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Numerical Analysis of Singular Weighted Integrals

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Dedicated to the memory of Prof. Peter Henrici

Abstract — Zusammenfassung

Numerical Analysis of Singular Weighted Integrals. In this article we investigate the numerical aspects of integrals of the form

$$\int_a^b f(x)\psi(x)dx \tag{1}$$

where f is an unobjectionable function and ψ is singular, i.e. ψ is oscillating with high frequency, is discontinuous or unbounded. Suitable integration algorithms are presented.

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Numerik singulär gewichteter Integrale. In diesem Artikel wird die Numerik von Integralen der Form (1) untersucht, wobei f eine numerisch unbedenkliche Funktion und ψ eine singuläre Funktion ist, d.h. ψ oszilliert mit hoher Frequenz, ist unstetig oder unbeschränkt. Geeignete Integrationsalgorithmen werden entwickelt.

1. Introduction

In different fields of applied mathematics and physics the following problem arises: Find a numerical approximation of the integral (1) where f is supposed to be a "nice" function whereas ψ may be discontinuous, unbounded or oscillating with high frequency (e.g. in the calculation of Fourier transforms). Then the standard integration algorithms as Simpson-, Romberg- or adaptive quadrature method do not converge in an appropriate way. In the case of an oscillating function ψ, we have to choose the interval length of the order of the period of ψ which may be much smaller than the regularity of f would admit. In case of a discontinuous or unbounded ψ the step-length at least in a neighborhood of the singular points of ψ has to be very small—although f could be nice all over the interval of integration.

As an example we mention computerized tomography where the weightfunction ψ comes from a so called *filter* which keeps to be the same for all density functions f. In that particular situation an algorithm which only evaluates f at equidistant points is required (see [4]).

A first approach to the numeric of singular integrals goes back to Lyness and Ninham: in [3] trapezoidal rules of the form

$$R^{[m,\alpha]}[g] = \frac{1}{m}\sum_{j=1}^{m} g\left(\frac{2j-1+\alpha}{2m}\right), \quad |\alpha| < 1$$

and

$$R^{[m,1]}[g] = \frac{1}{m}\sum_{j=1}^{m-1} g\left(\frac{j}{m}\right) + \frac{1}{2m}(g(0) + g(1))$$

for the numerical integration of $\int_0^1 g(x)dx$ with a singular integrand g are investigated. The asymptotic expansion of the corresponding error functional is discussed for special cases of algebraic and logarithmic singularities.

If the integrand is a product of a smooth function f and a singular function ψ the idea is to replace f by an approximation $\bar{f}$, usually an interpolation polynomial, and then integrating $\bar{f}\psi$ analytically (a simple example of this technique is Filon's method: see e.g. [1]). The result are rules which do no longer need to evaluate the integrand $f\psi$ but only the regular part f. The case of polynomial approximation of the smooth function f and a function ψ having algebraic or logarithmic singularities is discussed by de Hoog and Weiss in [2]. The method of de Hoog and Weiss allows the construction of integration algorithms of high order either by choosing a polynomial approximation of high order for f (which has the disadvantage that the weights which need to be calculated analytically get more and more difficult) or by explicit calculation of the error expansion (which is difficult and costly for general functions ψ). Schneider has pointed out that (in case of algebraic singularities) for an appropriate choice of evaluation points (in general not equidistant) there results some profit in the error order (see [5]).

Here we present methods which are applicable quite generally and an extrapolation method which does not require the explicit calculation of the error expansion.

2. Trapezoidal Rule for Product Integration

The trapezoidal rule we present here can already be found in [2]. But we want to give it a new interpretation and also give a slightly different derivation:

Let $f \in C^2([a,b])$ and $\theta'' = \psi \in L^1([a,b])$. Then we have

$$\int_a^b f(x)\psi(x)dx = f(x)(\theta'(x) + c)|_a^b - f'(x)(\theta(x) + cx + d)|_a^b + \int_a^b f''(x)(\theta(x) + cx + d)dx. \quad (2)$$

Now we choose the constants c and d such that $-(cx + d) = i(x)$ is the interpolation polynomial i of degree one for the function θ in the points a and b. Thus the second term in (2) vanishes and by partial integration we obtain, with $h = b - a$,

$$\int_a^b f(x)\psi(x)dx = f(x)\left(\theta'(x) - \frac{\theta(b) - \theta(a)}{h}\right)\Big|_a^b + \int_a^b \theta''(x)(f(x) - j(x))dx. \quad (3)$$

Here, j is the interpolation polynomial of degree one for the function f in the points a and b. Hence for all $x \in [a, b]$ there exists $\xi(x) \in [a, b]$ such that

$$f(x) - j(x) = \frac{1}{2}(x - a)(x - b)f''(\xi).$$

Thus the error term is estimated by

$$\left|\int_a^b \theta''(x)(f(x) - j(x))dx\right| \leq M_a^b(f'')\frac{h^2}{8}\int_a^b |\theta''(x)|dx,$$

where we use the shorthand notation $M_a^b(g) = \sup\{|g(x)|; x \in [a, b]\}$. Now let $f \in C^2([A, B])$ and $\theta'' = \psi \in L^1([A, B])$. Dividing the interval $[A, B]$ by the points $a_i = A + hi$ for $i = 0, \ldots, n$ with $h = \frac{B - A}{n}$ and summing up (3) for each interval leads to

$$\int_A^B f(x)\psi(x)dx = h\sum_{i=1}^{n-1} f(a_i)\Delta_h^2\theta(a_i) + T[f] + R[f]. \quad (4)$$

Here, Δ_h^2 denotes the central second difference quotient

$$\Delta_h^2\theta(x) = \frac{\theta(x - h) - 2\theta(x) + \theta(x + h)}{h^2}.$$

The boundary terms $T[f]$ which vanish for $f \in C_0^2([A, B])$ are

$$T[f] = f(B)\theta'(B) - f(A)\theta'(A) + \frac{1}{h}(f(A)(\theta(a_1) - \theta(A)) + f(B)(\theta(a_{n-1}) - \theta(B))).$$

The error term $R[f]$ is estimated by

$$|R[f]| \leq \frac{h^2}{8}M_A^B(f'')\int_A^B |\psi(x)|dx.$$

Definition: We call

$$J[f] := h\sum_{i=1}^{n-1} f(a_i)\Delta_h^2\theta(a_i) + T[f] \quad (5)$$

trapezoidal rule. We shall use the notation $J_A^B[f]$, $J_h[f]$ or $J_A^B[f, \psi]$ when we want to emphasize the dependence on A, B, h or ψ.

Interpretation: When we integrate $\int_A^B f(x)\theta''(x)dx$ for $f \in C_0^2([A, B])$ we have to replace the second differential quotient θ'' by the second difference quotient $\Delta_h^2\theta$ and proceed as in the ordinary trapezoidal rule with mesh constant h (when f does not vanish at the endpoints of the interval a boundary term $T[f]$ has to be added). The error order is $O(h^2)$ as for the classical trapezoidal rule.

3. Higher Order Methods

3.1 Simpson's Rule for Product Integrals

Let $f \in C^3([A,B])$ and $\theta''' = \psi \in L^1([A,B])$. Dividing the interval $[A,B]$ by the points $a_i = A + i\frac{h}{2}$ for $i = 0, 1, \ldots, n$, n even and $h = 2\frac{B-A}{n}$ we can interpolate f on every interval $[a_{i-1}, a_{i+1}]$ (i odd) by a polynomial of second degree coinciding with f at a_{i-1}, a_i, a_{i+1} ($i = 1, \ldots, n-1$). Integrating on each interval and summing up yields

$$\begin{aligned}\int_A^B f(x)\theta'''(x)dx = &\sum_{i=1,\mathrm{odd}}^{n-1} f(a_i)\left(\frac{8}{h^2}(\theta(a_{i-1}) - \theta(a_{i+1}))\right.\\ &\left.+\frac{4}{h}(\theta'(a_{i-1}) + \theta'(a_{i+1}))\right)\\ &+\sum_{i=2,\mathrm{even}}^{n-2} f(a_i)\left(\frac{4}{h^2}(\theta(a_{i+2}) - \theta(a_{i-2}))\right.\\ &\left.-\frac{1}{h}(\theta'(a_{i-2}) + 6\theta'(a_i) + \theta'(a_{i+2}))\right) + T + R. \end{aligned} \tag{6}$$

The boundary terms are

$$\begin{aligned}T = &f(A)\left(\frac{4}{h^2}(\theta(a_2) - \theta(A)) - \frac{1}{h}(3\theta'(A) + \theta'(a_2)) - \theta''(A)\right)\\ &+ f(B)\left(\frac{4}{h^2}(\theta(B) - \theta(a_{n-2})) - \frac{1}{h}(3\theta'(B) + \theta'(a_{n-2})) - \theta''(B)\right). \end{aligned} \tag{7}$$

The error term R may be estimated by

$$|R| \le \frac{h^3}{72\sqrt{3}} M_A^B(f''') \int_A^B |\psi(x)|\,dx. \tag{8}$$

The formulas (6)–(8) correspond to the classical Simpson rule. However notice the following differences to the classical case:

Remark: Suppose p_3 is an arbitrary polynomial of third degree. Then we can write $p_3 = \tilde{p}_3 + p_2$ where p_2 is a polynomial of second degree which coincides with p_3 in the points a_{i-1}, a_i, a_{i+1} and hence $\tilde{p}_3 = 0$ in the points a_{i-1}, a_i, a_{i+1}, i.e. $\tilde{p}_3$ is odd with respect to the point a_i. Thus we have

$$\int_{a_{i-1}}^{a_{i+1}} p_3(x)\psi(x)dx = \int_{a_{i-1}}^{a_{i+1}} \tilde{p}_3(x)\psi(x)dx + \int_{a_{i-1}}^{a_{i+1}} p_2(x)\psi(x)dx = I + II. \tag{9}$$

If ψ is an even function with respect to the point a_i (as for $\psi \equiv 1$ in the classical situation) we have that $I = 0$ in (9) and hence that integration rule (6) is exact even if f is a polynomial of third degree. But in general (i.e. if the weightfunction does not have the mentioned special symmetries) the rule (6) integrates only polynomials of second degree exactly. The same effect is responsible for the fact that the error order (8) is only $O(h^3)$ (the classical Simpson rule has error order $O(h^4)$).

For higher order rules of the Newton-Cotes type see [2].

3.2 Extrapolation Methods for Product Integrals

3.2.1 Linear Extrapolation

The trapezoidal integration formula (5)

$$\int_a^b f(x)\psi(x)dx = J_a^b[f] + R_a^b[f]$$

is linear and of order two, i.e. $J_a^b[\cdot]$ is linear and R satisfies $R_a^b[x^n] = 0$ for $n \in \{0, 1\}$. Defining a new integration rule by

$$\tilde{J}_a^b[f] := pJ_a^b[f] + q(J_a^v[f] + J_v^b[f])$$

with $v = \dfrac{a+b}{2}$ we choose p and q such that $\tilde{J}$ integrates exactly polynomials of degree two, i.e.

$$pR_a^b[x^2] + q(R_a^v[x^2] + R_v^b[x^2]) = 0.$$

Together with $p + q = 1$ an elementary calculation leads to

$$p = \frac{2}{h}\,\frac{2(\theta(a) - \theta(b)) + \frac{h}{2}(\theta'(a) + 2\theta'(v) + \theta'(b))}{\theta'(a) - 2\theta'(v) + \theta'(b)} \tag{10}$$

$$q = \frac{2}{h}\,\frac{2(\theta(a) - \theta(b)) - h(\theta'(a) + \theta'(b))}{\theta'(a) + 2\theta'(v) + \theta'(b)}. \tag{11}$$

Now $\tilde{J}$ is of order three. The same procedure repeated with $\tilde{J}$ would give a rule of order four and so on. Unfortunately the formulas corresponding to (10) and (11) get very extensive and as for the Simpson- and corresponding rules of higher orders, primitives θ with $\theta^{(n)} = \psi$ of corresponding order n need to be calculated analytically.

3.2.2 Nonlinear Extrapolation

In order to get an easier extrapolation scheme for the trapezoidal formula (5) let us consider its asymptotic error expansion which we infer from [2]: For the case of the singular function $\psi(x) = x^\beta(1-x)^\omega$, β, $\omega > -1$, and a C^∞-function $f(x)$ on $x \in [0, 1]$ de Hoog and Weiss obtain for rule (5) with mesh length $h = \dfrac{1}{n}$

$$
\begin{aligned}
R_h[f] &= J_h[f] - \int_0^1 f(x)\psi(x)dx \\
&= \sum_{r=0}^{p-2} h^{2+r} \int_0^1 \omega_r(s)ds \int_0^1 \psi(s) f^{(2+r)}(s)ds \\
&+ \sum_{r=0}^{p-2} h^{2+r+\beta+1} \sum_{l=0}^{r} \frac{\phi_{0l}^{(r-l)}(0)}{(r-l)!} \int_0^1 \omega_l(s)\tilde{\zeta}(-\beta - r + l, s)ds \\
&+ \sum_{r=0}^{p-2} h^{2+r+\omega+1} \sum_{l=0}^{r} \frac{(-1)^{r-l}\phi_{1l}^{(r-l)}(1)}{(r-l)!} \int_0^1 \omega_l(s)\tilde{\zeta}(-\omega - r + l, 1-s)ds \\
&+ O(h^{p+1})
\end{aligned}
$$

where $\omega_0(s) = 1 - s$, $\omega_1(s) = s$, $\tilde{\zeta}$ are periodic generalized zeta functions and

$$
\begin{aligned}
\phi_{0r}(x) &= f^{(2+r)}(x)(1-x)^{\omega} \\
\phi_{1r}(x) &= f^{(2+r)}(x)x^{\beta}.
\end{aligned}
$$

Analogous expansions hold when more algebraic singularities (in the interior of the interval) are considered. Instead of trying to calculate this expansion (which gets more difficult for more general ψ) explicitly as in [2] we shall make use of its structure, namely

$$
J_h[f] = \int_0^1 f(x)\psi(x)dx + \sum_{i=1}^{\infty} c_i h^{\alpha_i}.
$$

Let us first do some heuristic consideration: If we would know the exponents α_i (this is not always so obvious as in the above trivial example) then we could eliminate the leading error term by considering the linear combination

$$
\tilde{J}[f] := \frac{J_h[f] - 2^{\alpha_1} J_{h/2}[f]}{1 - 2^{\alpha_1}}. \tag{12}
$$

On the other hand we can get an approximation of the exponent α_1 by

$$
\frac{J_h[f] - J_{h/2}[f]}{J_{h/2}[f] - J_{h/4}[f]} \approx \frac{1 - \dfrac{1}{2^{\alpha_1}}}{\dfrac{1}{2^{\alpha_1}} - \dfrac{1}{4^{\alpha_1}}}
$$

and hence

$$
2^{\alpha_1} \approx \frac{J_h[f] - J_{h/2}[f]}{J_{h/2}[f] - J_{h/4}[f]}. \tag{13}
$$

Let us look at what happens if we use approximation (13) for 2^{α_1} in (12): We obtain

$$
\tilde{J}[f] = \frac{J_h[f] J_{h/4}[f] - (J_{h/2}[f])^2}{J_h[f] - 2J_{h/2}[f] + J_{h/4}[f]}.
$$

To avoid cancellation we rewrite this and obtain Aitken's "Δ^2"-structure:

$$\tilde{J}[f] = J_h[f] - \frac{(J_h[f] - J_{h/2}[f])^2}{J_h[f] - 2J_{h/2}[f] + J_{h/4}[f]}.$$

Since we only use an approximation for α_1 there is little hope to eliminate the leading error term $c_1 h^{\alpha_1}$ completely and obtain a higher order rule. It is much more likely that the order remains α_1 (maybe with smaller leading coefficient $\tilde{c}_1$, $|\tilde{c}_1| \ll |c_1|$). But in fact $\tilde{c}_1$ *is* zero as the following theorem shows.

Theorem: *Suppose* $\xi(k) = c_0 + \sum_{i=1}^{\infty} \frac{c_i}{k^{\alpha_i}}$ *with* $0 < \alpha_1 < \alpha_2 < \cdots \to \infty$ *is converging for* $k \in \mathbb{N}$. *Let*

$$T_{1,n} = \xi(2^n) = c_0 + \sum_{i=1}^{\infty} \frac{c_i}{2^{n\alpha_i}}$$

for $n = 0, 1, \ldots$. *Then there exist constants* $\tilde{\alpha}_i$ *with* $\alpha_2 < \tilde{\alpha}_3 < \tilde{\alpha}_4 < \cdots \to \infty$ *and constants* $\tilde{c}_i$ *such that*

$$T_{2,n} = T_{1,n} - \frac{(T_{1,n} - T_{1,n+1})^2}{T_{1,n} - 2T_{1,n+1} + T_{1,n+2}} = c_0 + \frac{\tilde{c}_2}{2^{n\alpha_2}} + \sum_{i=3}^{\infty} \frac{\tilde{c}_i}{2^{n\tilde{\alpha}_i}}.$$

Especially $\tilde{\alpha}_3 = 2\alpha_3 - \alpha_1$ *and* $\tilde{c}_2 = c_2 \frac{2^{2\alpha_1} + 2^{2\alpha_2} - 2^{\alpha_1+\alpha_2+1}}{2^{2\alpha_2}(2^{\alpha_1} - 1)^2}$, *i.e.* $\tilde{c}_2 \leq \frac{1}{9} c_2$ *if* $\alpha_1 \geq 2$.

Proof: By rearranging the series we find

$$T_{2,n} = c_0 + \frac{\sum_{1 \leq i < j} \frac{c_i c_j}{2^{n(\alpha_i + \alpha_j - \alpha_1)}} \left(\frac{1}{2^{2\alpha_i}} + \frac{1}{2^{2\alpha_j}} - \frac{2}{2^{\alpha_i + \alpha_j}} \right)}{c_1 \left(1 - \frac{1}{2^{\alpha_1}}\right)^2 + \sum_{i>1} \frac{c_i}{2^{n(\alpha_i - \alpha_1)}} \left(1 - \frac{1}{2^{\alpha_i}}\right)^2}.$$

Expanding the fraction on the right hand side of this expression we obtain

$$T_{2,n} = c_0 + \frac{\tilde{c}_2}{2^{n\alpha_2}} + \frac{\tilde{c}_3}{2^{n\tilde{\alpha}_3}} + \frac{\tilde{c}_4}{2^{n\tilde{\alpha}_4}} + \cdots \tag{14}$$

with exponents $\tilde{\alpha}_i$ being the sums of exponents occurring in the numerator and multiples of the exponents occurring in the denominator of the fraction. For n large enough the series in (14) converges. □

Summary: Let ψ have finitely many algebraic singularities on an integration interval I of length l. Let f be smooth and $T_{1,n} = J_{l/2^n}[f]$, $n \in \mathbb{N}$, the numerical approximations for $\int_I f(x)\psi(x)dx$ obtained by the trapezoidal rule (5) applied with steplength $h = \frac{l}{2^n}$. If we denote by $T_{m+1,n}$, $m = 1, 2, \ldots$, the Aitken transformation of the sequence $T_{m,n}$, i.e.

$$T_{m+1,n} = T_{m,n} - \frac{(T_{m,n} - T_{m,n+1})^2}{T_{m,n} - 2T_{m,n+1} + T_{m,n+2}}$$

then the sequences $T_{m,n}$ for fixed m are integration rules of increasing order $O(h^{\tilde{\beta}_m})$.

Remarks: (1) To eliminate the leading error term $c_2 h^2$ of the trapezoidal approximation in the very first step there may be used the corresponding *classical* Romberg step.

(2) The fact stated above is also true for logarithmic singularities as we shall see below. However the acceleration of convergence is of different kind.

Example: We use this method on the integral

$$\int_0^1 \frac{\exp x}{\sqrt{x}} dx = -i\sqrt{\pi}\,\mathrm{Erf}(ix)|_0^1 = 2.92530349181436\ldots$$

Erf denotes the error function. To use the trapezoidal rule we need a second primitive of $\psi(x) = 1/\sqrt{x}$, e.g. $\frac{4x^{3/2}}{3}$. We start with a step length $h = \frac{1}{2}$.

$T_{1,n}$	$T_{2,n}$	$T_{3,n}$	$T_{4,n}$
2.9811732544	2.9252857083	2.9253071463	2.9253034950
2.9395615282	2.9252965978	2.9253035659	2.9253034918
2.9289322995	2.9253019559	2.9253034964	
2.9262232288	2.9253031939	2.9253034921	
2.9255357475	2.9253034370		
2.9253619756	2.9253034819		
2.9253181878			
2.9253071791			

The situation is more difficult when ψ includes logarithmic singularities. As a model case let us consider $\psi(x) = \log|x - x_0|$, x_0 in the integration interval. From [2] we infer the structure of the corresponding error expansion for the trapezoidal rule

$$T_{1,n} = J_{l/2^n}[f] = \int_0^1 f(x)\psi(x)dx + \frac{c_2}{2^{2n}} + \sum_{i=3}^{\infty}\left(c_i + d_i \log\frac{1}{2^n}\right)\frac{1}{2^{in}}$$

which is of order $O(h^2)$, $h = \frac{l}{2^n}$. The Aitken transformation $T_{2,n}$ of the sequence $T_{1,n}$ has the expansion

$$T_{2,n} = \int_0^1 f(x)\psi(x)dx + \sum_{i=3}^{\infty}\frac{1}{2^{in}}\sum_{k=0}^{i-2} c_{i,k}\left(\log\frac{1}{2^n}\right)^k,$$

i.e. the leading error term has disappeared and $T_{2,n}$ is an integration rule of order $O(h^3 \log h)$. The coefficient of the leading term $\frac{1}{2^{3n}}$ in $T_{2,n}$ is $\frac{c_3 + d_3 \log 4}{36} + \frac{d_3}{36}\log\frac{1}{2^n}$.

For $T_{3,n}$ we obtain

$$T_{2,n} = \int_0^1 f(x)\psi(x)dx + \frac{c}{d + e\log\frac{1}{2^n}}\frac{1}{2^{3n}} + \sum_{i=4}^{\infty}\frac{1}{2^{in}}\frac{p_i\left(\log\frac{1}{2^n}\right)}{q_i\left(\log\frac{1}{2^n}\right)}$$

where p_i and q_i are polynomials of the same degree. Now the leading error term $\frac{1}{2^{3n}}$ has a coefficient which may be expressed in terms of the coefficients of $T_{1,n}$ as follows

$$\frac{c}{d + e\log\frac{1}{2^n}} = -\frac{d_3^2(\log 2)^2}{252\left(7c_3 + 16d_3\log 2 + 7d_3\log\frac{1}{2^n}\right)}.$$

The rule $T_{3,n}$ is of the higher order $O(h^3/\log h)$. By induction we find that $T_{m,n}$ is a rule of order $O(h^3/(\log h)^{2m-5})$. We close this consideration with a further numerical example which illustrates the extrapolation method for a logarithmic singularity.

Example: We use this method on the integral

$$-\int_{-1}^{1} \exp x \log|x|\,dx = e^x\log|x|\big|_{-1}^{1} - \mathrm{Ei}(x)\big|_{-1}^{1} = \mathrm{Ei}(-1) - \mathrm{Ei}(1)$$
$$= 2.114501750751457\ldots$$

Ei denotes the exponential integral function. To use the trapezoidal rule we need a second primitive of $\psi(x) = \log x$, e.g. $\frac{x^2}{2}\log|x| - \frac{3x^2}{4}$. We start with a step length $h = 1$.

$T_{1,n}$	$T_{2,n}$	$T_{3,n}$	$T_{4,n}$
2.27154031740	2.11434648737	2.11461629087	2.11450176386
2.15542261657	2.11443208069	2.11450214197	2.11450175093
2.12508004091	2.11449052011	2.11450176511	2.11450175075
2.11719806201	2.11450021412	2.11450175145	
2.11518278781	2.11450155119	2.11450175079	
2.11467290986	2.11450172536		
2.11454465485	2.11450174755		
2.11451249118			
2.11450443766			

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