = \frac{\beta}{\ell!}\, Q_{C_n}(f_\alpha \sum_{i_1,\ldots,i_\ell=1}^{s} x_{i_1}\cdots x_{i_\ell}\, \frac{\partial^\ell g}{\partial x_{i_1}\ldots\partial x_{i_\ell}}(\mathbf{x}_0)),\; \ell = 1, 2, \ldots p-1. \\ \hat{c}_0 = \beta \int_{C_n} f_\alpha g(\mathbf{x}_0) d\mathbf{x}, \\ \hat{c}_\ell = \frac{\beta}{\ell!}\int_{C_n} f_\alpha \sum_{i_1,\ldots,i_\ell=1}^{s} x_{i_1}\cdots x_{i_\ell}\, \frac{\partial^\ell g}{\partial x_{i_1}\ldots\partial x_{i_\ell}}(\mathbf{x}_0)\; d\mathbf{x},\; \ell = 1, 2, \ldots p-1. \end{cases}$$

The extrapolation scheme will be based the error expansion (12). Using linear extrapolation just as before: it is well known that considering each h-exponent to appear twice will remove both the constant and the $\ln h$ term in front of the $h^{\alpha+s+\ell}$. We will give one example where we apply this idea in the next section.

5. Numerical Examples

In this section we will demonstrate, on a few examples in 2 and 3 dimensions, how efficient this approach may be. We will for this illustrative purpose apply the highest degree basic rule Q implemented in DCUHRE [2] (Berntsen et al. 1991) and furthermore not subdivide any of the rectangles which does not contain the singularity any further.

1) In the first example we look at a problem with a line singularity in C_2 combined with a nice function $g(x, y)$

$$\int_{C_2} x^{-1/2} e^{2x+y}\, dxdy \approx 8.1255\ 96316\ 47 \tag{13}$$

We give the Tail tableau in Table 2. The number of function evaluations (nfe) is given in the left column.

nfe				
65	8.13780021352			
195	8.13431250231	8.12589242260		
325	8.13179057440	8.12570210185	8.12559801197	
455	8.12998733056	8.12563391482	8.12559662210	8.12559632365
585	8.12870513608	8.12560964477	8.12559637104	8.12559631712
	8.12559631649			

Table 2. The Tail extrapolation tableau T_{ij} on (13).

DCUHRE uses in this example a degree 13 rule Q based on 65 evaluation points. Thus, dividing in two pieces and computing $\hat{U}_k$ and Q_k in each step cost 130 function evaluations per step.

As mentioned in Section 2 we can deal with this problem with the technique given in [7]. Using the transformation $y = t/x$ in (13) we get

$$\int_0^1 (\int_0^x x^{-3/2} e^{2x+t/x}\, dt)\, dx \approx 8.1255\ 96316\ 47 \tag{14}$$

and applying the tail approach described in [7] gives

nfe				
37	7.65148426982			
185	7.79175999005	8.13041553629		
333	7.89003397527	8.12728836320	8.12557805545	
481	7.95920320233	8.12619248842	8.12559313459	8.12559637265
629	8.00800024677	8.12580673327	8.12559575677	8.12559631985
	8.12559631473			
777	8.04246510858	8.12567064538	8.12559621644	8.12559631515
	8.12559631469	8.12559631469		

Table 3. The Tail extrapolation tableau T_{ij} on (14).

In this example a 37 point rule of degree 13 is used on each triangle (DCUTRI, Berntsen and Espelid 1992 [1]) and we divide each triangle into 4 subtriangles in each step by connection the midpoints of the 3 sides. Thus the cost per step is $4 \times 37 = 148$ evaluation points.

We get an impression of the efficiency of these two approaches by plotting, in Figure 2, the true error for the diagonals in these two tableaus versus the cost of computing these diagonals elements.

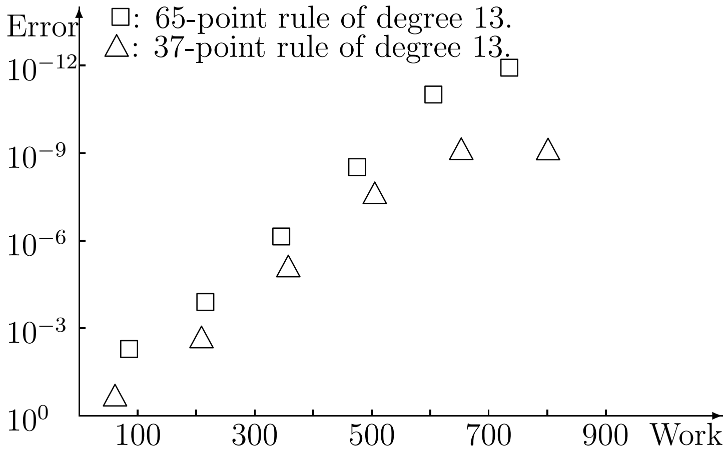

Figure 2. The true error in the diagonal elements in Table 2 (□) and Table 3 (△) versus the number of function values used to produce these elements.

Both techniques demonstrate fast convergence, however they will both converge to a "wrong" answer. Figure 2 indicates that the error in $\hat{U}_\ell$ is $O(10^{-8})$ in the triangle version and much smaller in the rectangle approach. This difference in behavior probably stems from the Hølder discontinuity introduced by the transformation. Thus it looks like the direct treatment of the integration problem (13) is to be preferred. In order to achieve a similar accuracy using adaptive codes, e. g. DCUTRI on (14) or DCUHRE on (13), we need in both cases at least ≈ 20,000 function evaluations.

2) In the next example we integrate a face singularity in C_3

$$\int_{C_3} x^{-1/2} e^{x+xy+z/3}\, dxdydz \approx 4.4191\ 59656\ 80 \tag{15}$$

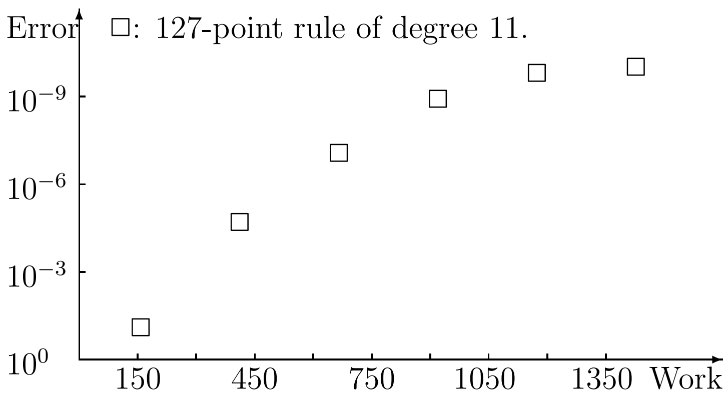

Figure 3. The true error in the diagonal elements in the T-tableau versus the number of function values used to produce these elements.

In this example the error in $\hat{U}_1$ is $O(10^{-10})$ and we see that after 4-5 extrapolation steps we reach this limit.

3) In this example we integrate a face singularity in C_3 created by a logarithmic singularity and a homogeneous function

$$-\int_{C_3} x^{-1/2} \ln x \, e^{x+xy+z/3} \, dxdydz \approx 5.8401\ 12318\ 46 \tag{16}$$

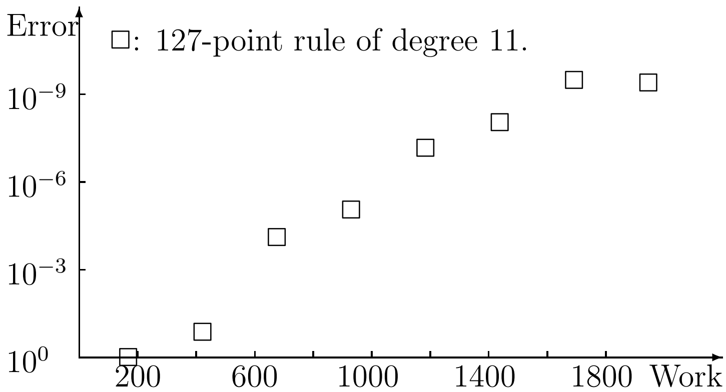

Figure 4. The true error in the diagonal elements in the T-tableau versus the number of function values used to produce these elements.

In this example the error in $\hat{U}_1$ is $O(10^{-9})$ and we see that after 6 extrapolation steps we reach this limit.

4) In the last example we integrate a line singularity in 3 dimensions

$$\int_{C_3} (x+y)^{-1/2} \, e^{x+xy+z/3} \, dxdydz \approx 2.7878925361\ldots \tag{17}$$

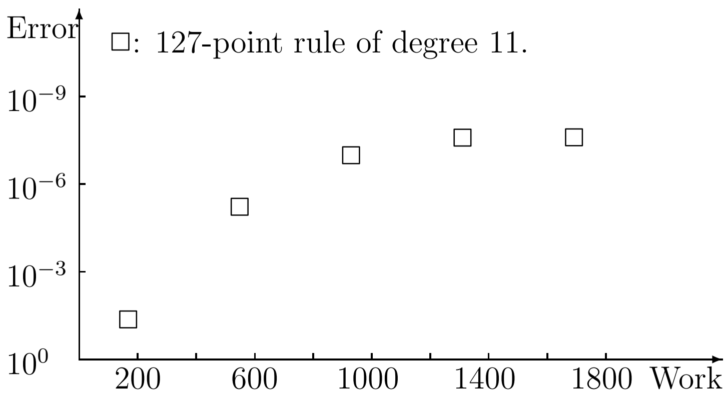

Figure 5. The true error in the diagonal elements in the T-tableau versus the number of function values used to produce these elements.

In this example the error in $\hat{U}_1$ is $O(10^{-8})$ and we see that after 3 extrapolation steps we reach this limit.

6. Conclusions

The power of this technique is clearly demonstrated through these examples. Using a high degree rule gives good accuracy in the computation of $\hat{U}_\ell$ and will in addition give small constants a_i in the error expansion which in turn will reduce the number of extrapolation steps needed. In practice it may be difficult to choose the best rule Q to use and it seems natural to combine an adaptive strategy and extrapolation.

It is essential though, in order to apply the technique, that we have all information about the singularity in C_n. We have used that knowledge in our examples creating two sequences $\hat{U}_1, \hat{U}_2, \hat{U}_3 \ldots$ and $Q_1, Q_2, Q_3, \ldots$. The $\hat{U}_\ell$'s are estimates to integrals over a sequence of non-overlapping regions *all of the same form, but non of them containing the singularity*. Similarly, the Q_ℓ's are estimates to integrals, *over overlapping regions, all of the same form and containing the singularity*.

Having more than one singularity in a region complicates the integration problem considerably. If we can separate these singularities, that is: subdivide the region such that each subregion has at most one singularity the problem can be handled. If this is not the case then further research is needed in order to handle such problems by this non-uniform subdivision technique.

Extrapolation is, as we have seen, the key to the success of both the uniform and non-uniform approaches. We have, in our examples, used the value of α combined with linear extrapolation. If we do not know the value of α, only the position of the singular point, then a pre-computation of function values in selected points along a straight line ending in a singular point, combined with extrapolation, will provide accurate estimates of α. This seems to be a good way to compute α and then use this value in the described linear extrapolation. One would expect such an approach to be at least as efficient as many of the non-linear extrapolation techniques available which do not need a value of α and therefore can be applied directly on the Tail-sequence created by the Q- and U-sequences.

Finally the non-uniform approach fits well with the general strategy one finds in adaptive codes and therefore it is reasonable to expect that these codes can be modified to handle these types of singular integrands quite well.

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