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Note

Numerical Evaluation of a Class of Integrals by Integrating along a String of Saddle Points*

1. INTRODUCTION

This note is concerned with the numerical integration of a class of slowly convergent integrals of the form

$$F(y) = \int_{-\infty}^{\infty} e^{-iuy+\phi(u)}\, du, \tag{1}$$

where y is large and positive. As stated in Section 2, the function $\phi(u)$ must be analytic and such that $\phi'(u) = iA(iu)^{-\nu} e^{iu}[1 + o(1)]$ as $u \to -i\infty$ where the numerical values of A and ν are known. Although these conditions restrict the method to a narrow class of integrals, such integrals do occur in a variety of technical problems [1–4]. For instance, in the phase modulation example discussed in Section 8, $\phi(u)$ is $(b \sin u)/u$, or in noise problems, $\phi(u)$ may be a combination of exponential and Bessel functions. It should be noted that a separate calculation is required for each value of y.

A number of methods have been proposed for dealing with (1). The Fast Fourier Transform works well if the convergence is not too slow or $F(y)$ not too small. Integration formulas of Filon's type can sometime be used (see [5, Sect. 2.10], where several methods of integrating rapidly oscillating functions are discussed). Other methods deal with the slow convergence by inserting convergence factors or by subtracting known integrals that converge at the same rate as (1).

When y is large and positive, as will be assumed throughout this paper, it is often desirable to deform the path of integration in (1) so as to take advantage of the fact that $\exp(-iuy)$ becomes small when $\mathrm{Im}(u) \to -\infty$. When $\phi(u)$ is such that it can be done, a simple procedure is to tilt the positive and negative u portions of the path so that they remain straight lines along which $\mathrm{Im}(u) \to -\infty$. The variable of integration can then be changed so as to take advantage of the exponential decrease of $\exp(-iuy)$ [6, Sect. 6]. Unfortunately when $\phi(u)$ is of the type of interest here, the integrals taken along the tilted straight lines do not converge. However, by curving the path as discussed in Section 2 we can often get the integrand to decrease as $O(|u|^{-\nu y})$ where ν is a positive parameter appearing in the asymptotic expansion of $\phi(u)$.

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The curved path of integration runs close to a string of saddle points of $\exp[-iuy + \phi(u)]$. These saddle points are discussed in Sections 3 and 4 and their properties are used to obtain an estimate of the truncation error in Section 5. The path of integration described in Section 2 can be improved by making it pass close to saddle points near near $u = 0$. This is studied in Section 6. Some remarks are made in Section 7 about choosing a step size for the numerical integration and the example $\phi(u) = (b \sin u)/u$ is discussed in Sections 8 and 9.

2. Conditions Satisfied by $\phi(u)$ and the New Path of Integration

We assume that $\phi(u)$ is such that (i)

$$d\phi(u)/du = iA(iu)^{-\nu} e^{iu}[1 + o(1)], \qquad \nu > 0 \tag{2}$$

as $u \to -i\infty$, and (ii) $\phi(u)$ is analytic in a region such that the path of integration in (1) can be deformed into the curve

$$u = x - i \ln(y/|A|) - \tfrac{1}{2}i\nu \ln(1 + x^2), \tag{3}$$

where x is real and runs from $-\infty$ to $+\infty$. To make condition (i) precise, we take $\arg(iu)$ to be zero on the negative imaginary u-axis, and assume that there is a non-negative number a such that the term $o(1)$ in (2) tends to zero uniformly with respect to $\mathrm{Re}(u)$ as $\mathrm{Im}(u) \to -\infty$ in the region $|\mathrm{Re}(u)| \geqslant a$.

Curve (3) is the result of a search for a path of integration that passes close to the saddle points of the integrand $\exp[-iuy + \phi(u)]$ when $|u|$ is large. It is shown in the next section that (3) does indeed do this. Since saddle points are not singularities, there is no difficulty in deforming the original path, the real u-axis, into curve (3). Changing the variable of integration in (1) from u to x and using Jordan's lemma carries (1) into

$$F(y) = \int_{-\infty}^{\infty} e^{-iuy + \phi(u)} \left(1 - \frac{i\nu x}{1 + x^2}\right) dx, \tag{4}$$

in which u is regarded as a function of x defined by (3). Integral (4) is suited to machine calculation because u can be obtained readily from (3). The calculations show that (4) converges faster than (1), and that the larger y is, the more rapid is the convergence.

The number of points required in the numerical evaluation can be reduced by modifying (4) as discussed in Section 6. However, this improvement requires a study of the saddle points near $u = 0$.

3. The Saddle Points

The saddle points of $\exp[-iuy + \phi(u)]$ are defined as the zeros of the derivative of the exponent; i.e., as the roots of

$$0 = -iy + d\phi(u)/du. \tag{5}$$

When u lies in the region where (2) holds, the saddle point equation becomes

$$0 = -y + A(iu)^{-\nu} e^{iu}[1 + o(1)]. \tag{6}$$

An equation satisfied by the kth saddle point, u_k, when $|u_k|$ is large, can be obtained by solving (6) for e^{iu}, using $\exp(iu) = \exp(iu - i2\pi k)$, $A = |A| \exp(i \arg A)$, and taking logarithms:

$$u_k = 2\pi k - \arg A + \nu(\tfrac{1}{2}\pi + \arg u_k) - i \ln(y/|A|) - i\nu \ln |u_k| + o(1). \tag{7}$$

Equation (7) shows that $|\mathrm{Re}(u_k)|$ increases linearly and $|\mathrm{Im}(u_k)|$ increases logarithmically as $|k|$ tends to ∞.

It is convenient to associate the value

$$x_k = 2\pi k - \arg A \pm \tfrac{1}{2}\pi\nu \tag{8}$$

of x with u_k. The $+$ sign is used when $k > 0$ and the $-$ sign when $k < 0$. This is suggested when we compare (7) and (8) and note that $\arg u_k \to 0$ as $k \to \infty$ and $\arg u_k \to -\pi$ as $k \to -\infty$. With the help of (8) we can rewrite (7) as

$$u_k = x_k - i \ln(y/|A|) - i\nu \ln |x_k| + o(1), \tag{9}$$

where $o(1) \to 0$ as $|x_k| \to \infty$.

The value of u on curve (3) corresponding to $x = x_k$ differs by $o(1)$ from u_k given by (9). Therefore u_k lies close to curve (3) when $|k|$ is large.

4. Contribution of the kth Saddle Point

The integrand in (4) oscillates as $|x|$ increases. Its peak values can be estimated if, in addition to condition (2), $\phi(u)$ also satisfies

$$\phi(u) = A(iu)^{-\nu} e^{iu}[1 + o(1)] + o(1) \tag{10}$$

on (3) as $|x| \to \infty$. Far out on (3) the largest values of the integrand occur near the saddle points. At u_k the saddle point equation (6) shows that

$$A(iu_k)^{-\nu} \exp(iu_k) = y[1 + o(1)]. \tag{11}$$

Therefore when u is at x_k on curve (3) we have

$$\begin{aligned}\exp[-iuy+\phi(u)] &= \exp[-iu_k y+\phi(u_k)+o(1)]\\ &= \exp[-iu_k y+y(1+o(1))+o(1)]\\ &= \left(\frac{|A|\,e}{y}\right)^y \frac{\exp[-iyx_k+o(1)]}{|x_k|^{\nu y}},\end{aligned} \tag{12}$$

where (10) and (11) have been used in going from the first to the second line, and (9) has been used in going to the third line.

Consequently the integrand in (4) decreases as $O(|x|^{-\nu y})$ when $|x|\to\infty$. Even when (10) is not satisfied the rate of decrease may be rapid. For example, if $\phi(u)$ is such that the rightmost $o(1)$ in (10) is replaced by $-C(iu)^{1/2}$, where $C>0$ the integrand will decrease as $O[|x|^{-\nu y}\exp(-C\,|x/2|^{1/2})]$.

The contribution of the region around u_k to the value of the integral (4) is approximately equal to the leading term in the classical saddle point expansion. This leading term is $[-2\pi/\phi''(u_k)]^{1/2}$ times expression (12). Taking the logarithmic derivative of (2) and assuming $d\,o(1)/du=o(1)$ leads to

$$\phi''(u_k)=-y+o(1). \tag{13}$$

Using this and Stirling's approximation for $\Gamma(1+y)$ shows that the contribution is approximately

$$\frac{2\pi}{\Gamma(1+y)}\,|A|^y\,|x_k|^{-\nu y}\exp[-iyx_k+o(1)]. \tag{14}$$

This expression can also be obtained by considering the integral taken along the path of steepest descent through u_k.

5. The Truncation Error

Let $F(y; x_{\min}, x_{\max})$ be the value of integral (4) when it is truncated at $x=x_{\min}$ on the left and at $x=x_{\max}$ on the right. Let $x_{l'}\leqslant x_{\min}<x_{l'+1}$ define the integer l' (large and negative), where $x_{l'}$ is given by (8). Similarly, let $x_{l-1}<x_{\max}\leqslant x_l$ define the integer l.

Then an estimate of the truncation error

$$E_t=F(y)-F(y; x_{\min}, x_{\max})$$

can be obtained by adding the contributions (14) of the appropriate saddle points:

$$E_t\approx\frac{2\pi\,|A|^y}{\Gamma(1+y)}\left(\sum_{k=-\infty}^{l'}+\sum_{k=l}^{\infty}\right)\frac{\exp[-iyx_k+o(1)]}{|x_k|^{\nu y}}. \tag{15}$$

The terms in (15) can add in any phase, depending on y and x_k. In the worst case they will add in phase and, for $\nu y > 1$ and large l' and l,

$$|E_t| \approx \frac{|A|^y}{\Gamma(1+y)} \frac{1}{\nu y - 1} (|x_l|^{1-\nu y} + |x_{l'}|^{1-\nu y}). \tag{16}$$

This is a rough upper bound for the truncation error.

6. Improving the Path of Integration

The path of integration (3) is a special case ($B = 1$, $C = 0$) of the path

$$u = x - i\ln[y/|A|] - \tfrac{1}{2}i\nu\ln[B + (x-C)^2] \tag{17}$$

where B and C are real and $B > 0$. Changing the variable of integration in (1) from u to x by using (17) gives the generalization

$$F(y) = \int_{-\infty}^{\infty} e^{-iuy+\phi(u)} \left[1 - \frac{i\nu(x-C)}{B+(x-C)^2}\right] dx \tag{18}$$

of (4). When B and C are chosen so that the path (17) passes closer to the important saddle points near $u = 0$ than does (3), the points used in the numerical integration can usually be spaced farther apart. However, the truncation error remains about the same because the two curves approach each other when $|x| \to \infty$.

The determination of the saddle points requires the solution of the saddle point equation (5) which is usually transcendental. Even after a saddle point has been determined, some judgement is required to decide whether or not is is "important." A straightforward but laborious decision procedure would be, first to determine all of the saddle points and the paths of steepest descent from them (see the Appendix of Ref. [6]); then to deform the path of integration in (1), the real u-axis, into a path consisting of paths of steepest descent. A saddle point is not "important" if the deformed path does not pass through it. Fortunately we can often guess from its location whether or not it is important.

When the saddle points are symmetrically located with respect to the imaginary u-axis we can take $C = 0$. If, in addition, an important saddle, point, say $u_0 = iv_0$, lies on the imaginary axis, putting $x = 0$ in (17) and solving for B gives

$$B = (|A|\, y^{-1} e^{-v_0})^{2/\nu}. \tag{19}$$

7. Choosing the Step Size for Numerical Integration

The integrals (4) and (18) are both well suited to numerical integration by the trapezoidal rule. One of the factors that determine the step size $h = \Delta x$ is the value of h suited to integration near the saddle points far out on the tails. Experience indicates that a satisfactory first trial value of h for numerical integration over a saddle point u_k is

$$h = [2/|\phi''(u_k)|]^{1/2}. \tag{20}$$

When u_k is large we have $\phi''(u_k) \approx -y$ from (13). This suggests that in the evaluation of (18) we first try

$$h = [2/y]^{1/2}, \tag{21}$$

then try successively smaller values of h until the desired accuracy is attained. We might expect the initial value of h to work better for (18) than for (4) because its path passes closer to the saddle points.

8. Example – Phase Modulation Integral

As an example consider the integral

$$G(y) = \int_{-\infty}^{\infty} e^{-iuy}[e^{(b \sin u)/u} - 1]\, du \tag{22}$$

which occurs in phase modulation problems [2]. When $y > 1$ the path of integration can be deformed into (3) or (17) and the -1 within the brackets can be omitted. Then $G(y)$ is given by either integral (4) or integral (18) with

$$\phi(u) = bu^{-1} \sin u. \tag{23}$$

As $\operatorname{Im}(u) \to -\infty$,

$$(d/du)\,\phi(u) = i(b/2)(iu)^{-1}\, e^{iu}(1 + o(1)) \tag{24}$$

and comparison with (2) gives

$$\begin{aligned} A &= b/2, \\ v &= 1. \end{aligned} \tag{25}$$

For our example, (4) becomes

$$\begin{aligned} G(y) &= \int_{-\infty}^{\infty} \exp[-iuy + bu^{-1} \sin u] \left(1 - \frac{ix}{1 + x^2}\right) dx, \qquad y > 1, \\ u &= x - i \ln(2y/|b|) - (i/2) \ln(1 + x^2). \end{aligned} \tag{26}$$

When we apply the trapezoidal rule to (26) for the case $y = 5$, $b = 5$ with truncation at $x_{\min} = -50$, $x_{\max} = 50$, we obtain the results shown in the left-hand portion of the table below. Here $h = \Delta x$ is the spacing, N is the number of points used, $N = 2x_{\max} + 1$, and $\tilde{G}(y; x_{\min}, x_{\max}, h)$ is the value given by the trapezoidal rule. Actually when b is real only half as many points are needed because of the symmetry of the integrand. Since $\phi(u)$ satisfies (10), (16) gives the rough upper bound

$$\frac{|b/2|^y}{\Gamma(1+y)} \frac{2}{y-1} |x_{\max}|^{1-y}, \qquad y > 1, \tag{27}$$

for the error due to truncation at $x = \pm x_{\max}$.

Before we can use (18) we have to choose values of B and C that will make the path (17) pass through, or close to, the important saddle points near $u = 0$. From (5) the saddle points are the roots of

$$iy = bu^{-1} \cos u - bu^{-2} \sin u. \tag{28}$$

When b is real, the saddle points are located symmetrically with respect to imaginary u-axis so that we can take $C = 0$. Furthermore, an important saddle point, say, u_0, lies on the negative imaginary axis at $u = -i2.03$ when $y = 5$ and $b = 5$. In this case we can use (19) and get $B = 14.5$. Putting $B = 14.5$ and $C = 0$ in (18) (with $v = 1$ and $\phi(u) = (b \sin u)/u$) and using the trapezoidal rule gives the values shown on the right hand side of the table. The "exact" $G(5)$ is the value of $\tilde{G}(5, -200, 200, 0.35)$.

h	N	$\tilde{G}(5; -50, 50, h)$ $b = 5$, $B = 1$ from (26)	h	N	$\tilde{G}(5; -50, 50, h)$ $b = 5$, $B = 14.5$ from (18)
1.0	101	5.63648 8274	1.0	101	0.48151 0140
0.50	201	0.59944 4300	0.75	135	0.47241 6228
0.25	401	0.47182 4812	0.50	201	0.47181 9965
0.125	801	0.47181 9239	0.35	287	0.47181 9239
Trunc. error			Exact $G(5)$		0.47181 9266
bound (27)		0.00000 0065	Trunc. Error		0.00000 0027

Note that the truncation error bound given by (27), 6.5 (−8), is about 2.4 times as large as the actual truncation error, 2.7 (−8).

Computations for the cases $y = 5$, $b = -5$, and $y = 5$, $b = i5$ give results similar to those shown in the above table for $y = 5$, $b = 5$.

Comparison of the two sides of the table shows that a good choice of B and C produces an appreciable increase in the efficiency of the numerical integration. Whether one should use (4) or (18) appears to depend on whether the cost of the extra points needed by (4) outweights the labor of determining the saddle points needed by (18).

6. Integration Along the Real u-Axis

It is interesting to compare integration along the string of saddle points, which is suited to large values of y, to integration along the real u-axis, which is suited to small values of y.

Before we can use our example (22) for the comparison, we must deal with its slow convergence along the real axis. We shall use a common subtraction method and rewrite (22) as

$$G(y)=\int_{-\infty}^{\infty} e^{-iuy}\left\{e^{\phi(u)}-1-\sum_{k=1}^{K}\frac{1}{k!}[\phi(u)]^k\right\}du+\sum_{k=1}^{K}\frac{\Phi_k(y)}{k!}, \tag{29}$$

where $\Phi_k(y)$ is the Fourier transform of the kth power of $\phi(u)$. When $\phi(u)=(b\sin u)/u$ and K is chosen to make $K\leqslant|y|$, all of the terms in the last series in (29) vanish. Furthermore, the integrand ultimately decreases as $O(1/|u|^{K+1})$.

When we put $\phi(u)=(b\sin u)/u$ in (29), set $y=5$, $b=5$, $K=5$ and make several trial integrations with the trapezoidal rule we get (with $h=\Delta u=0.25$ and truncation at $x=\pm 60$) $G(5)$ to nine significant figures. As it should be, this value of $G(5)$ is equal to $\tilde{G}(5,-200,200,0.35)$, the "exact" $G(5)$ stated in Section 8 and obtained by integration (18).

For the case $y=10$, $b=5$, and $K=10$, single precision numerical integration of (29) gave only three significant figures of $G(10)$ because of large cancellation errors. On the other hand, integration of (18) with $C=0$ and $B=19.1$ corresponding to the saddle point $u_0=-i2.86$ gave nine significant figures ($G(10)=0.13339\,4446(-5)$, with $h=\Delta x=0.25$ and truncation at $x=\pm 15$).

This suggests that when $b=5$ in our example, a good place to switch from (29) to (18), i.e., from integration along the real u-axis to integration along the string of saddle points, is around $y=5$ or 6.

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