JOURNAL OF COMPUTATIONAL PHYSICS 37, 264–267 (1980)

Note

Use of Gaussian Convergence Factors in the Numerical Evaluation of Slowly Converging Integrals*

1. *Introduction*

A number of methods have been proposed for the numerical evaluation of slowly converging integrals with infinite limits. Here we describe a method based on extrapolation. The convergence factor $\exp(-\frac{1}{2}\sigma^2 u^2)$ is inserted in the integrand, the integral is evaluated for several small values of σ, and the results are extrapolated to $\sigma = 0$. The point of the method is that it is often computationally easier to evaluate the several integrals than to try to evaluate the original integral directly.

2. *The Extrapolation Procedure*

It is convenient to base the description of extrapolation method on the integral

$$F(y) = \int_0^\infty e^{-iuy} f(u)\, du, \tag{1}$$

which is of a type that often converges slowly. Let

$$F(y, \sigma) = \int_0^\infty \exp[-iuy - \tfrac{1}{2}\sigma^2 u^2] f(u)\, du \tag{2}$$

and let $F(y, \sigma_k)$, $k = 1, 2,..., N$, be the values of $F(y, \sigma)$ obtained by numerical integration of (2) for a sequence of decreasing values of σ. Then extrapolating the values of $F(y, \sigma_k)$ to $\sigma = 0$ gives an approximation for $F(y)$. From the second mean-value theorem and the fact that $\exp[-\sigma^2 u^2/2]$ is a monotonic function of u it can be shown that if the integral (1) converges then the integral (2) for $F(y, \sigma)$ converges and tends to $F(y)$ as $\sigma \to 0$.

The extrapolation formulas are based upon the fact that $F(y, \sigma)$ can also be expressed as

$$F(y, \sigma) = \frac{1}{\sigma(2\pi)^{1/2}} \int_{-\infty}^\infty F(y') \exp[-(y - y')^2/(2\sigma^2)]\, dy'. \tag{3}$$

This follows from (2) and the convolution theorem for Fourier integrals [1, pp.

* This research was sponsored by the Air Force Office of Scientific Research, Air Force Systems Command, USAF, under Grant AFOSR 74-2689.

0021-9991/80/110264-04$02.00/0

25–27]. Expanding $F(y')$ in a Taylor's series about y and integrating termwise gives the formal result

$$F(y,\sigma)=F(y)+\sum_{n=1}^{N-1} C_{2n}(y)\,\sigma^{2n}+O(\sigma^{2N}). \tag{4}$$

Ignoring $O(\sigma^{2N})$, putting $\sigma=\sigma_k$, $k=1, 2,\ldots, N$, and solving the resulting N equations for $F(y)$ gives an Nth-order extrapolation to $\sigma=0$ [2].

When $\sigma_k=\sigma_1 r^{k-1}$ with $0<r<1$, the extrapolation can be cast in the form of a sequence of approximations similar to the ones appearing in Romberg integration [3]. Denote the values of $F(y,\sigma_k)$ by $F_a(1,k)$ (the first approximations). The second approximations, obtained by eliminating $C_2(y)$ between successive pairs of equations (4), are

$$F_a(2,k)=\frac{F_a(1,k+1)-r^2F_a(1,k)}{1-r^2}, \qquad k=1, 2,\ldots, N-1. \tag{5}$$

The $(j+1)$st set of approximations can be obtained from the jth set by using

$$F_a(j+1,k)=\frac{F_a(j,k+1)-r^{2j}F_a(j,k)}{1-r^{2j}}, \tag{6}$$

where $j=1, 2,\ldots, N-1$ and $k=1, 2,\ldots, N-j$.

A convenient arrangement of these approximations is

k	$j=1$	$j=2$	$j=3$	$j=4$
1	$F_a(1,1)$	$F_a(2,1)$	$F_a(3,1)$	$F_a(4,1)$
2	$F_a(1,2)$	$F_a(2,2)$	$F_a(3,2)$	
3	$F_a(1,3)$	$F_a(2,3)$		
4	$F_a(1,4)$			

(7)

where $N=4$ has been taken for illustration. When the extrapolation is working well, the entries in the columns either increase or decrease regularly, and $F_a(3,1)$ and $F_a(3,2)$ are nearly equal to the final approximation $F_a(4,1)$ to $F(y)$. Furthermore for the larger values of k the ratios

$$[F_a(j,k+1)-F_a(4,1)]/[F_a(j,k)-F_a(4,1)] \tag{8}$$

obtained from the jth column are nearly equal to r^{2j}.

If $F(y,\sigma)$ decreases steadily as $\sigma\to 0$, (4) suggests that $(d/dy)^2\,F(y)\geqslant 0$, and vice versa. When $F(y)$ has a finite jump at $y=y_1$, the integral (1) does not converge at $y=y_1$ but (3) suggests that

$$\operatorname*{limit}_{\sigma\to 0} F(y_1,\sigma)=\tfrac{1}{2}[F(y_1-0)+F(y_1+0)].$$

We have been unable to find a straightforward procedure for selecting the best values of σ_1 and N. In the uses we have made of the extrapolation method we have arbitrarily taken $N = 4$ (i.e., the array (7)) and $r^2 = 1/2$. Different values of σ_1 were tried until an array was obtained whose regularity indicated that $F_a(4, 1)$ did indeed give $F(y)$ to within the required accuracy. It was observed that when y was near a singularity of $F(y)$, say at y_1, a value of σ_1 that made

$$\exp[-(y - y_1)^2/(2\sigma_1^2)] \tag{9}$$

equal to the allowable error was satisfactory.

3. *Example*

To illustrate the extrapolation method we use it to evaluate the integral

$$K_0(y) = \int_0^\infty (1 + u^2)^{-1/2} \cos(yu)\, du, \qquad y > 0, \tag{10}$$

where $K_0(y)$ is the modified Bessel function (Eq. 9.6.21 in [4]). The integral corresponding to (2) is

$$F(y, \sigma) = \int_0^\infty \exp[-\tfrac{1}{2}\sigma^2 u^2](1 + u^2)^{-1/2} \cos(yu)\, du. \tag{11}$$

Suppose we are interested in accuracies of order 10^{-6}. Since $K_0(y)$ is known to have a singularity at $y = 0$, we set $y_1 = 0$ in (9) and then set the expression (9) equal to 10^{-6}. This gives an equation whose solution is approximately $\sigma_1 = y/5$.

To illustrate the computation we take $y = 1$, $\sigma_1 = 0.2$, and $r^2 = 0.5$. Evaluating (11) for $\sigma_k = 0.2\, r^{k-1}$, $k = 1, 2, 3, 4$, leads to the following array of approximations to $K_0(1)$:

N	k	σ_k	$j = 1$	$j = 2$	$j = 3$	$j = 4$
80	1	0.2000	0.442999	0.420205	0.421058	0.421023
110	2	0.1414	0.431602	0.420844	0.421028	
160	3	0.1000	0.426223	0.420982		
220	4	0.0707	0.423603			

(12)

The first column shows the number of points used to evaluate the integral (11) by the trapezoidal rule with a spacing of $\Delta u = 0.4$ (the integral is suited to evaluation by the trapezoidal rule because the integrand is an even analytic function). The entries in the $j = 1$ column are the values of $F(y, \sigma_k)$ calculated from (11) with $y = 1$. They correspond to the $F_a(1, k)$'s in array (7). The following columns are obtained step by step using (6). The entry in the last column agrees well with the exact value $K_0(1) = 0.421014\ldots$. Note the regularity of the entries in the array.

REFERENCES

1. A. PAPOULIS, "The Fourier Integral and Its Applications," McGraw–Hill, New York, 1962.
2. D. C. JOYCE, Survey of extrapolation processes in numerical analysis, *SIAM Rev.* **13**, No. 4 (1971), 435–490.
3. E. ISAACSON AND H. B. KELLER, "Analysis of Numerical Methods," Wiley, New York, 1966.
4. M. ABRAMOWITZ AND I. A. STEGUN, "Handbook of Mathematical Functions," Dover, N.Y., 1972.

RECEIVED: March 1, 1978; REVISED: October 31, 1979

ROBERT LUGANNANI AND STEPHEN RICE

Department of Electrical Engineering and Computer Sciences
University of California, San Diego
La Jolla, California 92093