Efficient Evaluation of Integrals of Analytic Functions by the Trapezoidal Rule

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Definite integrals of analytic functions can often be evaluated efficiently by the trapezoidal rule after a suitable transformation. Here the work of Moran[1] and Schwartz[2] along this line is extended. First the dependence of the error on the spacing is discussed, and then several types of transformations are described and applied to integrals of technical interest.

I. INTRODUCTION

Quite often the problem of determining the value of a definite integral arises. When the integral cannot be readily evaluated by analysis, we must resort to numerical methods. Here we discuss a method of numerical quadrature which gives promise of being useful in evaluating some types of integrals that are difficult to handle by conventional numerical methods.

In particular, we consider the problem (Moran[1] and Schwartz[2]) of transforming a given integral of an analytic function $f(x)$ into a rapidly converging one (with limits $\pm \infty$) which can be efficiently evaluated by the trapezoidal rule,

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

The integral and series are assumed to converge. In addition to the trapezoidal error E, a second error is introduced when the series is truncated in the process of computation. It is supposed that both errors are made negligible, E by taking h small, and the truncation error by taking enough terms in the series. The feature which makes the use of (1) attractive is that E often decreases in proportion to $\exp(-C/h)$ as h decreases, C being a constant. Thus if h gives three-figure accuracy, $h/2$ will give six-figure accuracy in many cases.

The transformations, i.e., the changes of variable of integration used to carry the limits of the given integral into $\pm \infty$, are usually constructed by combining functions which are readily computed, such as powers and exponential functions.

Schwartz[2] recommends the following procedure for evaluating the integral of an analytic function $f(u)$: (i) change the variable from u to v so as to make the integration with respect to v extend from $-\infty$ to $+\infty$, (ii) make the further transformation

$$v = e^x - e^{-x}$$

to increase the rate of convergence, and then (iii) evaluate the trapezoidal sum, truncating when contributions fall below the desired accuracy, and reduce the spacing h until the answer has the desired accuracy.

Here we present a summary of several variations of Schwartz's procedure. Details are given in a report by the author.[3] The dependence of the error E on the spacing h is first reviewed, and then examples are used to illustrate the evaluation of various types of integrals.

II. THE DEPENDENCE OF E ON h

The trapezoidal error E can be expressed in several ways. For example, it is the remainder in the Euler-Maclaurin sum formula. Again, it can be written as the sum of contour integrals with integrands $f(z)/[\exp (\pm i2\pi z/h) - 1]$ (Ref. 4, p. 145, Problem 7, and Refs. 5, 6, 7, 8, and 9). Here we follow Fettis[5] and use Poisson's summation formula which, when applied to (1), gives

$$E = \left(\sum_{k=-\infty}^{-1} + \sum_{k=1}^{\infty} \right) \int_{-\infty}^{\infty} f(z) \exp (i2\pi zk/h)dz. \tag{2}$$

Let $f(z)$ be analytic throughout a strip in the z-plane containing the real z-axis and assume that suitable convergence conditions are satisfied. Then the paths of integration in the terms for $k > 0$ in (2) can be displaced upwards to make Im $(z) > 0$. It follows that $|\exp (i2\pi kz/h)|$ $= \exp (-2\pi k$ Im $(z)/h)$ becomes small when h becomes small and z is on the path. Furthermore, as $h \to 0$ the terms for $k > 1$ become negligible in comparison with the term for $k = 1$. A similar argument holds for the $k < 0$ terms, and as $h \to 0$ we have the asymptotic result

$$E \sim R_+ + R_-$$

where R_+ and R_- are the $k = 1$ and $k = -1$ terms, respectively, in (2). For the important case in which $f(z)$ is real on the real z-axis, R_-

is equal to the conjugate complex R_+^* of R_+ and E is given asymptotically by

$$E \sim R_+ + R_+^*,$$

$$R_+ = \int_{-\infty}^{\infty} f(z) \exp{(i2\pi z/h)}dz. \tag{3}$$

When h is small, the trapezoidal error E given by (3) can be viewed as the sum of contributions from singularities of $f(z)$ and saddle points of $f(z) \exp{(i2\pi z/h)}$. At the saddle points the derivative $d\varphi(z)/dz$ is zero, $\varphi(z)$ being defined to within a multiple of $2\pi i$ by $\exp{[\varphi(z)]}$ $= f(z) \exp{(i2\pi z/h)}$.

This picture of E is suggested by the following remarks. The path of integration in (3) can be deformed upwards towards $z = i\infty$ in the complex z-plane until it becomes an optimal path comprised of paths of steepest descent and ascent passing through one or more saddle points. The path runs from $-\infty$ to $+\infty$ and may have detours running out to, and returning from, infinity. It may also have loops around some of the singularities of $f(z)$. When h is small, the factor $\exp{(i2\pi z/h)}$ decreases rapidly as Im (z) increases, and the only significant contributions to R_+ come from the portions of the path near the singularities and near the saddle points not associated with singularities.

An approximate expression for a typical contribution can be obtained by expanding the contribution about the corresponding singularity or saddle point and taking the leading term. Such expansions are usually asymptotic in h. For estimating orders of magnitude we can use the dominant factors in the leading terms:

(Contribution to R_+ of a saddle point at z_0) $\approx \exp{[\varphi(z_0)]}$,

(Contribution to R_+ of a singularity at z_1) $\approx \exp{(i2\pi z_1/h)}$.

As h decreases, E may either decrease steadily or may oscillate with decreasing amplitude depending upon how the dominant contributions combine.

If there are no singularities or saddle points in the finite part of the z-plane, the trapezoidal rule may give the exact value of the integral when h is less than some fixed value. This is associated with the sampling theorem for band-limited functions. For example, if m and n are positive integers such that $m - n = 0$ or $2, 4, \cdots$, the integral

$$I = \int_{-\infty}^{\infty} \sin^m x dx/x^n \tag{4}$$

is exactly equal to the trapezoidal sum when $h < 2\pi/m$ (h can equal

$2\pi/m$ if $n \geq 2$). The proof follows from the fact that all of the terms in the series (2) for E vanish when $h < 2\pi/m$, as can be shown by deforming the paths of integration into infinite semicircles and using Jordan's lemma (Ref. 4, p. 115). As a check, note that for $m = n = 1$ or 2 we can take $h = \pi$. Then $I = \pi$ because there is only one nonzero term in the sum.

The foregoing discussion shows that the structure of E can be determined by computing the saddle points and associated paths of steepest descent for $f(z) \exp(i2\pi z/h)$. This is done in the report[3] for the examples (6) and (25) given below. The path for example (6) is shown in Fig. 1 and discussed in the appendix. However, computations of this sort are laborious. In practice it appears that the dependence of E on h is most easily determined by computing the trapezoidal sum for a sequence of decreasing values of h, bearing in mind the possibility that E may go through zero for some values of h.

Incidentally, arguments similar to those given in this section show that the trapezoidal rule also works well when it is used to evaluate integrals of periodic analytic functions in which the integration extends over a period.

III. CONTRIBUTIONS TO E—EXAMPLE

Goodwin[6] has pointed out that the trapezoidal rule usually performs well for integrals of the type

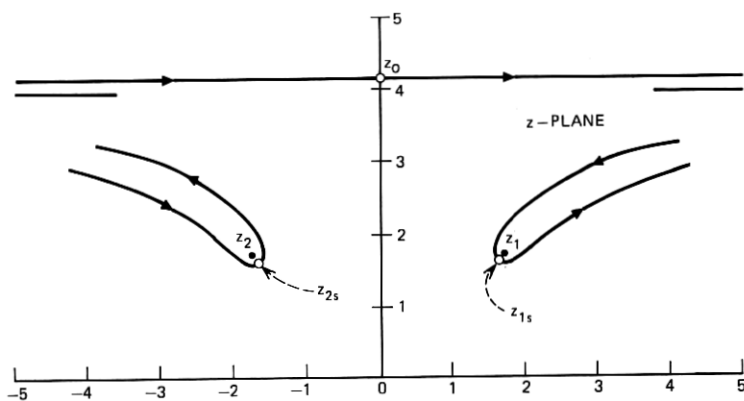$$I = \int_{-\infty}^{\infty} g(x) \exp(-bx^2) dx. \tag{5}$$

Fig. 1—Steepest descent paths for $\exp[\varphi(z)]$ when $a = 2.4$ and $h = 0.8$ in both (30) and example (6). The points z_0, z_{1s}, z_{2s} are saddle points; z_1, z_2 are branch points.

Computations[3] made with $b = 1$,

$$g(x) = (x^4 + a^4)^{-\frac{1}{2}}, \tag{6}$$

and $a = 2.4$ show that, as h decreases, E first decreases steadily and then near $h = 1$ (where $E/I \approx 10^{-4}$) E starts to oscillate with decreasing amplitude. This behavior can be explained in terms of a contribution to E of approximately

$$2\pi^{\frac{1}{2}} \operatorname{Re} \left[g(i\pi/h) \exp \left(-\pi^2/h^2 \right) \right] \tag{7}$$

from a saddle point near $z = i\pi/h$ (see Fig. 1, eq. (32), and Goodwin[6]) and contributions from the branch points at $z_1 = a \exp (i\pi/4)$ and $z_2 = a \exp (i3\pi/4)$. The expressions for the branch point contributions are somewhat more complicated than (7), but all that need be noted here is that they contain $\exp (i2\pi z_k/h)$, $k = 1, 2$, as a dominant factor. Adding the three contributions and neglecting multipliers such as $g(i\pi/h)$ in (7) shows that E is roughly

$$\exp \left(-\pi^2/h^2 \right) + (\cos \alpha) \exp \left(-\beta \right) \tag{8}$$

where $\beta = 2^{\frac{1}{2}}\pi a/h$ and $\cos \alpha$ oscillates with increasing frequency as h decreases. The steady decrease of E with h, dominated by $\exp \left(-\pi^2/h^2 \right)$, changes to an oscillating decrease when $\beta = \pi^2/h^2$. Solving for h with $a = 2.4$ gives $h = 0.93$, which agrees with the observed $h \approx 1.0$.

When $g(x)$ in (5) is algebraic and $g(z)$ has no singularities inside the rectangle with corners at $\pm z_0$, $\pm |z_0|$, where $z_0 = i\pi/(bh)$ and $\operatorname{Re} (b) > 0$, the error E tends to be dominated by the saddle point contribution. This contribution is approximately $|\exp (bz_0^2)|$ in the sense that $\exp \left(-\pi^2/h^2 \right)$ approximates the approximation (7). When the rectangle contains singularities, their contributions dominate. For the example (6), $z_0 = i\pi/h$ and the rectangle becomes a square which expands as h decreases. The behavior of E changes when the sides of the square sweep across the branch points.

IV. INTEGRALS WITH BOTH LIMITS FINITE

Consider the integral

$$I = \int_a^b (u - a)^{\alpha-1}(b - u)^{\beta-1} f(u) du, \qquad \alpha, \beta > 0, \tag{9}$$

where $f(u)$ is analytic and $0(1)$, $f(a)$ and $f(b) \neq 0$, and a and b are finite. The transformation

$$u = (be^v + ae^{-v})/(e^v + e^{-v}),$$
$$du/dv = 2(b - a)/(e^v + e^{-v})^2, \tag{10}$$

carries the limits into $v = \pm\infty$. The associated equations

$$u - a = e^v(b - a)/(e^v + e^{-v}),$$
$$b - u = e^{-v}(b - a)/(e^v + e^{-v}),$$

and du/dv show that the dominant factors in the integrand when $v \to +\infty$ and $v \to -\infty$ are $\exp(-2\beta v)$ and $\exp(2\alpha v)$, respectively. One might expect, and it is confirmed by computation, that in a good transformation the final integral should converge at $-\infty$ at nearly the same rate as it does at $+\infty$. Therefore the further change of variable

$$v = c(\beta^{-1}e^x - \alpha^{-1}e^{-x})$$
$$dv/dx = c(\beta^{-1}e^x + \alpha^{-1}e^{-x}) \tag{11}$$

is made to equalize the rates of convergence at $x = \pm\infty$. The transformation (11) makes the integrand behave roughly as $\exp[-2c\exp|x|]$ as $x \to \pm\infty$ when the effect of $f(u)$ is ignored.

The constant c in (11) can be chosen somewhat arbitrarily. It is helpful, but not necessary, to have

$$c \leqq \pi(\beta\alpha)^{\frac{1}{2}}/4. \tag{12}$$

The inequality (12) for c guarantees that the singularities in the complex x-plane due to the vanishing of $e^v + e^{-v}$ are at least $\pi/2$ distant from the real x-axis. It says nothing about the singularities and saddle points introduced by $f(u)$.

Thus the integral to be evaluated by the trapezoidal rule is

$$I = \int_{-\infty}^{\infty} (u - a)^{\alpha-1}(b - u)^{\beta-1} f(u) \frac{du}{dv} \frac{dv}{dx} dx \tag{13}$$

which can also be written as

$$I = 2(b - a)^{\alpha+\beta-1} \int_{-\infty}^{\infty} \frac{e^{(\alpha-\beta)v}}{(e^v + e^{-v})^{\alpha+\beta}} f(u) \frac{dv}{dx} dx.$$

Here x is the variable of integration and, in writing the program, u, v, du/dv, and dv/dx are given by (10) and (11).

As an example of (9) and (13), consider the beta function

$$I = \int_0^{\pi/2} [\sin u]^{\alpha-1} \left[\sin\left(\frac{\pi}{2} - u\right) \right]^{\beta-1} du$$

$$= \int_{-\infty}^{\infty} [\sin u]^{\alpha-1} \left[\sin\left(\frac{\pi}{2} - u\right) \right]^{\beta-1} \frac{du}{dv} \frac{dv}{dx} dx$$

$$= \pi c \int_{-\infty}^{\infty} [\sin u]^{\alpha-1} \left[\sin\left(\frac{\pi}{2} - u\right) \right]^{\beta-1} \left[\frac{\beta^{-1}e^x + \alpha^{-1}e^{-x}}{(e^v + e^{-v})^2} \right] dx$$

where the third line is to be evaluated by the trapezoidal rule. For $\alpha = 0.95$ and $\beta = 0.05$, the value of I is known to be $20.748\,732 \cdots$ and the inequality (12) for the multiplier c gives $c \leqq 0.171$.

Computations show that the values 0.171, 0.1, and 0.05 for c all give six-figure accuracy with $h = 0.5$ and about 20 terms in the trapezoidal sum (e.g., for $c = 0.1$, $h = 0.5$, and 21 terms, the computed value is 20.748 729). When $c = 1$, about 70 terms (with $h = 0.075$) are required to achieve the same accuracy.

Instead of computing the $\alpha - 1$ power of simply $[\sin u]$, it was found better to compute the $\alpha - 1$ power of $[(e^v + e^{-v})^2 \sin u]$, and similarly for $\sin \left(\dfrac{\pi}{2} - u \right)$. In general, it is usually helpful to combine as much as possible of the $1/(e^v + e^{-v})^2$ contained in du/dv with other factors in the integrand in order to avoid underflow and overflow.

When $\alpha = \beta = 1$, the transformations (10) and (11) reduce to the ones used by Schwartz[2] except for the coefficient $c \leqq \pi/4 = 0.785$. To illustrate this case take (Kajfez[10])

$$ I = (-\pi/40) \int_{10}^{15} \exp(u/4) \sin[0.4\pi \exp(u/4)] du $$

in which the integrand oscillates through about 6 cycles. Using (10) and (11) with $a = 10$, $b = 15$, $c = 0.785$ shows that the trapezoidal rule with $h = 0.09$ and 60 terms gives $I = -0.0195495$ compared with the true value $-0.0195488 \cdots$. For relative errors less than about 0.01, the trapezoidal rule requires less terms than the spline quadrature methods considered in Ref. 10, but this is offset somewhat by the more complicated terms introduced by (10) and (11).

V. INTEGRALS WITH LIMITS 0, ∞ CONTAINING $u^{\alpha-1}(1 + u)^{-\alpha-\beta}$

The integral

$$ I = \int_0^\infty u^{\alpha-1}(1 + u)^{-\alpha-\beta} f(u)du, \qquad \alpha, \beta > 0, \tag{14} $$

where $f(0) \neq 0$ and $f(u)$ is analytic and $0(1)$, can be handled by the transformations

$$ u = e^v, \qquad v = c(\beta^{-1}e^z - \alpha^{-1}e^{-z}) \tag{15} $$

where $c \leqq \pi(\alpha\beta)^{\frac{1}{2}}/2$. For $\alpha = 3$, $\beta = 2$ the inequality for c becomes $c \leqq 3.85$, and for $\alpha = 0.2$, $\beta = 0.1$ it becomes $c \leqq 0.222$. Computations were made for these values of α and β with $f(u) = 1$. Values of h and the number of terms N in the trapezoidal sum required for seven-

figure accuracy were found to be as follows:

α	β	c	h	N
3.0	2.0	3.85	0.25	15
		2.00	0.35	15
		5.00	0.10	40
0.2	0.1	0.22	0.45	25
		0.08	0.45	25
		0.45	0.25	35

VI. INTEGRALS WITH LIMITS 0, ∞ CONTAINING $u^{\alpha-1} \exp(-u)$

For the integrals

$$I = \int_0^\infty u^{\alpha-1} e^{-u} f(u) du, \qquad \alpha > 0, \tag{16}$$

where $f(0) \neq 0$ and $f(u)$ is analytic and $0(1)$, we can use

$$u = e^v, \qquad v = x - \alpha^{-1}e^{-x}. \tag{17}$$

Computations for the case $f(u) = 1$ and $\alpha = 1$ gave the following results:

h	$N =$ No. of terms	Trap. values of I
0.4	15	0.9999 9997
0.6	10	0.9999 8711
0.8	7	0.9998 2442

Repeating the computations with $u = c \exp [x - c \exp(-x)]$ and $c = 0.5$, 2.0, and 4.0 showed that the magnitude of the error depends only slightly on c.

VII. INTEGRANDS WHICH CHANGE RAPIDLY NEAR A POINT

When the integrand contains a factor, say $F(t)$ where t is the variable of integration, which changes rapidly near a point it is sometimes helpful to change to a new variable of integration u where $du/dt = F(t)$ and the constant of integration is chosen at our convenience. The success of the transformation depends upon the ease of inverting to get t as an easily computed function of u.

As an example, consider

$$I = \int_{-1}^1 e^t(t^2 + a^2)^{-\frac{1}{2}}dt \tag{18}$$

where a is small (Smith and Lyness[11]). Taking $du/dt = F(t) = (t^2 + a^2)^{-\frac{1}{2}}$, $u = \operatorname{arcsinh}(t/a)$, and $t = a \sinh u$ carries (18) into an

integral of the form (9) with $b = -a = A$ and $\alpha = \beta = 1$:

$$I = \int_{-A}^{A} e^t du = \int_{-\infty}^{\infty} e^t \frac{du}{dv} \frac{dv}{dx} dx$$

$$= 4Ac \int_{-\infty}^{\infty} e^t(e^x + e^{-x})dx/(e^v + e^{-v})^2.$$

Here $A = \text{arcsinh }(1/a)$, $t = a \sinh (A \tanh v)$, $v = 2c \sinh x$, and $c \leq \pi/4 = 0.785$. Computations with $c = 0.3$, $h = 0.2$, and 40 terms in the trapezoidal sum show that $I = 29.538\,618 \pm 10^{-6}$ when $a = 10^{-6}$.

If the rapidly changing factor has the more general form

$$F(t) = (t^2 + a^2)^{-\theta},$$

the transformation $t = a \sinh u$ can still be used to carry the integral into the form (9), but computation shows that the trapezoidal rule requires more terms as θ moves away from $\frac{1}{2}$. For example, when the exponent $-\frac{1}{2}$ in (18) is replaced by $-\frac{3}{4}$, i.e., $\theta = \frac{3}{4}$, computations with $a = 10^{-6}$, $c = 0.785$, and $h = 0.03$ show that 100 terms give the value 5240.808 for I whereas the true value is $5240.806 \cdots$.

VIII. THE FERMI-DIRAC INTEGRAL

The Fermi-Dirac integral (tabulated by Blakemore[12])

$$I = \frac{1}{\Gamma(\alpha)} \int_0^{\infty} t^{\alpha-1} dt/(1 + e^{t-a}), \qquad \alpha > 0, \tag{19}$$

has an integrand which changes rapidly near $t = a$ when a is large. Section VII suggests taking $du/dt = F(t) = 1/(1 + e^{t-a})$. Choosing the constant of integration to make $u = 0$ at $t = 0$ gives

$$u = \ln(1 + e^{-a}) - \ln(e^{-t} + e^{-a}),$$
$$t = -\ln(e^{-u} + e^{-u-a} - e^{-a}), \tag{20}$$
$$I = \frac{1}{\Gamma(\alpha)} \int_0^b t^{\alpha-1} du,$$

where $b = \ln(1 + e^a)$. When u tends to 0, $t \to (1 + e^{-a})u$, and hence the integral (20) is of the form (9) with $\beta = 1$.

The transformations (10) and (11) carry I into

$$I = \frac{1}{\Gamma(\alpha)} \int_{-\infty}^{\infty} t^{\alpha-1} \frac{du}{dv} \frac{dv}{dx} dx$$

$$= \frac{2bc}{\Gamma(\alpha)} \int_{-\infty}^{\infty} t^{\alpha-1}(e^x + \alpha^{-1}e^{-x})dx/(e^v + e^{-v})^2 \tag{21}$$

where $c \leqq 0.785\alpha^{\frac{1}{2}}$, t is defined in terms of u by (20), and

$$u = be^v/(e^v + e^{-v}), \qquad v = c(e^x - \alpha^{-1}e^{-x}).$$

The integral (21), with $c = 0.5$, was used to compute I for $\alpha = \frac{1}{2}$ and $\frac{3}{2}$ with a between 0 and 20. Difficulty in computing t for small values of u was avoided by using three terms in the expansion of $\ell n(1 - z)$ when $z = \exp(u - a) - \exp(-a)$ was less than 0.001. The following tabulation shows the results for the typical values $\alpha = \frac{1}{2}$ and $a = 10$.

h	N = No. of terms	Trap. values of I
0.2	34	3.5527 792
0.3	22	792
0.4	17	795
0.5	14	742

The above transformation has been used by W. K. Kent in a study of the charge distribution in a charge coupled device and I am indebted to him for helpful discussions regarding his experience with (21).

IX. INTEGRALS WITH LIMITS 0, ∞ AND OSCILLATING INTEGRANDS

Kluyver's Bessel function (random walk) integral for the probability P that the resultant of the sum of m randomly phased unit vectors in a plane be less than r in length is (Bennett[13], Greenwood and Durand[14])

$$P = \int_0^\infty rJ_1(ru)[J_0(u)]^m du. \qquad (22)$$

This integral is typical of a class of integrals that are difficult to evaluate by any means. They are characterized by rather slow convergence and an integrand which tends to oscillate at a regular rate as $u \to \infty$. In this section we consider the evaluation of such integrals by the trapezoidal rule when the rate of convergence is not too slow.

Some general remarks can be made concerning integrals that behave like (22). In order that

$$I = \int_0^\infty f(u)du$$

may represent the typical integral of this section, $f(u)$ must tend, as $u \to \infty$, to a form that can be written as a steadily decreasing factor times the sum of a finite number of sinusoidal terms whose periods tend to constant values (as $u \to \infty$). Define h_0 to be the shortest constant period (so that the most rapidly oscillating term varies as $\cos[(2\pi u/h_0) + \beta]$). The interval h_0 is related to the sampling theorem

for band-limited functions in that $1/h_0$ plays the role of the "bandwidth" of $f(u)$ at $u = \infty$. Quite often the required accuracy in I can be obtained by using values of h which are close to h_0.

If the integrand is an even function of u, the trapezoidal rule can be applied directly. If the integrand is not even, the integral can be evaluated by setting

$$u = a\ell n(1 + e^{x/a}), \qquad du/dx = e^{x/a}/(1 + e^{x/a}) \qquad (23)$$

and then using the trapezoidal rule. Computations described below show that the choice $a = 1$ works well for (22). More will be said later about the choice of a. The transformation (23) takes advantage of the fact that the trapezoidal error E is often small, or zero, for regularly oscillating integrands. Although many terms may be needed in some cases, the present method compares favorably with competing ones.

The choice of a in (23) depends upon the behavior of $f(u)$ near $u = 0$. Suppose that $f(u)$ tends to Cu^ν as $u \to 0$. Here C is a constant and $\nu > -1$. After the change of variable (23), the integrand is a function of x which approaches 0 as $\exp\left[(\nu + 1)x/a\right]$ when $x \to -\infty$. When $(\nu + 1)h/a$ is too small, successive terms in the negative x portion of the trapezoidal sum are nearly equal and an unduly large number of terms must be taken to achieve a small truncation error on the left. When $(\nu + 1)h/a$ is too large, the successive terms differ by a large amount and the trapezoidal error E tends to be large. The problem is to choose a value of a which balances these two effects and at the same time allows h to be large. The choice $a = (\nu + 1)h_0$ works well for all of the cases that have been tried.

Some insight regarding a good choice of h for (22) can be obtained as follows. Consider the integral, say K, obtained by replacing $J_1(ru)$ by $J_0(ru)$ in (22) and taking the limits of integration to be $u = \pm\infty$. With the help of the asymptotic expression for $J_0(z)$ and the procedure used to deal with (4), it can be shown that when K is evaluated by the trapezoidal rule the error is zero if $h < h_0$ where $h_0 = 2\pi/(r + m)$. Furthermore, when P is transformed by (23) and then evaluated by the trapezoidal rule the error E is relatively small when h is only slightly less than h_0—as might be hoped from the similar behavior of the integrands in P and K as $u \to \infty$. A saddle point analysis of R_+ in (3) leads to the rough estimate

$$|E| \approx 2r^{\frac{1}{2}}(2\pi^2)^{-(m+1)/2} \exp\left[\pi(r + m - 2\pi h^{-1})\right] \qquad (24)$$

for the error in the trapezoidal sum for P when $a = 1$.

In the example (22) the asymptotic expression for the integrand con-

tains the product $\cos\left[ru - (3\pi/4)\right]\cos^m\left[u - (\pi/4)\right]$ which can be written as the sum of $m + 1$ sinusoidal terms. The most rapidly oscillating term is proportional to $\cos\left[(r + m)u - (m + 3)(\pi/4)\right]$ and the quantity $h_0 = 2\pi/(r + m)$ now appears as the shortest period.

Now we turn to the details of the evaluation of the integral (22) for P. Let r and m have the representative values $r = 4$ and $m = 6$. Then $h_0 = 2\pi/(r + m) = 0.628$. Since $J_0(z) \to 1$ and $J_1(z) \to z/2$ as $z \to 0$, the exponent ν is 1. The suggested value $a = (\nu + 1)h_0$ gives $a = 2h_0 = 1.26$, and since the choice of a is not critical, we take $a = 1$. Putting $a = 1$ in (23), substituting in (22), and using the trapezoidal rule gives the values of P shown in column 3:

h	No. of terms	P	Error: Col. 3	$|E|$ from (24)
0.475	286	0.9375 5485		
0.500	272	5475	$-10. \times 10^{-8}$	3.5×10^{-8}
0.525	259	5437	-4.8×10^{-7}	2.8×10^{-7}
0.550	247	5354	-1.3×10^{-6}	1.3×10^{-6}
0.575	236	5791	$+3.1 \times 10^{-6}$	6.9×10^{-6}
0.600	226	0.9375 9798	$+4.3 \times 10^{-5}$	2.4×10^{-5}
0.625	217	0.9376 9974	$+1.4 \times 10^{-4}$	0.94×10^{-4}

The fourth column gives the error estimated from column 3. The fifth column shows the approximation (24) for $|E|$. The trapezoidal sum was truncated at $x = 124$. Beyond 124 the absolute value of the integrand remains less than 2×10^{-8} and its amplitude decreases as $x^{-7/2}$. Note that the error starts to be appreciable as h approaches the critical value $h_0 = 2\pi/(r + m) = 0.628$.

X. THE INTEGRAL OF $u^k \exp(-u^2 - au^{-1})$ FROM 0 TO ∞

The integral

$$I_k(a) = \int_0^\infty u^k \exp(-u^2 - au^{-1})du, \qquad \text{Re } (a) \geq 0, \qquad (25)$$

is of interest in some physical problems (I wish to thank J. N. Lyness for calling my attention to this example). First let k be 0 and a be positive real. We seek a change of variable from u to x, with new limits $x = \pm\infty$, which will make u^2 tend to $\exp(2x)$ as $x \to \infty$ and a/u tend to $\exp(-2x)$ as $x \to -\infty$. This leads to

$$u = ae^x/(a + e^{-x}). \qquad (26)$$

Substituting (26) in (25), taking the special case $k = 0$, $a = 1$, and applying the trapezoidal rule gives the values of $I_o(1)$ shown in column 3:

h	No. of terms	$I_o(1)$	Obs. error	$|E|$ from (27)
0.1	38	0.1500 4597	2×10^{-8}	
0.2	19	0.1500 4597	2×10^{-8}	5×10^{-9}
0.3	12	0.1500 4835	2.40×10^{-6}	7×10^{-6}
0.4	10	0.1501 2711	8.12×10^{-5}	20×10^{-5}

The last column lists a rough approximation obtained by saddle point analysis:

$$|E| \approx \exp\left[-\frac{\pi^2}{2h} + \left(\frac{2\pi}{h}\right)^{\frac{1}{2}} \right]. \tag{27}$$

The observed error shown in column 4 is the trapezoidal sum (column 3) minus the value 0.1500 4595 of $I_o(1)$ computed from

$$I_k(a) = \frac{1}{4\pi i} \int_{c-i\infty}^{c+i\infty} \Gamma(-s)\Gamma\left(\frac{k-s+1}{2}\right) a^s ds$$

$$= \sum_{n=0}^{k} \frac{(-a)^n}{2(n!)} \Gamma\left(\frac{k-n+1}{2}\right) + \sum_{n=1}^{\infty} \frac{\pi}{2} \frac{(-1)^{n+k}a^{2n+k}}{(2n+k)!\Gamma(n+\frac{1}{2})}$$

$$+ \sum_{n=0}^{\infty} \frac{[\ln(a) - \psi(2n+k+2) - \frac{1}{2}\psi(n+1)]}{n!(2n+k+1)!} (-1)^{n+k}a^{2n+k+1}$$

where $c < \min(0, k+1)$, $\psi(x) = (d\Gamma(x)/dx)/\Gamma(x)$, and the series holds for $k = -1, 0, 1, 2, 3, \cdots$ except that the first sum is omitted when $k = -1$.

When a is complex, say $a = \rho e^{i\alpha}$ where $|\alpha| \leq \pi/2$, we tilt the path of integration in (25) by setting $u = v e^{i\theta}$ where $|\theta| \leq \pi/4$ and $|\alpha - \theta| < \pi/2$. If we choose θ to be $\alpha/3$, the new integral

$$I_k(\rho e^{i\alpha}) = \exp\left[i(k+1)\alpha/3\right] \int_0^\infty v^k \exp[-(v^2 + \rho v^{-1})e^{i2\alpha/3}]dv \tag{28}$$

can be evaluated by using the substitution (26) with u and a replaced by v and ρ, and then applying the trapezoidal rule. For the physically important case of $k = 3$ and imaginary a [$I_3(i\rho)$ and $I_k(a)$, $k = 1, 2, 3$, are tabulated in NBS Handbook,[15] Section 27.5], the error can be kept below 1×10^{-6} for $a = i0.001$ by using $h = 0.04$ and 95 terms in the trapezoidal sum. As a increases to $i10.0$, h can increase to 0.08 and the required number of terms decrease to 40.

APPENDIX

Examples of Paths of Steepest Descent for R_+

For the example (6), the integral (3) for R_+ becomes

$$R_+ = \int_{-\infty}^{\infty} \exp\left[\varphi(z)\right]dz, \tag{29}$$

$$\varphi(z) = -z^2 + i2\pi h^{-1}z - \tfrac{1}{2}\ell n(z^4 + a^4). \tag{30}$$

The saddle point equation $d\varphi(z)/dz \equiv \varphi'(z) = 0$ is of the 5th degree in z. Solving by Newton's rule or otherwise gives 5 saddle points, 3 of which are in the half-plane Im $(z) > 0$. They are shown as small circles in Fig. 1 for the case $a = 2.4$ and $h = 0.8$. One is on the imaginary z-axis at $z_0 = i4.14$, and the other two (z_{1s}, z_{2s}) are at $\pm 1.648 + i1.629$ near the branch points (z_1, z_2) at $a(\pm 1 + i)/2^{\frac{1}{2}} = 1.697(\pm 1 + i)$.

The path of steepest descent through the saddle point z_0 (a path on which Im $\left[\varphi(z) - \varphi(z_0)\right] = 0$) was computed by: (*i*) evaluating the phase of the coefficient $\left[-2\pi/\varphi''(z_0)\right]^{\frac{1}{2}}$ in the saddle point contribution

$$\int \exp[\varphi(z)]dz \sim \left[-2\pi/\varphi''(z_0)\right]^{\frac{1}{2}} \exp\left[\varphi(z_0)\right] \tag{31}$$

to determine the direction of the path through z_0; (*ii*) selecting two starting points (one for each branch of the path) on opposite sides of, but close to, z_0; and (*iii*) applying

$$z_\ell = z_{\ell-1} + d_{\ell-1}, \qquad d_\ell = -\left|\varphi'(z_\ell)\right|\Delta/\varphi'(z\ell)$$

to compute the path step by step, Δ being the step length. The other paths of steepest descent shown in Fig. 1 were computed in the same way. Paths of steepest descent through a saddle point may run down into a "lower" saddle point, i.e., one having a more negative Re $\varphi(z)$, or may end at a point (possibly $z = \infty$) where Re $\varphi(z) = -\infty$.

Figure 1 shows that the path of integration for R_+ can be deformed in a natural way into three portions: the loop around z_2 (which encloses the branch cut from z_2), the path from $-\infty + i\pi h^{-1}$ through z_0 to $+\infty + i\pi h^{-1}$, and lastly the loop around z_1. The path directions are denoted by arrows.

As h increases (from 0.8), z_0 in Fig. 1 moves downward towards the origin. Eventually h reaches a critical value at which the path of steepest descent from z_0 runs directly into z_{1s} and z_{2s}. For still larger values of h, the loops around z_1 and z_2 lie above the path through z_0, and the deformed path of integration for R_+ consists only of the path running from $-\infty + i\pi h^{-1}$ to $+\infty + i\pi h^{-1}$ through z_0. The sudden

change in the path as h passes through the critical value is related to Stokes phenomena in the theory of asymptotic expansions.

The approximation (7) for the contribution of z_0 to $E \sim 2\,\mathrm{Re}\,(R_+)$ can be obtained by approximating the saddle point equation $\varphi'(z) = 0$ by $\varphi_A'(z) = 0$ where

$$\varphi_A(z) = -z^2 + i2\pi h^{-1}z \tag{32}$$

is the most important part of the expression (30) for $\varphi(z)$ near $z = z_0$. The equation $\varphi_A'(z) = 0$ gives the approximation $z_A = i\pi/h$ for z_0. Substituting $\varphi_A''(z_A) = -2$ and $\varphi(z_A)$ from (30) in place of $\varphi''(z_0)$ and $\varphi(z_0)$, respectively, in the saddle point contribution (31) to R_+ leads to (7).

Figure 2 shows the paths of steepest descent and the path of integration used to estimate E for the integral (25), $I_o(1)$, when $h = 0.2$. For $k = 0$ and $a = 1$, the $\varphi(z)$ in the integral (29) for R_+ is

$$\varphi(z) = -u^2 - u^{-1} + i2\pi zh^{-1} + \ell n\left[\frac{e^{2z}(e^z + 2)}{(e^z + 1)^2}\right] \tag{33}$$

where u is given by (26) with z in place of x. The deformed path of integration for R_+ shown in Fig. 2 contains the arbitrary bridging segment AB and shows that the saddle points z_1 and z_3 are the main contributors to R_+.
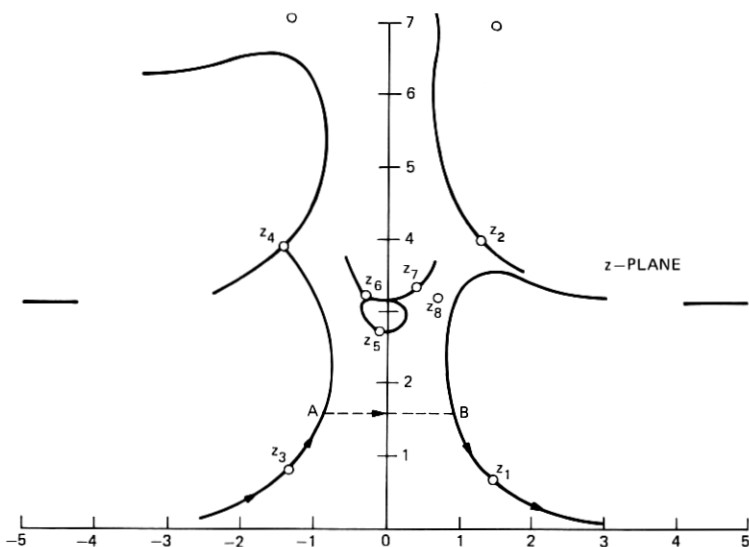

Fig. 2—Steepest descent paths for $\exp\left[\varphi(z)\right]$ when $h = 0.2$ in (33). The arrows mark a deformed path of integration for R_+ corresponding to $I_o(1)$ in (25). The points $z_1, z_2, \cdots, z_8$ are saddle points.

Finally, if one wishes to integrate along a path of steepest descent, a combination of the above path computation and the trapezoidal rule with spacing Δ suggests itself. However, greater accuracy can be achieved by either (*i*) first computing the entire path, approximating it by several straight-line segments (sometimes one will do), and using Romberg integration on each segment, or (*ii*) taking the step size Δ relatively large in the path computation, and then using Romberg integration over each linear segment of length Δ (by dividing d_l into lengths of, say, $\Delta/8$).

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