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APPLICATIONS OF PADÉ APPROXIMATION TO NUMERICAL INTEGRATION

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1. **Introductory Remarks.** The work reported in this lecture has been done during the past two or three years in collaboration with research students Glenys Rowlands, Alan Genz and Graham Matthews. Alan Genz is now a member of staff in the University of Kent at Canterbury, and has contributed a great deal to the work. Both Glenys Rowlands and Alan Genz were supported as students by a U.S.A.A.F. grant, through the European office.

The work performed in collaboration with Glenys Rowlands and Alan Genz has been published, [1], and was reported last year to the second Marseilles colloquium on computational physics [2]. For this reason, I shall only summarise this part of my lecture in the written report. I shall give a full written account of the results obtained so far by Graham Matthews.

2. **Accelerated Convergence of Quadrature Approximants.** In this section I shall summarise the results obtained in collaboration with Glenys Rowlands and Alan Genz.

The basic idea is to use Wynn's ϵ-algorithm, related to the use of Padé Approximants, [3], to accelerate the convergence of a sequence $\{S_p\}$ of quadrature approximants to an integral

$$S = \int_a^b f(x)\,dx \tag{2.1}$$

For finite-range integrals, the range was taken to be $(0, 1)$, and the study centred on sequences $\{S_p\}$ defined by using generalised trapezoidal rules, [4], in particular using the two-point Legendre-Gauss formula on 2^p equal subintervals. Then using error formula of Lyness and Ninham, [4], and Fox, [5], Genz has shown that, for integrands with certain types of end-point singularities, the ϵ-algorithm eliminates successive error terms. Comparison is made with the original Romberg [6] and the Bulirsch-Stoer [7] methods of acceleration, both of which also eliminate successive error terms when the integrand is well-behaved. It is found that, as expected, the ϵ-algorithm method is inferior for well-behaved integrands, but that it is the only method that works well for integrands with infinite singularities at end-points, for example $x^{-1/2}$, $x^{-1/6}$ and $x^{-1/2}\log x$; for these integrands, Gaussian integration gives poor results. The conclusion is that using a generalized trapezoidal rule, together with ϵ-algorithm acceleration, is a good universal method of evaluating integrands with end-point singularities.

A second successful application of ϵ-algorithm acceleration concerns sequences of Laguerre-Gauss quadratures to integrals over the range $(0, \infty)$; the method was remarkably successful for integrands which oscillated infinitely, for example $J_{1/2}(x)$, $J_{3/2}(x)$ and x^{-1}. The sequence of quadratures has an arithmetically increasing number of points. What is remarkable is that accurate results are obtained from few points, using quadrature approximants which are themselves extremely inaccurate. The reason for this success is unknown; we have been unable to produce any convincing error analysis.

3. **Evaluation of Fourier Transforms.** Padé approximants and Fourier transforms were linked together in work which Alan Common and I carried out a few years ago, [8]. We were concerned with the interpretation of the infinte series of generalized functions (physically, a one-dimensional multipole expansion)

$$g(k) = 2\pi \sum_{n=0}^{\infty} a_n(-1)^n \delta^{(n)}(k), \tag{3.1}$$

where $\delta^n(k)$ is the nth derivative of the Dirac δ-function. One can interpret (3.1) in two ways:

(a) By integrating term by term with test functions $\{\psi(k)\}$ forming a suitable space; we showed that such spaces exist. Then we obtain

$$g(k)\psi(k) = 2\pi \sum_{n=0}^{\infty} a_n \psi^{(n)}(0). \tag{3.2}$$

When

$$\lim_{n\to\infty} n! a_n = 0, \tag{3.3}$$

the generalized function is localized at $k = 0$. But when $a_n \geqq (n!)^{-1}$, it represents a generalized function with non-compact support, of the form

$$g(k) = 2\pi a_0 \delta(k) - 2\pi [g_0(k)\, \theta(k)]\,', \tag{3.4}$$

where $g_0(k)$ has an integral representation

$$g_0(k) = \int_{0+}^{\infty} e^{-k/u}\, d\phi(u), \tag{3.5}$$

and $\phi(u)$ is a measure function to be defined.

(b) By defining a term-by-term Fourier transformed series

$$f(x) = \sum_{n=0}^{\infty} a_n(-ix)^n. \tag{3.6}$$

When (3.3) is satisfied, the integral

$$g(k) = \int_{-\infty}^{\infty} dx\, e^{ikx} f(x), \tag{3.7}$$

can be evaluated term-by-term. We considered the difficult case for which (3.3) does not hold; to evolve rigorous proofs, we had to assume that (3.6) was a Series of Stieltjes in ix. Then writing

$$f(x) = \int_0^{\infty} \frac{d\phi(u)}{1 + iux} \tag{3.8}$$

defines the unique measure function $\phi(u)$ occurring in (3.5). We were able to show that forming the $(N, N-1)$ Padé approximant to the series (3.6), and substituting in (3.7), gives an approximation to $g(k)$.

In detail, if the approximant to (3.8) is

$$\sum_{m=1}^{N} \frac{\alpha_m}{1 + ix\sigma_m}, \tag{3.9}$$

then the corresponding approximant to the function (3.5) is

$$\sum_{m=1}^{N} \alpha_m e^{-k/\sigma_m}. \tag{3.10}$$

This is a Gammel-Baker approximant [9] to (3.5). Alan Common and I had to modify Baker's proofs to establish our approximation theorem.

In effect, Gammel-Baker approximants have been proved to be good approximants to the Fourier transform (3.7), for this particular class of generalized functions. Graham Matthews has therefore been investigating the possibility of using the same technique to approximate other Fourier transforms. Suppose that $f(x)$ has a power series expansion

$$f(x) = \sum_{n=0}^{\infty} b_n x^n \tag{3.11}$$

and the $(N, N-1)$ Padé approximant to this series is

$$f_{N,N-1}(x) \equiv \sum_{m=1}^{N} \frac{\gamma_m}{x - \sigma_m}. \tag{3.12}$$

Then we might expect that a well-defined Fourier transform

$$g(k) = \int_{-\infty}^{\infty} dx f(x) e^{ikx}$$

would be approximated by the Gammel-Baker approximant

$$g_{N,N-1}(k) = \sum_{m=1}^{N} \int_{-\infty}^{\infty} dx \frac{\gamma_m}{x - \sigma_m} e^{ikx}. \tag{3.13}$$

In general, the poles σ_m can lie anywhere in the x-plane. If they do not lie on the real axis, the integrals in (3.13) can be evaluated explicitly by contour integration to give

$$g_{N,N-1}(k) = \sum_{\substack{\sigma_m \text{ in} \\ \frac{1}{2}\text{-plane}}} \gamma_m e^{ik\sigma_m}, \tag{3.14}$$

the direct analogue of (3.10). If a pole σ_m lies on the real axis, we would expect half of the corresponding term to occur in (3.14). Since one cannot prove in general that (3.12) approximates (3.11), it is not established that (3.14) is a good approximation to $g(k)$. We have therefore experimented by applying the method to evaluate Fourier transforms of functions $J_1(x)$, $J_2(x)$ and $e^{-|x|}$. For various values of k and N, the errors

$$|g(k) - g_{N,N-1}(k)|$$

are given in Tables 1, 2 and 3. These errors are compared with those arising in two other procedures for evaluating $g(k)$: a standard quadrature formula with Romberg acceleration, and the Filon method. For $e^{-|x|}$, we have also used ϵ-algorithm acceleration in N. One can see that, in these examples, the Padé method gives better results than the other two methods, especially for low values of k. The Filon method gives the poorest results. The Padé method uses about three times as much computer time as the quadrature method; most of this time is spent in finding the roots of the Padé denominator. We would welcome an improved method of factoring polynomials!

Graham Matthews has generalized this method to evaluate Fourier transforms of functions of the type

$$F_1(x) = x^{1/2} f(x)$$

$$F_2(x) = x^{-1/2} f(x)$$

and

$$F_3(x) = (1 + x^2)^{-1/2} f(x),$$

where $f(x)$ is given as a power series (3.11). Forming $(N, N-1)$ and $(N, N-2)$ Padé approximants then leads to approximations which are linear combinations of the standard integrals

$$\int_{-\infty}^{\infty} \frac{|x|^{1/2} e^{ikx}}{x^2 - \alpha}\, dx,$$

$$\int_{-\infty}^{\infty} \frac{|x|^{-1/2} e^{ikx}}{x - \beta}\, dx$$

and

$$\int_{-\infty}^{\infty} \frac{e^{ikx}}{(1 + x^2)^{1/2}(x - \beta)}\, dx.$$

The errors using this method, and the two alternative methods, to evaluate the Fourier transforms of $J_{1/2}(x)$ and $J_{3/2}(x)$, are given in Tables 4 and 5. Once again we see that the Padé method gives the best results, especially for low values of k.

The accuracy to which we have been able to calculate has been limited by the precision attainable using our own fairly small computer; it is not yet fully equipped to deal with double precision arithmetic of complex variables, so that round-off error has been a problem. The results given in this section may therefore be improved upon in later work.

4. **Conclusions.** It seems that both the ϵ-algorithm acceleration of sequences of quadrature approximants, and the approximation of integrand factors by Padé approximants, are useful methods of performing certain classes of integrals. The ϵ-algorithm method has been extended by Alan Genz to deal with multiple integrals, [1]. Further work on all of these problems is still proceeding.

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TABLE 1. Errors for $\int_{-\infty}^{\infty} J_1(x)e^{ikx}\,dx = 0$.

$k=$	1	2	3	4	5	6
Using $f_{2,1}(x^2)$	$-1{\cdot}0.10^{-6}$ $+i\,22{\cdot}4$	0 $+i\,2{\cdot}2.10^{-2}$	0 $+i\,2.10^{-5}$	0	0	0
Using $f_{3,2}(x^2)$	$-2{\cdot}0.10^{-6}$ $+i\,8{\cdot}33$	0 $+i\,2{\cdot}01.10^{-3}$	0 $+i\,4{\cdot}3.10^{-6}$	0	0	0
Quad + Romberg	$1{\cdot}62.10^{-4}$ $+i\,238{\cdot}1$	$1{\cdot}6.10^{-5}$ $+i\,1{\cdot}23$	$3{\cdot}61.10^{-6}$ $+i\,3{\cdot}1.10^{-3}$	0 $+i\,1{\cdot}33.10^{-5}$	0 $+i\,6{\cdot}2.10^{-7}$	0
Filon	$17{\cdot}3$ $+i\,820$	$1{\cdot}79.10^{-1}$ $+i\,3{\cdot}1$	$4{\cdot}13.10^{-3}$ $+i\,8.10^{-2}$	$2{\cdot}12.10^{-5}$ $+i\,3{\cdot}5.10^{-4}$	$1{\cdot}1.10^{-6}$ $+i\,8.10^{-6}$	0

TABLE 2. Errors for $\int_{-\infty}^{\infty} J_2(x)e^{ikx}\,dx = 0$.

$k=$	1	2	3	4	5	6
Using $f_{3,2}(x^2)$	$6{\cdot}10^{-7}$ $-i\,2{\cdot}265$	0 $-i\,2.10^{-8}$	0	0	0	0
Using $f_{4,3}(x^2)$	0 $-i\,0{\cdot}316$	0 $-i\,1{\cdot}7.10^{-8}$	0	0	0	0
Quad. + Romberg	$4{\cdot}77.10^{-2}$ $-i\,34{\cdot}2$	$2{\cdot}18.10^{-4}$ $-i\,2{\cdot}13.10^{-2}$	$7{\cdot}11.10^{-6}$ $-i\,1{\cdot}8.10^{-5}$	0 $-i\,3{\cdot}1.10^{-7}$	0 $-i\,10^{-8}$	0
Filon	$79{\cdot}17$ $-i\,6{\cdot}3.10^{-4}$	$1{\cdot}37$ $-i\,1{\cdot}8.10^{2}$	$5{\cdot}92.10^{-3}$ $-i\,0{\cdot}875$	$7{\cdot}34.10^{-6}$ $-i\,3{\cdot}4.10^{-3}$	$1{\cdot}2.10^{-8}$ $-i\,6{\cdot}6.10^{-6}$	

TABLE 3. Errors for $\int_{-\infty}^{\infty} e^{-|x|}e^{ikx}\,dx$.

	Using $f_{5,4}(x)$	Using $f_{6,5}(x)$	ϵ-alg. up to $f_{5,4}$*	Quad + Romberg	Filon	Exact
$k = 1$	2.10^{-4}	0	10^{-5}	$4 \cdot 7.10^{-3}$	$1 \cdot 2.10^{-2}$	$1 \cdot 0000$
$k = 2$	$2 \cdot 7.10^{-2}$	$5 \cdot 5.10^{-3}$	$2 \cdot 8.10^{-3}$	$4 \cdot 1.10^{-3}$	$1 \cdot 3.10^{-2}$	$0 \cdot 4000$
$k = 3$	$2 \cdot 1.10^{-2}$	$2 \cdot 3.10^{-3}$	3.10^{-3}	$1 \cdot 7.10^{-2}$	$2 \cdot 3.10^{-2}$	$0 \cdot 6000$

*round-off error involved

TABLE 4. Errors for $\int_{-\infty}^{\infty} J_{1/2}(x)e^{ikx}\,dx$.

$k=$	1	2	3	4	5	6
Using $f_{2,1}(x^2)$	$-1 \cdot 5.10^{-5}$ $+i\,1 \cdot 75$	-1.10^{-8} $+i\,0 \cdot 35$	0 $+i\,4 \cdot 7.10^{-4}$	0 $-i\,5 \cdot 4.10^{-6}$	0 $-i\,1 \cdot 8.10^{-8}$	0
Using $f_{3,2}(x^2)$	6.10^{-7} $-i\,1 \cdot 53$	0 $-i\,5 \cdot 2.10^{-7}$	0	0	0	0
Quad. + Romberg	$1 \cdot 25$ $+i\,8 \cdot 7.10^{2}$	$4 \cdot 5.10^{-2}$ $+i\,1 \cdot 41$	$7 \cdot 11.10^{-4}$ $+i\,9 \cdot 2.10^{-3}$	$2 \cdot 7.10^{-6}$ $+i\,1 \cdot 6.10^{-5}$	3.10^{-8} $+i\,3 \cdot 7.10^{-8}$	0
Filon	$4 \cdot 38.10^{2}$ $+i\,6 \cdot 6.10^{4}$	$0 \cdot 377$ $+i\,3 \cdot 5.10^{-2}$	$1 \cdot 16.10^{-2}$ $+i\,1 \cdot 2.10^{-2}$	$2 \cdot 19.10^{-3}$ $+i\,2 \cdot 15.10^{-2}$	$3 \cdot 11.10^{-4}$ $+i\,1 \cdot 5.10^{-3}$	

TABLE 5. Errors for $\int_{-\infty}^{\infty} J_{3/2}(x)e^{ikx}\,dx$.

$k =$	1	2	3	4	5	6
Using $f_{2,0}(x^2)$	$1\cdot63.10^{-4}$ $+i\,0\cdot27$	$6\cdot2.10^{-7}$ $-i\,4\cdot9.10^{-5}$	0 $+i\,3.10^{-8}$	0	0	0
Using $f_{3,1}(x^2)$	$5\cdot5.10^{-5}$ $+i\,3\cdot4$	0 $-i\,4\cdot1.10^{-5}$	0 $+i\,.10^{-8}$	0	0	0
Using $f_{4,2}(x^2)$	$2\cdot7.10^{-5}$ $+i\,1\cdot18$	0 $-i\,8\cdot2.10^{-6}$	0	0	0	0
Quad. + Romberg	$9\cdot73$ $+i\,15\cdot24$	$7\cdot72.10^{-2}$ $-i\,1\cdot127$	$4\cdot79.10^{-4}$ $-i\,6\cdot6.10^{-3}$	$2\cdot29.10^{-6}$ $-i\,2\cdot18.10^{-5}$	$1\cdot18.10^{-8}$ $+i\,1\cdot75.10^{-6}$	0 $-i\,1\cdot3.10^{-8}$