THE EVALUATION OF INTEGRALS OF THE FORM $\int_{-\infty}^{\infty} f(x)\, e^{-x^2} dx$

By E. T. GOODWIN

Received 28 February 1948

1. *Introduction.* It is well known to computers that the approximate formula

$$\int_{-\infty}^{\infty} e^{-x^2}\, dx \doteqdot h \sum_{n=-\infty}^{\infty} e^{-n^2h^2} \tag{1·1}$$

yields a surprising degree of accuracy even for quite large values of the interval h; for example, if $h = 1$ the error is one unit in the fourth decimal.

The connexion between (1·1) and the standard formulae for numerical quadrature is interesting, and not immediately apparent. For example, the formula for numerical integration using central differences is

$$\int_a^{a+h} f(x)\, dx = \tfrac{1}{2}h[f(a)+f(a+h)] + h\sum_{s=1}^{\infty} \frac{B_{2s}^{(2s)}(s)}{(2s)!}[\mu\delta^{2s-1}f(a+h) - \mu\delta^{2s-1}f(a)] \tag{1·2}$$

for integration over one interval and, by summing m such formulae, is

$$\int_a^{a+mh} f(x)\, dx = h[\tfrac{1}{2}f(a)+f(a+h)+\ldots+\tfrac{1}{2}f(a+mh)] + h\sum_{s=1}^{\infty} \frac{B_{2s}^{(2s)}(s)}{(2s)!}[\mu\delta^{2s-1}f(a+mh) - \mu\delta^{2s-1}f(a)] \tag{1·3}$$

for integration over m intervals. In both these formulae $B_{2s}^{(2s)}(s)$ denotes the Bernoulli polynomial*.

Now e^{-x^2} and its differences approach zero rapidly as $x \to \pm\infty$, so that a naïve application of (1·3) would lead to the formula (1·1) with the sign of equality; it is apparent that this is incorrect. In fact the infinite series of (1·2) does not converge, but is asymptotic, and an indication of the error caused by using (1·1) can be obtained from a consideration of the size of the remainder term.

If $n-1$ terms are taken in the infinite series of (1·2) the remainder is given by

$$R_n = h^{2n+1}\frac{B_{2n}^{(2n)}(n)}{(2n)!} f^{(2n)}(\xi), \tag{1·4}$$

where ξ is some point lying within the range $a \pm nh$. Now in the case $f(x) \equiv e^{-x^2}$,

$$f^{(2n)}(\xi) = \frac{d^{2n}}{d\xi^{2n}} e^{-\xi^2} = e^{-\xi^2} H_{2n}(\xi),$$

where $H_{2n}(\xi)$ is the Hermite polynomial. Accordingly, for large n,

$$f^{(2n)}(\xi) \sim (-)^n 2^{2n+\frac{1}{2}} \left(\frac{n}{e}\right)^n e^{-\frac{1}{2}\xi^2} \cos 2\xi\sqrt{n}. \tag{1·5}$$

Also the asymptotic form of $B_{2n}^{(2n)}(n)/(2n)!$ for large n is

$$B_{2n}^{(2n)}(n)/(2n)! \sim (-)^{n-1} n^{-\frac{1}{2}} \pi^{-\frac{1}{2}} 2^{-2n+1}. \tag{1·6}$$

* See, for example, L. M. Milne-Thomson, *The calculus of finite differences* (Macmillan, 1933).

On substituting (1·5) and (1·6) into (1·4) the asymptotic form of the remainder term for large n is obtained as
$$R_n \sim -\frac{2^{\frac{1}{2}}h}{n^{\frac{1}{4}}\pi^{\frac{1}{4}}}\left(\frac{h^2n}{e}\right)^n e^{-\frac{1}{2}\xi^2}\cos 2\xi\sqrt{n}. \tag{1·7}$$

From (1·7) it is apparent that, however small the interval h is taken to be, R_n will eventually increase without limit. The expression $(h^2n/e)^n$ has a minimum for $n = 1/h^2$, for which its value is e^{-1/h^2}, and the least value of R_n for varying n is accordingly $O(h^4e^{-1/h^2})$, if it is assumed that the terms in ξ are $O(1)$. (It may be noted that for the central interval with $a = 0$, ξ lies between $\pm nh$, that is, in this case, between $\pm 1/h$ so that the least value of the exponential term would be $e^{-1/2h^2}$.) There is thus a limit to the accuracy obtainable in this case from the formula (1·2) and, correspondingly, (1·1) is only approximately true.

It is clear that the estimate $O(h^4e^{-1/h^2})$ for the least remainder of the series (1·2) may appreciably exceed the error in using (1·1) since when a number of remainders R_n are summed in forming (1·1) the highly oscillatory cosine term may be expected to cause considerable cancellation. No very reliable estimate can be obtained in this way, in view of the uncertainty of the exact value of ξ, but, on making the most reasonable assumption that ξ lies at the mid-point a of the range $a \pm nh$, and since the successive values of a taken in forming (1·1) are of the form mh, the summation $h\sum_\xi e^{-\frac{1}{2}\xi^2}\cos 2\xi\sqrt{n}$ involved becomes
$$h\sum_{m=-\infty}^{\infty} e^{-\frac{1}{2}m^2h^2}\cos 2mh\sqrt{n},$$
which is equal to
$$\sqrt{(2\pi)}\sum_{m=-\infty}^{\infty} e^{-2(\sqrt{n}+m\pi/h)^2}.$$

For values of h less than about unity at most two terms of this series will be significant, and in this way an estimate for the error in (1·1) is obtained in the form
$$\text{Remainder} \sim -\frac{64h^3}{\pi^5}\left(\frac{\pi^2}{4e^3}\right)^{\frac{1}{4}\pi^2/h^2}$$
which is approximately $O(h^3e^{-\frac{1}{4}\pi^2/h^2})$. This, as has been anticipated, is of an order appreciably smaller than (1·7).

The practical excellence of the formula (1·1) for values of h as large as unity confirms that this smaller estimate of the error is likely to be the more correct. In fact the actual error is $O(e^{-\pi^2/h^2})$, and a proof of this is contained in a paper by Turing*. In this paper he points out that his argument can be used in more general cases, and it is the purpose of the present paper to give the details of the trivial extension to the important class of integrals $\int_{-\infty}^{\infty} f(x)\,e^{-x^2}\,dx$. These occur quite frequently in practical calculations, and the summation of the rapidly convergent series (1·1) at a fairly wide interval in h provides a very rapid and satisfactory method for their evaluation. A number of examples are given showing how this method can be, and has been, applied in cases of practical interest.

* A. M. Turing, 'A method for the calculation of the zeta-function', *Proc. London Math. Soc.* (2), 48 (1943), 180.

2. *Estimation of the error.* In this section Turing's method for the formula (1·1) is extended to estimate the error term $E(h)$ in the corresponding formula

$$\int_{-\infty}^{\infty} f(x)\, e^{-x^2}\, dx = h \sum_{n=-\infty}^{\infty} f(nh)\, e^{-n^2h^2} - E(h). \tag{2·1}$$

Clearly, without any loss of generality, $f(x)$ may be taken to be an even function. Now integrate the function $f(x)\, e^{-x^2}/(1-e^{-2\pi i x/h})$ round a rectangular contour with vertices at $\pm\infty \pm i\pi/h$. Then

$$\left\{\int_{-\infty-i\pi/h}^{\infty-i\pi/h} + \int_{\infty+i\pi/h}^{-\infty+i\pi/h}\right\} \frac{f(x)\, e^{-x^2}}{1-e^{-2\pi i x/h}}\, dx = h \sum_{n=-\infty}^{\infty} f(nh)\, e^{-n^2h^2}; \tag{2·2}$$

thus

$$h \sum_{n=-\infty}^{\infty} f(nh)\, e^{-n^2h^2} - \int_{-\infty-i\pi/h}^{\infty-i\pi/h} f(x)\, e^{-x^2}\, dx$$

$$= \int_{-\infty-i\pi/h}^{\infty-i\pi/h} \frac{f(x)\, e^{-x^2}\, e^{-2\pi i x/h}}{1-e^{-2\pi i x/h}}\, dx + \int_{\infty+i\pi/h}^{-\infty+i\pi/h} \frac{f(x)\, e^{-x^2}}{1-e^{-2\pi i x/h}}\, dx = 2\int_{-\infty-i\pi/h}^{\infty-i\pi/h} \frac{f(x)\, e^{-x^2}}{e^{2\pi i x/h}-1}\, dx, \tag{2·3}$$

since $f(x)$ is an even function. It has here been assumed that $f(x)$ has no poles between the real axis and the lines $x = \pm i\pi/h$. The integral on the left-hand side may therefore be taken along the real axis and the left-hand side is $E(h)$. If $f(x)$ has such poles then the formula (2·1) breaks down completely and must be modified by the inclusion of a term corresponding to the appropriate residues.

The integral on the right-hand side can be written as

$$2e^{-\pi^2/h^2} \int_{-\infty}^{\infty} f(y - i\pi/h)\, \frac{e^{-y^2}}{1-e^{-2\pi i y/h - 2\pi^2/h^2}}\, dy.$$

Now in all cases of interest $e^{-2\pi^2/h^2}$ is negligible compared with unity, and the term in the denominator involving it can be neglected. This leads to

$$E(h) = 2e^{-\pi^2/h^2} \int_{-\infty}^{\infty} f(y - i\pi/h)\, e^{-y^2}\, dy. \tag{2·4}$$

In the particular case $f(x) \equiv 1$ this gives $2\sqrt{\pi}e^{-\pi^2/h^2}$ for the error; thus the error in using (1·1) is $1{\cdot}8 \times 10^{-4}$ if the interval is unity and $2{\cdot}5 \times 10^{-17}$ if $h = \frac{1}{2}$.

In more general cases a good estimate to $E(h)$ can be obtained by approximating for the integral in (2·4), though the most convenient method of doing so will in general depend on the precise form of $f(x)$. One very simple approximation gives a satisfactory result for a very large variety of forms of f. This consists of assuming that the main contribution to the integral in (2·4) arises from the neighbourhood of $y = 0$, the factor f is taken outside the integral in the form $f(i\pi/h)$ and a very simple expression for $E(h)$ is obtained.

$$E(h) = 2\sqrt{\pi}e^{-\pi^2/h^2} f(i\pi/h). \tag{2·5}$$

This expression is only likely to underestimate the error seriously when $f(x)$ tends rapidly to infinity with x. If $f(x) = x^2$, (2·5) is still quite accurate giving

$$E(h) = -2\sqrt{\pi}\frac{\pi^2}{h^2} e^{-\pi^2/h^2}$$

instead of the accurate value

$$E(h) = -2\sqrt{\pi}\left(\frac{\pi^2}{h^2} - \frac{1}{2}\right) e^{-\pi^2/h^2}.$$

However, if $f(x) = \cosh kx$, and $\cos k\pi/h$ is replaced by unity, (2·5) underestimates the error by a factor $e^{-\frac{1}{4}k^2}$ which is appreciable for large values of k. Such an underestimate could, however, be anticipated by anyone using these formulae. If, for example, $f(x)$ were of the form $\phi(x) \cosh kx$, (2·5) could be replaced by

$$E(h) \sim 2\sqrt{\pi} e^{-\pi^2/h^2} e^{\frac{1}{4}k^2} \phi(i\pi/h), \tag{2·6}$$

which would almost certainly give a good estimate.

3. *Applications of the formula.*

(1) $$\int_{-\infty}^{\infty} \cos x \, e^{-x^2} dx = \sqrt{\pi} \, e^{-\frac{1}{4}}, \quad E(h) \sim 2\sqrt{\pi} \, e^{-\pi^2/h^2} \cosh(\pi/h) \sim \sqrt{\pi} \, e^{\pi/h - \pi^2/h^2}.$$

For $h = 1$ the estimated error is 21 in units of the fourth decimal and the actual error is 16. For $h = 0{\cdot}9$ the figures are 3 and 2 respectively.

(2) $$\int_{-\infty}^{\infty} x^2 \cos x \, e^{-x^2} dx = \tfrac{1}{4}\sqrt{\pi} \, e^{-\frac{1}{4}}, \quad E(h) \sim \sqrt{\pi} \left(\frac{\pi^2}{h^2}\right) e^{\pi/h - \pi^2/h^2}.$$

For $h = 1$ the estimated error is 209 in units of the fourth decimal and the actual error is 107. For $h = 0{\cdot}9$ the figures are 36 and 19 respectively, and for $h = 0{\cdot}8$ they are 5 and 3.

(3) $$\int_{-\infty}^{\infty} J_0(x) \, e^{-x^2} dx = \sqrt{\pi} \, e^{-\frac{1}{8}} I_0(\tfrac{1}{8}), \quad E(h) \sim 2\sqrt{\pi} \, I_0\left(\frac{\pi}{h}\right) e^{-\pi^2/h^2} \sim \sqrt{\left(\frac{2h}{\pi}\right)} \, e^{\pi/h - \pi^2/h^2}.$$

For $h = 1$ the estimated error is 10 in units of the fourth decimal and the actual error is 8. For $h = 0{\cdot}9$ the figure is 1 in each case.

The three examples given above have all been chosen because the exact value of the integral is known. They suffice to show that the formula (2·5) gives an estimate $E(h)$ which is sufficiently accurate for general purposes. It may be emphasized at this point that quite a small decrease in h causes a very large increase in the accuracy. This means that if there is any doubt of the required accuracy being obtained by summation at any particular interval h, a small decrease in the interval will suffice to ensure that it is, in fact, obtained.

Finally, two examples are given illustrative of the type of integral for which this method has been used with success in practice.

(4) $$\frac{1}{\sqrt{\pi}} \int_0^{\infty} e^{-\frac{1}{4}u^2} \cos xu \, J_0(yu) \, du.$$

It was found that four-decimal accuracy could be obtained by quadrature of this integral at an interval of $\frac{1}{2}$ for values of x, y up to $x = 1$, $y = 5$. Formula (2·5) gives

$$E(h) \sim \frac{1}{2\pi} \left(\frac{h}{y}\right)^{\frac{1}{2}} e^{2\pi(x+y)/h - \pi^2/h^2},$$

where h is the interval in $\frac{1}{2}u$. This was $\frac{1}{4}$, and the error is then estimated as

$$(4\pi\sqrt{y})^{-1} \, e^{8\pi(x+y-2\pi)} \quad \text{or} \quad 0{\cdot}00003 \qquad \text{for} \qquad x = 1, \; y = 5.$$

(5) $$\int_0^{\infty} e^{-x^2}(x^2 - \tfrac{1}{2}) \, [Y_0(|a + bx|) + Y_0(|a - bx|)] \, dx.$$

This integral can be quadratured by this method provided that b/a is sufficiently small (actually less than 4) for the infinity in the Bessel function to be neglected. The largest value of b was 2, and if the simple approximation of replacing Y_0 by a cosine term is made, an estimate for the error is obtained as

$$E(h) \sim \sqrt{\pi}\left(\frac{\pi^2}{h^2}+\tfrac{1}{2}\right) e^{2\pi/h-\pi^2/h^2}.$$

This shows that the interval of $\frac{1}{2}$ which was actually used is quite small enough to provide a high degree of accuracy.

The work described above has been carried out as part of the research programme of the National Physical Laboratory, and this paper is published by permission of the Director of the Laboratory.

Mathematics Division, National Physical Laboratory
Teddington, Middlesex