Numer. Math. 57, 139–145 (1990)

Numerische Mathematik

Calculating Singular Integrals as an Ill-posed Problem

A. G. Ramm[1] **and A. van der Sluis**[2]

[1] Department of Mathematics, Kansas State University, Cardwell Hall, Manhattan, KS 66506, USA
[2] Mathematical Institute, University of Utrecht, P.O. Box 80.010, NL-3508 TA Utrecht, the Netherlands

Received April 5, 1988/September 18, 1989

Dedicated to Professor G. Hämmerlin on the occasion of his 60th birthday.

Summary. Applying numerical quadrature to singular integrals in a straightforward way leads to uncontrolled instability with respect to data errors. In this paper we describe how to control this instability.

Subject Classifications: AMS(MOS): 65D32; CR: G1.4.

1 Introduction

Hadamard Finite Part Integrals (HFP integrals, for short), denoted as

$$\fint_a^b g(x)\,\mathrm{d}x \tag{1}$$

may be defined in a few different, but equivalent ways (cf. [1, p. 309], [3, book III, Ch. I]; cf. [2, Ch. I, §§ 1.7, 2.2, 3.3, 4.2] for still other ways of regularizing divergent integrals). For our purposes the following definition is appropriate: for μ non-integer, $\mu>1$, $f\in C^{(k)}[0,b]$, $k>\mu-1$, $b>0$

$$\fint_0^b \frac{f(x)}{x^\mu}\,\mathrm{d}x \equiv \int_0^b \frac{f(x)-f_k(x)}{x^\mu}\,\mathrm{d}x + \sum_{i=0}^{k} \frac{f^{(i)}(0)b^{-\mu+i+1}}{i!(-\mu+i+1)} \tag{2}$$

with $f_k(x)=\sum_{i=0}^{k} f^{(i)}(0)x^i/i!$; for integer $\mu\geqq 1$ and $f\in C^{(k+1)}[0,b]$, $k\geqq\mu-1$, the term with $-\mu+i+1=0$ in $\sum_{i=0}^{k}$ should be replaced by $f^{(i)}(0)\ln(b)/i!$.

For general a and b the HFP integral is defined from (2) using translation and reflexion.

We note that the definition does not depend on the particular choice of k when there is any choice.

Offprint requests to: A. van der Sluis

Obviously, when the integral in the right-hand side is approximated by numerical quadrature, stability problems should be expected because of the small numbers now occurring in the denominator.

We shall first show that, indeed, errors in the data will always give rise to unbounded errors in the quadrature result if we use a sequence of numerical quadratures which, in the absence of data errors, converges to the true integral. Subsequently we will show in a fairly general setting how HFP integrals may be computed in a stable way.

In the existing literature on the numerical evaluation of HFP integrals little or no attention is given to this stability issue (cf., e.g., [4, 5, 6, 7, 8, 12]). We mention in passing that in [5] and [6], where the stability problem is at least mentioned, the erroneous advice is given to add the positive and negative terms separately and then to perform a single subtraction (it is better to add them in such a way as to keep the partial sums as small as possible).

To conclude this introduction we note that our considerations may also be useful for integrals $\int_a^b \frac{f(x)}{g(x)}\,\mathrm{d}x$ with a regular integrand (as is the case for the integral in the right-hand side of (2)) where f and g vanish at the same point of the interval.

In the sequel we restrict ourselves to the case that μ is non-integer. The other case is quite similar.

2 Unstable Computation

Let instead of the true values $f(x)$ values $f_\varepsilon(x)=f(x)+\varepsilon(x)$ be available with $|\varepsilon(x)|\leqq\delta$. Let a convergent family of quadrature formulae $(Q_n)_{n\geqq 1}$ for the interval $[0,b]$ be given, i.e. a family of functionals such that

$$Q_n g=\sum_j w_{nj}\,g(x_{nj}) \tag{3}$$

and

$$\lim_{n\to\infty} Q_n g=\int_0^b g(x)\,\mathrm{d}x \quad \text{for all } g\in C[0,b]. \tag{4}$$

Note that (4) implies $\lim_{n\to\infty} x_{n1}=0$.

Now suppose we apply this family (Q_n) to the integral in the right-hand side of (2). With $\varphi(x)\equiv[f(x)-f_k(x)]x^{-\mu}$ and $\varphi_\varepsilon(x)\equiv[f_\varepsilon(x)-f_k(x)]x^{-\mu}$ we define

$$\beta_n(\delta)=\max_{|\varepsilon(x)|\leqq\delta}|Q_n(\varphi_\varepsilon)-Q_n(\varphi)| \tag{5}$$

(i.e., we only consider the effects of the noise on f, we disregard possible noise in the $f^{(i)}(0)$). Then we make the following observation:

$$\lim_{n\to\infty}\beta_n(\delta)=\infty. \tag{6}$$

In order to see that this is true, choose a number $a\in(0,b]$, define $\varepsilon(x)=\delta$ for $a\leqq x\leqq b$, $\varepsilon(x)=\delta(x/a)^\mu$ for $0<x\leqq a$. Then the function $x\mapsto\varepsilon(x)x^{-\mu}$ is continuous,

hence $\lim_{n\to\infty} \sum_j w_{nj}\varepsilon(x_{nj})x_{nj}^{-\mu} = \int_0^b \varepsilon(x)x^{-\mu}\mathrm{d}x > \delta a^{-\mu+1}$, and the right-hand side can be made arbitrarily large by taking a small enough, which proves (6).

Thus, as we proceed with the family of quadrature formulae, the effect of data errors blows up.

Now, of course, if δ is known, we might assess the effect of the data errors during the process of numerical quadrature, and stop when the combined effect of data errors and quadrature errors no longer decreases. In order to get reasonable results, however, this requires a rather careful choice of quadrature formulae, which should have no nodes unduly close to 0 (e.g., in the class of quadrature formulae $\frac{b}{n}\sum_{j=0}^{n-1} f[(j+\theta)b/n]$, $0 \leqq \theta \leqq 1$, it would be bad to take θ small). But as yet there is no theory for this. Moreover there should be a rather sharp error estimate for the quadrature result.

Similar observations can be made if, instead of applying numerical quadrature to the integral in the right-hand side of (2), the left-hand side of (2) is considered as a case for product integration (as, e.g., is done in [5] and [6]), i.e. a family $(\tilde{Q}_n)_{n\geq 1}$, $\tilde{Q}_n f = \Sigma \tilde{w}_{nj} f(\tilde{x}_{nj})$, is constructed such that

$$\fint_0^b \frac{f(x)}{x^\mu}\,\mathrm{d}x \cong \tilde{Q}_n f. \tag{7}$$

If this is done in such a way that $\lim_{n\to\infty} \tilde{Q}_n f = \fint_0^b f(x)x^{-\mu}\mathrm{d}x$ for any $f \in C^{(k)}[0,b]$, $k > \mu - 1$, we would also have $\lim_{n\to\infty} \tilde{Q}_n f = \int_0^b f(x)x^{-\mu}\mathrm{d}x$ for any $f \in C^{(k)}[0,b]$ for which the integral exists in the ordinary sense. Now choosing $\varepsilon(x) = x^k/(a^k + x^k)$, $a \in (0,b]$ we have $\lim_{n\to\infty} \tilde{Q}_n \varepsilon = \int_0^b \varepsilon(x)x^{-\mu}\mathrm{d}x$ which again can be made arbitrarily large by taking a small enough.

In the next section we discuss another way for optimizing the error.

3 Stabilized Computation

We will now show that HFP integrals may be computed with an error $O(\delta^\alpha)$ for $\delta \to 0$, α a given number < 1, provided f is sufficiently smooth and a bound for a relevant derivative is known.

Moreover we will not assume the necessary values of $f^{(i)}(0)$ to be known but assume them to be computed by numerical differentiation from noisy data.

We first discuss the numerical differentiation formulae for $f'(0), \ldots, f^{(k)}(0)$ for given k. We assume these formulae to have the form

$$f^{(i)}(0) \cong \sum_j \frac{a_{ij}}{h^i} f(hy_{ij}) \tag{8}$$

with h a (stepsize-) parameter, and we assume them to have polynomial degree of accuracy $K \geqq k$ (i.e. they give the true value of the derivative if f is a polynomial of degree $\leqq K$).

Then there are numbers α_i such that for any interval $[c,d]$ and any h_0 such that all $hy_{ij}\in[c,d]$ for $h\leqq h_0$ and any $f\in C^{(K+1)}[c,d]$ there holds

$$\left|\sum_j \frac{a_{ij}}{h^i} f(hy_{ij})-f^{(i)}(0)\right|\leqq \alpha_i h^{K+1-i}\max_{[c,d]}|f^{(K+1)}(x)|. \tag{9}$$

Now let $[c,d]$ and h_0 be as we just said, let $f\in C^{(K+1)}[c,d]$, let $M\geqq\max_{[c,d]}|f^{(K+1)}(x)|$, let $\delta>0$ be (as before) the noise level on f and let f_ε denote the noisy f-values.

Then we have the following lemma.

Lemma. *For any given constants* β_i and $h_i=\beta_i\delta^{1/(K+1)}$ *we have*

$$f^{(i)}(0)-\sum_j \frac{a_{ij}}{h_i^i} f_\varepsilon(h_i y_{ij})=O(\delta^{(K+1-i)/(K+1)})\quad \text{if } \delta\to 0. \tag{10}$$

Proof.

$$\left|f^{(i)}(0)-\sum_j \frac{a_{ij}}{h_i^i} f_\varepsilon(h_i y_{ij})\right|\leqq \alpha_i M h_i^{K+1-i}+\delta\sum_j |a_{ij}|/h_i^i. \quad \square \tag{11}$$

Remark 1. In any concrete situation where one has an a priori estimate for M one may determine the value of β_i which minimizes the right-hand side of (11) and get an estimate for the constant hidden in the O-term. This has been done in [9, 10, 11]. $\square$

Now suppose the derivatives $f^{(i)}(0)$, $i=1,2,\dots,k$, to be computed with (8) using noisy f-values and h_i as given in the lemma. Let the resulting values be denoted by $f_\varepsilon^{(i)}(0)$ and define $f_{k,\varepsilon}(x)\equiv\sum_{i=0}^{k} f_\varepsilon^{(i)}(0)x^i/i!$.

For any $a\in[0,b]$ let $(Q_{n,a,b})_{n\geqq 1}$ denote a convergent family of *positive* quadrature formulae for the interval $[a,b]$ with the nodes in $[a,b]$ (positive meaning that all the weights are positive, as is, e.g., the case for Gaussian formulae). Now suppose we approximate the HFP integral (1) by

$$Q_{n,a,b}\left(\frac{f_\varepsilon(x)-f_{k,\varepsilon}(x)}{x^\mu}\right)+\sum_{i=0}^{k}\frac{f_\varepsilon^{(i)}(0)b^{-\mu+i+1}}{i!(-\mu+i+1)} \tag{12}$$

for an appropriate value of a. Then we have the following theorem for the quality of this approximation:

Theorem. *Assume* $k>\mu-1$, $f\in C^{(K+1)}([0,b]\cup[c,d])$, $[c,d]$ *as above. Then for any* $\beta>0$ *and* $a=\beta\delta^{1/(k+1)}$ *there is an* $n_0=n_0(\delta,\mu,k,f,\beta)$ *such that*

$$\begin{aligned}&\,=\!\!\!\!\!\!\int_0^b \frac{f(x)}{x^\mu}\,\mathrm{d}x-Q_{n,a,b}\left(\frac{f_\varepsilon(x)-f_{k,\varepsilon}(x)}{x^\mu}\right)\\ &\qquad -\sum_{i=0}^{k}\frac{f_\varepsilon^{(i)}(0)b^{-\mu+i+1}}{i!(-\mu+i+1)}=O(\delta^{(k+2-\mu)/(k+1)}),\end{aligned} \tag{13}$$

for $\delta\to 0$ and $n\geqq n_0$.

Proof. Using (2) we write the left-hand side of (13) as $A+B+C+D$ with

$$A=\int_0^a \frac{f(x)-f_k(x)}{x^\mu}\,\mathrm{d}x$$

$$B=\int_a^b \frac{f(x)-f_k(x)}{x^\mu}\,\mathrm{d}x-Q_{n,a,b}\left(\frac{f(x)-f_k(x)}{x^\mu}\right)$$

$$C=Q_{n,a,b}\left(\frac{f(x)-f_\varepsilon(x)}{x^\mu}\right)$$

$$D=Q_{n,a,b}\left(\frac{f_{k,\varepsilon}(x)-f_k(x)}{x^\mu}\right)+\sum_{i=0}^{k}\frac{[f^{(i)}(0)-f_\varepsilon^{(i)}(0)]b^{-\mu+i+1}}{i!(-\mu+i+1)}.$$

Then

$$|A|\leqq M'\frac{a^{k+2-\mu}}{(k+1)!(k+2-\mu)}\quad\text{with } M'=\max_{[0,a]}|f^{(k+1)}(x)|$$

$$B\to 0\quad\text{for } n\to\infty$$

$$|C|\leqq\delta\sum_j\frac{w_{nj}}{x_{nj}^\mu}\to\delta\int_a^b x^{-\mu}\mathrm{d}x\leqq\delta\,\frac{a^{-\mu+1}}{\mu-1}\quad\text{for } n\to\infty$$

$$D=\sum_{i=0}^{k}\frac{1}{i!}[f_\varepsilon^{(i)}(0)-f^{(i)}(0)]\left[Q_{n,a,b}(x^{-\mu+i})-\frac{b^{-\mu+i+1}}{-\mu+i+1}\right]$$

$$\to\sum_{i=0}^{k}\frac{1}{i!}[f_\varepsilon^{(i)}(0)-f^{(i)}(0)]\,\frac{a^{-\mu+i+1}}{\mu-i-1}\quad\text{for } n\to\infty.$$

All these estimates are $O(\delta^{(k+2-\mu)/(k+1)})$ and this completes the proof. □

Remark 2. Using the optimal β_i from Remark 1 one may determine the value of β which minimizes the sum of the estimates for A, C and D given in the proof, and get an estimate for the constant hidden in the O-term. A simpler situation arises, however, if $K>k$ or if the $f^{(i)}(0)$ are known exactly or with a noise level proportional to δ. In the expression for $\lim_{n\to\infty} D$ the terms with $i>0$ will then be of higher order than the term with $i=0$, and the latter may be bounded by $\delta a^{-\mu+1}/(\mu-1)$. Hence in this case the optimal choice for β may be determined from this bound and the bounds for A and C. This gives $\beta=[2((k+1)!)/M']^{1/(k+1)}$ and for the hidden constant we now get $2\beta^{-\mu+1}(k+1)/[(k+2-\mu)(\mu-1)]$. □

Remark 3. Note that it is now no longer necessary to have a very sharp error estimate for the quadrature result, and that one may now take n as large as one pleases.

Remark 4. The requirement that the family $(Q_{n,a,b})_{n\geq 1}$ be positive is virtually necessary for optimal results. Indeed (cf. the proof of the theorem), A, $\lim_{n\to\infty} B$ and $\lim_{n\to\infty} D$ do not depend on the quadrature formulae. Now suppose we drop the positivity requirement. Then $\Sigma\frac{|w_{nj}|}{x_{nj}^\mu}$ is an upper bound for $|C|$ which is attained for suitable functions $x \mapsto \varepsilon(x)$. We note that $\Sigma \frac{|w_{nj}|}{x_{nj}^{\mu}} \geqq \left| \Sigma \frac{w_{nj}}{x_{nj}^{\mu}} \right|$ with equality only if all $w_{nj} > 0$, and that $\lim_{n\to\infty} \Sigma \frac{w_{nj}}{x_{nj}^{\mu}} = \int_a^b x^{-\mu} dx$ and $\lim_{n\to\infty} \Sigma w_{nj} = b - a$ for any choice of a convergent family of quadrature formulae. Hence $\limsup_{n\to\infty} \max_{|\varepsilon(x)| \leqq \delta} |C|$ has its minimum value only if $\lim_{n\to\infty} (\Sigma |w_{nj}| / \Sigma w_{nj}) = 1$.

Remark 5. Since μ was assumed to be non-integer, the integrand in the term B in the proof of the theorem has unbounded derivatives at 0, and therefore the convergence of the quadrature for $n \to \infty$ will be slow for the usual quadrature rules which are based on polynomial approximation. Likewise the limits in the estimates for C and D will be approximated rather slowly. However if, as often is the case, μ is a rational number, $\mu = p/q$ say, with integer p and q, the substitution $x = y^q$ in the integral in the right-hand side of (2) will speed up the convergence considerably. This virtually amounts to replacing the polynomial-type quadrature formulae $Q_{n,a,b}$ by

$$\tilde{Q}_{n,a,b} : \tilde{Q}_{n,a,b}\varphi(x) = Q_{n,a^{1/q},b^{1/q}}(qx^{q-1}\varphi(x^q)). \tag{14}$$

The family $(\tilde{Q}_{n,a,b})$ will then converge for all continuous functions φ and be positive if this is the case for the $Q_{n,a,b}$, and thus for this procedure our theorem is still valid.

Conclusion

Straightforward application of numerical quadrature to (2) leads to uncontrolled instability. A stable process is obtained by applying numerical quadrature to the integral in the right-hand side of (2) after deleting a suitable neighbourhood of 0 from the integration interval and using suitable numerical differentiation formulae for approximating the necessary derivatives of f at 0.

Nevertheless the process is still ill-conditioned in the sense that the error is of lower order than the data errors, and it necessarily should be since numerical differentiation is involved (cf., e.g., [11]). However, these orders can be arbitrarily close provided sufficient information is provided.

Acknowledgement. The first author thanks ONR and NSF for support.

References

1. Edwards, R.E.: Functional analysis. Holt etc. 1965
2. Gelfand, I.M., Shilov, G.E.: Generalized functions, vol. I. New York: Academic Press 1964
3. Hadamard, J.: Lectures on Cauchy's problem in linear partial differential equations. Yale Univ. Press 1923; Dover Publications 1952
4. Ioakimidis, N.I.: On the uniform convergence of Gaussian quadrature rules for Cauchy Principal Value integrals and their derivatives. Math. Comput. **44**, 191–198 (1985)
5. Kutt, H.R.: The numerical evaluation of principal value integrals by finite-part integration. Numer. Math. **24**, 205–210 (1975)
6. Kutt, H.R.: Quadrature formulae for finite-part integrals. CSIR Special Report WISK 178. Pretoria: National Research Institute for Mathematical Sciences 1975

7. Linz, P.: On the approximate computation of certain strongly singular integrals. Computing **35**, 345–353 (1985)
8. Paget, D.F.: The numerical evaluation of Hadamard finite – part integrals. Numer. Math. **36**, 447–453 (1981)
9. Ramm, A.G.: On numerical differentiation. Mathematics, Izvestija vuzov **11**, 131–135 (1968)
10. Ramm, A.G.: Stable solution of some ill-posed problems. Math. Methods in Appl. Sci. **3**, 336–363 (1981)
11. Ramm, A.G.: Estimates of derivatives of random functions. J. Math. Anal. Appl. **102**, 244–250 (1984)
12. Tsamasphyros, G., Theocaris, P.S.: On the convergence of some quadrature rules for Cauchy principal – value and finite – part integrals. Computing **31**, 105–114 (1983)