

Movable Singularities and Quadrature*

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Abstract. A general procedure is described for treating a movable singularity in an integral. This enables us to change the original integral I_0 into GI_1 , where G depends only on the parameters of the singularity and I_1 is a new integral which exists for all values of the parameters. The results are then applied to the particular problem of evaluating

$$\int_{-1}^1 \frac{f(x) dx}{\{(1-x^2)(1-k^2x^2)\}^{1/2}},$$

where f is entire and k varies between 0 and 1. Some new quadrature schemes and new effective methods of evaluating incomplete elliptic integrals are derived.

1. Introduction. In obtaining numerical solutions to certain three-dimensional diffraction problems, we found it necessary to evaluate integrals of the form

$$(1.1) \quad I(k) = \int_{-1}^1 \frac{f(x) dx}{\{(1-x^2)(1-k^2x^2)\}^{1/2}}, \quad 0 \leq k < 1.$$

The result $I(k)$ was to be subsequently integrated with respect to the parameter k , say,

$$(1.2) \quad J = \int_{\Omega} I(k)g(k) dk, \quad \Omega \subseteq [-1, 1].$$

To perform the second quadrature in the cases in which Ω includes the point $k = 1$, it is necessary to explicitly exhibit the logarithmic singularity of $I(k)$ as $k \rightarrow 1$.

For the particular form (1.1), this is readily done by noting that the transformation

$$x = \text{sn}(u); \quad u(x) = \int_0^x \frac{dt}{\{(1-t^2)(1-k^2t^2)\}^{1/2}},$$

where $\text{sn}(u)$ is the Jacobi elliptic function leads to

$$(1.3) \quad I(k) = \int_{-K(k)}^{K(k)} f(\text{sn } u) du,$$

where $K(k) = u(1)$ is the elliptic integral of the first kind. In fact, on putting $u = K(k)t$, we have

$$(1.4) \quad I(k) = K(k) \int_{-1}^1 f(\text{sn } Kt) dt.$$

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This form (1.4) then explicitly manifests the singular function $K(k)$ as a multiplicative factor, so that a logarithmic weight quadrature scheme can be used to evaluate (1.2).

At this point, we were faced with the problem of evaluating the Jacobi elliptic functions for the modulus k near 1, or, alternately, finding another scheme for treating the singularity in (1.1). This problem has led us to study more general cases of the same type as (1.1).

At the outset, in Section 2, we derive a simple error bound of quadrature which serves both as an intuitive guideline for obtaining the transformation, and as a tool by which we can quantitatively determine the effectiveness of a transformation.

In Section 3, we give a general transformation of the integral. The transformation of the independent variable is defined as an integral (see (3.6)). In this form, it is possible to deduce various properties of the transformation, although it is not generally possible to express the transformation or its inverse explicitly, both of which are eminently desirable in practice. It is expected, however, that in a number of instances in applications, it is worthwhile to compute the transformation and its inverse by a brute force technique. Whenever possible, we have tried to keep the proofs of Section 3 constructive.

The authors felt Section 3 to be important to numerical analysts, since this section exploits the connection between the region of analyticity of an integral and the rate of convergence of numerical quadrature, and, furthermore, this section leaves the numerical analyst with an intuitive approach towards choosing an effective transformation of the integral. In addition, he sees that transformations of the integral which remove the dominant effect of singularities exist in great profusion.

A byproduct of the analysis of Section 3 is an explanation of why the classical WKB method is effective in the asymptotic solution of differential equations [16].

The reader who is interested only in the integral (1.1) may skip Section 3 and proceed directly to Section 4. Here he finds various effective methods of evaluating (1.1), some new quadrature schemes, and some effective methods for evaluating elliptic integrals, together with error bounds.

2. An Error Bound. Let $E_n(g)$ be the error of a quadrature scheme, i.e.

$$(2.1) \quad E_n(g) = \int_{-1}^1 w(x)g(x) dx - \sum_{j=1}^n w_jg(x_j),$$

where $w(x)$ is integrable over $(-1, 1)$, the w_j are weights, and the x_j are points on the closed interval $[-1, 1]$, such that $E_n(g) = 0$ whenever g is a polynomial of degree p . Let $g(z)$ be holomorphic in the ellipse \mathcal{E}_ρ (of complex numbers $z = x + iy$) with foci at $z = \pm 1$ and sum of semiaxes equal to ρ , and let $g(x)$ be real. Define

$$(2.2) \quad A = \int_{-1}^1 |w(x)| dx, \quad B = \sum_{j=1}^n |w_j|,$$

$$M(\rho) = \sup_{z \in \mathcal{E}_\rho} |\operatorname{Re} g(z)|.$$

Then we have

THEOREM 2.1.

$$(2.3) \quad |E_n(g)| < \frac{8(A + B)}{\pi} \frac{M(\rho)}{\rho^{p+1}}.$$

Proof. The proof depends on a result of Achieser (see e.g. [17, p. 87], or [18, p. 309]). It is similar to the proof of Theorem 4 in [3] and is omitted here.

The bound in (2.3) is minimized with respect to p by the Gaussian quadrature scheme, and is, in fact,

$$(2.4) \quad E_n(g) < \frac{16\mu_0}{\pi} \frac{M(\rho)}{\rho^{2n}}; \quad \mu_0 = \int_{-1}^1 w(x) dx.$$

We have assumed in (2.4) that $w(x) > 0$ in $(-1, 1)$.

We remark that if $g(x)$ in (2.1) is not real when x is real the term ρ^{p+1} in (2.3) is replaced by $(\rho - 1)\rho^p$. This is readily verified by expanding $g(x)$ in a series of Chebyshev polynomials (see Barnhill [19] for the details).

3. The General Transformation. Let c be a vector in a domain C of complex numbers in a finite-dimensional space. Let $a = (a_1, a_2, \dots, a_m)$ be fixed real numbers and let x_1, x_2, \dots, x_m be m complex numbers which may depend upon c . Let us define

$$(3.1) \quad F(a, x) = r(x) \prod_{i=1}^m (x - x_i)^{a_i},$$

where $r(x)$ is an entire function. We shall assume that $x - x_i \neq 0$ for all $(x, c) \in (-1, 1) \times C$, and that the integral

$$(3.2) \quad \int_{-1}^1 F(a, x) dx$$

exists and is finite for all $c \in C$.

We consider evaluating the integral

$$(3.3) \quad \int_{-1}^1 F(a, x)f(x) dx,$$

where, for simplification of the developments of this section, we shall assume that $f(x)$ is an entire function.**

Quadrature schemes that are exact for polynomials of degree p are most extensively tabulated. Also inspection of (2.3) tells us that the larger the region in which g is analytic, the more rapidly the error of quadrature approaches zero as $p \rightarrow \infty$. In what follows, we shall, therefore, attempt to construct a transformation which reduces (3.3) to an integral of the form (2.1), and for which the resulting function $g(x)$ is analytic in as large a domain as possible. Best results would be achieved in this respect by choosing

$$w(x) = F(a, x)$$

as a weight function and constructing a set of quadrature formulas with respect to this weight function. We could achieve this by constructing quadrature formulas for certain fixed values of the parameters and then obtaining formulas for intermediate values of the parameters by use of polynomial interpolation. While this procedure may be worthwhile, particularly in the case when it is necessary to evaluate (3.3) for

**In practice, the functions $f(x)$ and $r(x)$ may have singularities in the finite plane, provided that these are far from the region of integration relative to those displayed in (3.1).

a large number of different functions f , in the present paper we study the use of a transformation, which we now describe.

Let \mathcal{P}_x be a path in the complex x -plane such that the segment of \mathcal{P}_x joining -1 and 1 is a straight line such that the integral

$$(3.4) \quad \int_{-1}^x F(a, t) dt,$$

taken along \mathcal{P}_x , exists for each x on \mathcal{P}_x , and such that the points x_0, x_1, \dots, x_r are on \mathcal{P}_x , where $x_0 = 1$. Let $w(y)$ be a function defined for complex y and independent of c such that $w(y) > 0$ if $-1 < y < 1$. Here $w(y)$ is any suitable weight function chosen by the user. Let \mathcal{P}_y be a path in the complex y plane such that the segment of \mathcal{P}_y joining -1 and 1 is a straight line and such that the $r + 1$ distinct points $\{y_i\}_{i=0}^r$ with $y_0 = 1$ are on \mathcal{P}_y . Let $\{h_j(y)\}_{j=0}^r$ be a set of functions such that $h_0(t) = 1$, such that $h_j(y)$ is real when y is real, such that each integral

$$(3.5) \quad H_{ij} = \int_{-1}^{y_{i-1}} w(t)h_{j-1}(t) dt, \quad (i, j = 1, 2, \dots, r + 1)$$

taken along \mathcal{P}_y exists, and such that the square matrix $[H_{ij}]$ of order $r + 1$ is non-singular for all $c \in \bar{C}$, the closure of C , where H_{ij} is the (i, j) th element of $[H_{ij}]$.

Note that \mathcal{P}_x and \mathcal{P}_y may depend continuously upon $c \in \bar{C}$, provided that the above conditions are satisfied.

Let us put

$$(3.6) \quad \int_{-1}^x F(a, t) dt = \int_{-1}^y G(e, t) dt,$$

$$G(e, y) = \left(e_0 + \sum_{j=1}^r e_j h_j(y) \right) w(y).$$

In this equation the constants e_j on the right are determined such that $y = y_j$ when $x = x_j, j = 0, 1, \dots, r$. This may be explicitly carried out as follows. Let \mathbf{x} denote the vector of order $r + 1$ with j th element equal to the left of (3.6) when x is replaced by x_{j-1} , and set*** $e = (e_0, \dots, e_r)^T$. Then, since $[H_{ij}]$ is nonsingular, the solution of $[H_{ij}]e = \mathbf{x}$ uniquely determines e for all $c \in C$.

THEOREM 3.1. *Let $x = x(y)$ be determined by (3.6) as described above. This transformation reduces the integral (3.3) to the integral*

$$(3.7) \quad I_0 = \int_{-1}^1 \left(e + \sum_{j=1}^r e_j h_j(y) \right) w(y) f(x(y)) dy.$$

Proof. The proof follows by direct substitution of (3.6) into (3.3).

The constants e_j in general depend on the parameters a_j . Hence, if $r > 0$, (3.7) offers no advantage over (3.3), if we attempt to evaluate (3.7) using

$$\left(e_0 + \sum_{j=1}^r e_j h_j(y) \right) w(y)$$

*** v^t denotes the transpose of the vector v .

as a weight function. We may, however, have gained over (3.3), if we either

- (i) replace (3.7) by $r + 1$ new integrals choosing $h_{j-1}(y)w(y)$ as a weight function in the j th. or
- (ii) choose $w(y)$ as a weight function to evaluate (3.7).

In order to minimize the bound (2.3), it is preferable in each of these cases that $x(y)$ be an analytic function in as large a region as possible. In the cases (ii) we also want the function $h_j(y)$ to be analytic in as large a region as possible.

Let $\mathcal{E}_\rho^{(x)}$ and $\mathcal{E}_\rho^{(y)}$ be ellipses of complex numbers with foci at ± 1 in the x and y planes respectively, such that for each ellipse the sum of its semiaxes is ρ , and such that $x(y)$ is analytic for $y \in \mathcal{E}_\rho^{(y)}$. Let $w = F(y)$ be a conformal map of $\mathcal{E}_\rho^{(y)}$ onto $|w| < 1$, such that $F(-1) = 0$. If we suppose that $x(y) \in \mathcal{E}_\rho^{(x)}$ whenever $y \in \mathcal{E}_\rho^{(y)}$, Schwarz's Lemma (see e.g. [4]), applied to the function $G(F(y)) = F(x(y))$, yields $|G(F(y))| \leq |F(y)|$ for all $y \in \mathcal{E}_\rho^{(y)}$. Since, moreover, $g(F(1)) = F(1)$ Schwarz's Lemma yields $G(F(y)) \equiv F(y)$, from which $x(y) \equiv y$.

We have thus proved the following negative result:

LEMMA 3.2. *Let $x(y)$ be analytic in $\mathcal{E}_\rho^{(y)}$. Unless $x(y) \equiv y$, there exist points $y \in \mathcal{E}_\rho^{(y)}$, such that $x(y) \notin \mathcal{E}_\rho^{(x)}$.*

Hence, if $x(y) \not\equiv y$, then, given any positive number B , there exist entire functions $f(t)$, such that

$$\sup_{y \in \mathcal{E}_\rho^{(y)}} |f(y)| = B, \quad \text{while} \quad \sup_{y \in \mathcal{E}_\rho^{(y)}} |f(x(y))| > B.$$

We have considerable freedom of choice in picking the weight function $w(t)$. In practice, we would be apt to pick a weight function for which quadrature formulas are extensively tabulated. On the other hand, since the bound (2.3) can in general be made smaller when $x(y)$ is analytic in a larger domain, picking a weight function $w(t)$, for which quadrature formulas are tabulated, does not always yield the most rapidly converging quadrature scheme.

By Lemma 3.2, the bound (2.3), applied to (3.7), in either case (i) or case (ii) above is in general minimal when $x(y) \equiv y$. Since the construction of high degree Gaussian quadrature formulas is no longer a formidable task (5), it is worthwhile to keep in mind the following result, the proof of which illustrates a construction of $x(y)$:

THEOREM 3.3. *Corresponding to any positive number ϵ , any compact subset U of the parameter domain C can be covered by a finite number of N neighborhoods U_j , $j = 1, 2, \dots, N$, such that for $c \in U_j$ there exists a function $w(t)$ and a set of functions $h_j(t)$ with the property that, if $x(y)$ is defined by (3.6), then $|x(y) - y| < \epsilon$, $-1 \leq y \leq 1$.*

Proof. The following proof of this theorem illustrates a construction of $w(t)$ for the transformation (3.6). Let c^0 be a point of S and let $\delta > 0$. Define U_j by

$$(3.8) \quad U_j = \left\{ c \in C : \sum_{j=1}^m |c_j - c_j^0|^2 < \delta \right\}.$$

Putting

$$(3.9) \quad w(t) = F_0(a, t) = F(a, t)_{c=c^0},$$

we choose e_0, e_1, \dots, e_r ($r \leq m$) in (3.6), such that

$$(3.10) \quad \begin{aligned} y &= 1, & \text{when } x &= 1, \\ y &= y_i(c_0), & \text{when } x &= x_i, \quad i = 1, 2, \dots, r. \end{aligned}$$

Here we assume that $r \geq 0$ is taken sufficiently small such that only integrable singularities are included on each side of (3.10) and such that in (3.6) $y = x_i(c_0)$ is a singularity of the same type as $x = x_i$. By our hypotheses on the independence of $h_j(t)$, the conditions (3.10) uniquely determine $e_j, j = 0, 1, \dots, r$ as continuous functions of c . When $c = c_0$, we have $e_0 = 1$ and $e_j = 0, j = 1, 2, \dots, r$. Consequently, if δ is chosen sufficiently small, e_j can be made to differ by as little as we please from its value when $c = c_0$. Hence, if δ is sufficiently small the assertion of Theorem 2.2 follows for $c \in U_j$. That U can be covered by a finite number of the U_j is a consequence of the compactness of U .

COROLLARY 3.4. *If the integral on the left of (2.9) becomes unbounded as c approaches certain boundary points of C then at least one of the e_j on the right of (3.6) becomes unbounded.*

Proof. That at least one of the e_j 's must become unbounded follows from the fact that

$$\int_{-1}^1 h_j(t)w(t) dt$$

exists for all $j = 0, 1, \dots, r$ and for all $c \in \bar{C}$.

We conclude this section with some additional remarks concerning the transformation (3.6).

Remarks. 1. The resulting transformation is often analytic in a larger domain if the b_i are chosen such that $-1 < b_i$. This choice can always be made by use of the following identity:

$$(3.11) \quad \frac{f(x)}{(1 - ux)^\omega} = \sum_{k=0}^{\mu-1} \frac{f^{(k)}(1/u)}{k!(-u)^\omega} \left(x - \frac{1}{u}\right)^{k-\omega} + \frac{F(x)}{(1 - ux)^{\omega-\mu}},$$

where $\mu = [\omega]$.† Given $f(x)$, (3.11) defines $F(x)$; further, with the exception of $x = 1/u$, the singularities of $F(x)$ are of the same type as those of $f(x)$, and $F(x)$ is holomorphic wherever $f(x)$ is holomorphic.

2. In the notation of Theorem 2.2 it is often the case that relatively few sets U_j are required to cover U , particularly if instead of “nearness of $x(y)$ to y ” we require “analyticity of $x(y)$ in some domain”. This leads us to the following.

THEOREM 3.5. *Let $x(y)$ be defined by (3.6) and let $r(x) \neq 0$ for all finite complex x . Set $x_{-1} = y_{-1} = -1, x_{m+1} = y_{m+1} = \infty$. Assume that for all $c \in C$*

- (a) $x \rightarrow x_i$ implies $y \rightarrow y_i, i = -1, 0, 1, \dots, m + 1$;
- (b)

$$(3.12) \quad F(a, x) = (x - x_i)^{a_i} g_i(x), \quad i = -1, 0, 1, \dots, m + 1,$$

$$G(e, y) = (y - y_i)^{d_i} h_i(y),$$

where $g_i(x)$ is analytic in a neighborhood of $x_i, g_i(x_i) \neq 0, h_i(y)$ is analytic in a neighborhood of $y_i, h_i(y_i) \neq 0$, and $(d_i + 1)/(a_i + 1)$ is a positive integer;

- (c) F and G have no singularities apart from those displayed in (3.12).

Then $x(y)$ is an entire function.

Proof. Let us examine the equation $dx/dy = G/F$. Under the assumptions of the

† $[\omega]$ is the greatest integer less than or equal to ω .

theorem it follows that dx/dy exists at all points of the complex plane with the exception of the singularities of F and G . Integration of F with respect to x and G with respect to y and inspection of $x(y)$ in a neighborhood of y_i , shows that $x(y)$ is analytic in a neighborhood of y_i .

4. Examples. In this section we illustrate the developments of Sections 2 and 3 with some examples. In Section 4.1 we give two examples illustrating that the theory of Section 3 does in fact include and extend well-known procedures. In Section 4.2 we develop some formulas to evaluate the integral (1.1).

4.1. *Well-Known Examples.* The example

$$(4.1) \quad I = \int_0^1 \frac{f(x)}{\sqrt{x}} dx$$

has been treated by Isaacson and Keller [13], where the singularity is removed by use of the transformation $x = y^2$, or equivalently using our general procedure

$$(4.2) \quad \int_0^x \frac{dt}{\sqrt{t}} = e_0 \int_0^y dt,$$

choosing e_0 such that $y = 1$ for $x = 1$.

We next examine the integral

$$(4.3) \quad I = x \int_0^1 \frac{f(t) dt}{1 - xt}, \quad 0 \leq x < 1.$$

The usual method of subtracting out the singularity in this integral is to write

$$(4.4) \quad I = -f(1/x)\ln(1 - x) + x \int_0^1 \frac{f(t) - f(1/x)}{1 - xt} dt$$

for x near 1. Note that the integrand in the integral on the right is now entire and we may use Legendre-Gauss quadrature to evaluate it. Using an n -point Gaussian formula, we get the error bound

$$(4.5) \quad |E_n(f)| < \frac{16}{\pi} e^{\beta(1/x+1/2)} \left(\frac{e\beta}{8n}\right)^{2n}; \quad f(x) = e^{\beta x}.$$

On the other hand, putting

$$(4.6) \quad x \int_0^t \frac{d\tau}{1 - x\tau} = e_0 \int_0^y d\tau,$$

and choosing e_0 such that $y = 1$ when $t = 1$, we obtain

$$(4.7) \quad t = 1 - (1 - x)^y/x, \quad e_0 = -\ln(1 - x),$$

$$I = -\ln(1 - x) \int_0^1 f\left(\frac{1 - (1 - x)^y}{x}\right) dy.$$

On evaluating

$$(4.4') \quad I_1 = \int_0^1 f\left(\frac{1 - (1 - x)^y}{x}\right) dy$$

by n -point Legendre-Gauss quadrature, we get the error bound

$$(4.8) \quad E_n(f) \leq \frac{16}{\pi} e^{\beta x} \left[\frac{e |\ln(1-x)|}{4 \ln 2nx/\beta} \right]^{2n}, \quad f(x) = e^{\beta x}, \quad \beta > 0.$$

Note that the function $t = t(y)$ defined by (4.7) is an entire function of y . Note also that although the bound on the right of (4.5) approaches zero faster as $n \rightarrow \infty$ than that given by (4.8), the form (4.4') has an advantage over (4.4) in the case when I is part of a repeated integral, and integration with respect to x is also required††, since an effective numerical integration of (4.4) with respect to x requires two different procedures, while the integration of (4.7) requires only one: Gaussian quadrature using $\log(1-x)$ as a weight function.

4.2. The Numerical Evaluation of

$$(4.9) \quad I = \int_{-1}^1 \frac{f(x) dx}{\{(1-x^2)(1-k^2x^2)\}^{1/2}}.$$

In this integral, k is a parameter such that $0 \leq k \leq 1$. We shall assume that $f(x)$ is an entire function, real when x is real.

An effective method of evaluating (4.9) would be of considerable value because of the frequent occurrence of elliptic integrals in practice. The above problem arose in our attempt to evaluate a three-dimensional integral connected with the solution of the reduced wave equation $(\nabla^2 + \lambda^2)u = 0$ in three dimensions (2). In that case, I was an inner integral and k a function of two other variables. As it was necessary to integrate the result also with respect to these other variables, a knowledge of the type of singularity that I has as $k \rightarrow 1$ was important. In evaluating (4.9), we wanted the number of evaluation points to be small, since the evaluation of I was an often used subroutine in a larger program. Also, it was necessary to compute I very accurately—to within 10^{-7} relative error.

In what follows, we illustrate several procedures for evaluating I . Some of these procedures are effective over the whole range of k , while others are effective only over a part of the range $0 \leq k < 1$.

4.3. *A Method for Small and Intermediate k .* We apply Chebyshev quadrature to (4.9) in the form

$$(4.10) \quad I = \frac{\pi}{n} \sum_{j=1}^n F(x_j) + E_n(F), \quad x_j = \cos \left[\frac{(2j-1)\pi}{2n} \right],$$

where

$$(4.11) \quad F(x) = f(x)/(1-k^2x^2)^{1/2}.$$

On applying the error bound of Section 2 with $f(x) = e^{\beta x}$, $\beta > 0$, we get

$$(4.12) \quad |E_n(F)| < \frac{16e^{\beta/2}}{\{1-k^2(4n/\beta)^2\}^{1/2}} \left(\frac{e\beta}{4n} \right)^{2n} \left(\frac{\beta}{4n} > k \right), \quad \text{or} \\ < 16 \left(\frac{2ne}{(1-k^2)^{1/2}} \right)^{1/2} \left[\frac{k}{1+(1-k^2)^{1/2}} \right]^{2n} e^{\beta/k}, \quad 0 < k < 1.$$

††Consider the case when $f(t) = f(t, x)$.

Thus, convergence is quite rapid when k is small. However when k is a function of other variables, and additional integrations are required with respect to these variables, the above method has a disadvantage for k near 1 since it does not display the singularity of I as a function of k .

4.4. *A Method for Large k .* In this section we use the procedure of Section 2 to develop a method suitable for k near 1. The method is, in fact, suitable for all k in the range $0 \leq k < 1$, although the rate of convergence is not as rapid as that of some of the other methods for intermediate and small values of k .

In view of (4.9), we have

$$(4.13) \quad I = \int_0^1 \frac{F(x) dx}{\{(1-x)(1-kx)\}^{1/2}},$$

$$F(x) = \frac{f(x) + f(-x)}{\{(1+x)(1+kx)\}^{1/2}}.$$

Thus, $F(x)$ has a singularity at the point $x = -1$; (since $f(x)$ is assumed to be entire by our assumptions of Section 3) this is the nearest singularity of $F(x)$ to the integration segment $[0, 1]$.

In (4.13) we put

$$(4.14) \quad \int_x^1 \frac{dt}{\{(1-t)(1-kt)\}^{1/2}} = \alpha \int_y^1 \frac{dt}{(1-t)^{1/2}},$$

choosing α so that $x = 0$ when $y = 0$. We then obtain

$$(4.15) \quad \frac{1}{\sqrt{k}} \sinh^{-1} \left(\frac{k(1-x)}{1-k} \right)^{1/2} = \alpha(1-y)^{1/2},$$

$$\alpha = \frac{1}{\sqrt{k}} \sinh^{-1} \left(\frac{k}{1-k} \right)^{1/2} = \frac{1}{\sqrt{k}} \ln \left(\frac{1+\sqrt{k}}{(1-k)^{1/2}} \right),$$

$$x = 1 - (1-k)/k \sinh^2[\alpha(k(1-y))^{1/2}].$$

With this transformation (4.13) becomes

$$(4.16) \quad I = \alpha \int_0^1 \frac{F(x(y))}{(1-y)^{1/2}} dy,$$

here $x(y)$ and α are given by (4.15).

Note that $x(y)$, defined in (4.15), is an entire function of y and also a one-to-one function mapping $0 \leq y \leq 1$ onto $0 \leq x \leq 1$. Hence, the integral on the right of (4.16) exists for all values of k . The dominant portion of the singularity of (4.9) as a function of k is contained in α , this being a particularly desirable feature from the point of view of repeated integration.

The integral on the right of (4.16) can now be evaluated by use of Gaussian quadrature with $1/(1-y)^{1/2}$ as a weight function (see (4.1), (4.2)). Setting

$$(4.17) \quad I = \sum_{j=1}^n w_j F(x(y_j)) + E_n(F),$$

we obtain

$$|E_n(F)| < \frac{64ne^{1+\beta/\pi}}{\alpha\{(1+k)(2-y_0)\}^{1/2}} (y_0 + (y_0^2 - 1)^{1/2})^{-2n},$$

(4.18)

$$y_0 = -1 + 2 \left(\frac{\sinh^{-1}(2k/(1-k))^{1/2}}{\alpha\sqrt{k}} \right)^2,$$

assuming again that $|f(x)| \leq e^{\beta|x|}$. The above bound is obtained again by use of (2.4) and minimization with respect to ρ . The bound on F used is $|F(x)| \leq 2e^{\beta|x|}/(1+x)$, $-1 < x \leq 0$. Under the transformation (4.15) the singularity at $x = -1$ in (4.13) becomes a function of k and approaches the region of integration arbitrarily closely as $k \rightarrow 1$. Consequently, y_0 defined in (4.18) approaches 1 as $k \rightarrow 1$. Note however that $E_n(F) \rightarrow 0$ as $k \rightarrow 1$.

4.5. *A Method for Intermediate and Large k .* Let us make the transformation $x = x(y)$ in (4.9), where $x(y)$ is determined from

$$(4.19) \quad \int_0^x \frac{dt}{\{(1-t^2)(1-k^2t^2)\}^{1/2}} = \int_0^y \frac{(\alpha + \beta t^2) dt}{\{(1-t^2)(1-k_0^2t^2)\}^{1/2}}.$$

In (4.19) k_0 is fixed, and α and β are determined such that

$$(4.20) \quad \begin{aligned} \text{(i)} \quad & y = 1 \quad \text{when } x = 1 \\ \text{(ii)} \quad & y = 1/k_0 \quad \text{when } x = 1/k, \quad 0 < k, k_0 < 1. \end{aligned}$$

We thus attempt to match up the singularities as described in Section 3. Using the notations

$$(4.21) \quad \begin{aligned} F(x, k) &= \int_0^x \frac{dt}{\{(1-t^2)(1-k^2t^2)\}^{1/2}}, \\ E(x, k) &= \int_0^x \left(\frac{1-k^2t^2}{1-t^2} \right)^{1/2} dt, \end{aligned}$$

together with

$$(4.22) \quad \begin{aligned} F(1, k) &= K, & F(1, k_0) &= K_0 \\ E(1, k) &= E, & E(1, k_0) &= E_0 \\ k' &= (1-k^2)^{1/2}, & F(1, k') &= K', & F(1, k'_0) &= K'_0 \\ E(1, k') &= E', & E(1, k'_0) &= E'_0 \\ F(1/k, k) &= K + iK', & E(1/k, k) &= E - i(E' - K'), \end{aligned}$$

we find, on substituting (4.20) into (4.19), that α and β satisfy a simultaneous pair of linear equations whose determinant is

$$(4.23) \quad E_0K'_0 + E'_0K_0 - K'_0K_0 = \pi/2,$$

the Legendre relation. Thus, the conditions (4.20) uniquely determine α and β in (4.19), and we obtain

$$(4.24) \quad F(x, k) = \frac{K}{K_0} F(y, k_0) + \frac{2}{\pi} [K_0 K' - K'_0 K] \left[\frac{E_0}{K_0} F(y, k_0) - E(y, k_0) \right],$$

or

$$(4.24') \quad x = \operatorname{sn} \left\{ \frac{K}{K_0} F(y, k_0) + \frac{2}{\pi} [K_0 K' - K'_0 K] \left[\frac{E_0}{K_0} F(y, k_0) - E(y, k_0) \right] \right\}.$$

The integral (4.9) is thus transformed into the integral

$$(4.25) \quad I = \int_{-1}^1 \frac{(\alpha + \beta y^2) F(x(y))}{\{(1 - y^2)(1 - k_0^2 y^2)\}^{1/2}} dy,$$

where

$$(4.26) \quad \alpha = \frac{K}{K_0} - \frac{2}{\pi} (K_0 K' - K'_0 K) \frac{E_0}{K_0}, \quad \beta = \frac{2k_0^2}{\pi} (K_0 K' - K'_0 K),$$

and where $x(y)$ is given by (4.24').

Let us check whether (4.24') is a one-to-one transformation. To this end we have

LEMMA 4.1. For a given $k_0 \in (0, 1)$, the transformation (4.24) maps $-1 \leq y \leq 1$ onto $-1 \leq x \leq 1$ in a one-to-one manner if and only if k is such that

$$(4.27) \quad \frac{K}{K'} \geq \frac{K'_0 E'_0}{K_0 E_0 - \pi/2}.$$

Proof. It is readily seen by use of (4.19) that (4.24) is one-to-one if and only if $dy/dx > 0$ a.e., which implies that both of the requirements (i) $\alpha \geq 0$ and (ii) $(\alpha + \beta) \geq 0$ are satisfied. For if $\alpha < 0$ we must have $\beta > 0$ in order to meet the first of (4.20); in this case $\alpha + \beta y^2$ has a simple zero in $(-1, 1)$. Similarly, if $\alpha = 0$, then $\beta > 0$. Clearly $\alpha + \beta \geq 0$ implies that $\alpha + \beta y^2 \geq 0$, $-1 \leq y \leq 1$, since††† there is at most one y in $(0, 1)$ such that $\alpha + \beta y^2 = 0$. Consequently, if $\alpha + \beta < 0$ then $\alpha + \beta y^2 < 0$ for $|y|$ ($|y| < 1$) sufficiently near 1. The inequality $\alpha + \beta \geq 0$ yields

$$(4.28) \quad K[E_0 - k_0^2 K'_0] + K'E_0 - (1 - k_0^2)K_0 \geq 0.$$

Since

$$(4.29) \quad E_0 - (1 - k_0^2)K_0 = k_0^2 \int_0^{K_0} \operatorname{cn}^2 u \, du,$$

where $\operatorname{cn} u (= \operatorname{cn}(u, k_0))$ is defined by $\operatorname{cn} u = (1 - \operatorname{sn}^2 u)^{1/2}$, $-K_0 < u \leq K_0$, it follows that $E_0 - (1 - k_0^2)K_0 \geq 0$ (> 0) for all k_0 in $0 \leq k_0 < 1$ ($0 < k_0 < 1$). Similarly, $E'_0 - k_0^2 K'_0 \geq 0$. Therefore, the only condition which may not be satisfied for all k in $0 \leq k < 1$ is the condition $\alpha \geq 0$. Using (4.26) we see that this condition is satisfied for all k such that (4.27) holds.

For example, when $k_0 = 1/\sqrt{2}$ (4.27) holds for all k such that $0.059 \dots \leq k < 1$.

Similarly, we are able to deduce the behavior of $x = x(y)$ defined by (4.24) when

††† I.e., from the above, since $\alpha \leq 0$ and $|x| + |\beta| < 0$.

y is complex by use of formulas in [7, pp. 12–13]. These formulas were used to obtain one of the graphs of Figure 1. Let $k_0 = 1/\sqrt{2}$ and let \mathcal{E}_ρ be defined as in Section 2. Then Figure 1 enables us to obtain for any given k in $0 < k < 1$ the value of ρ with the property that $x(y)$ is bounded if and only if $y \in \mathcal{E}_\rho$. In Section 4.6 we shall describe a method of using this graph for obtaining error bounds.

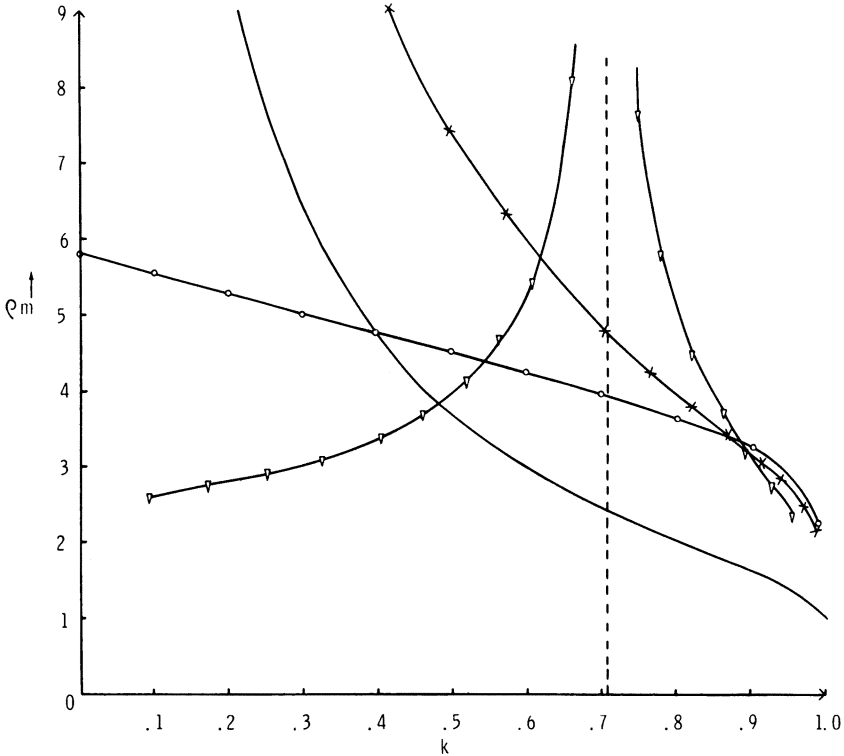


FIGURE 1. In the approximation of $\int_{-1}^1 w(y)F(y) dy$ by $\sum_{j=1}^n w_j F(y_j)$ these graphs show $\rho_m = \max\{\rho: F(y) \text{ is analytic in } \mathcal{E}_\rho\}$ as a function of k . The following notation is used with reference to formulas in Section 3: \cdot (4.10); \circ (4.17); \times (4.33); ∇ (4.39).

Figure 2 is a table of zeros and weights for applying Gaussian quadrature to (4.25), with weight function $1/\{(1 - y^2)(1 - k_0^2 y^2)\}^{1/2}$ and with $k_0 = 1/\sqrt{2}$. Gautschi's method [5] was used to obtain these formulas.

4.6. *A Method for all k.* In this section we describe the transformation

$$(4.30) \quad \int_0^x \frac{dt}{\{(1 - t^2)(1 - k^2 t^2)\}^{1/2}} = \int_0^y \frac{\alpha dt}{(1 - t^2)^{1/2}}$$

choosing α such that $x = 1$ when $y = 1$. We thus obtain $\alpha = 2K/\pi$, and

$$(4.31) \quad x = \operatorname{sn}\left(\frac{2K}{\pi} \sin^{-1} y\right),$$

and (4.9) is transformed into the integral

FIGURE 2

A Tabulation of Zeros and Weights for the formula (4.44).

x_i			w_i		
$n = 2$					
0.7369	21582	63652	1.854	07467	73012
$n = 4$					
0.3954	69781	80571	0.8425	64689	98211
0.9301	23603	28663	1.0115	09987	3191
$n = 6$					
0.2649	51587	16405	0.5451	74977	20330
0.7170	91637	67463	0.6099	34460	36376
0.9680	02002	48077	0.6989	65239	73418
$n = 8$					
0.1986	21001	15531	0.4036	60738	26268
0.5632	97934	36302	0.4324	38866	30620
0.8372	28694	04480	0.4845	76717	20760
0.9817	02539	55180	0.5333	98355	52475
$n = 10$					
0.1587	15892	17121	0.3207	08661	04100
0.4596	28626	03537	0.3357	07997	14341
0.7131	04989	96760	0.3647	39149	50250
0.8944	27331	04644	0.4019	89917	80663
0.9881	69228	53536	0.4309	28951	80771
$n = 32$					
0.0492	92858	71437	0.0986	84761	02046
0.1473	94213	81454	0.0991	54111	01528
0.2440	47560	36271	0.1000	94187	01064
0.3383	04451	55721	0.1015	06874	34035
0.4292	41652	76928	0.1033	92706	97865
0.5159	70971	01291	0.1057	47763	89022
0.5976	48818	41601	0.1085	58977	12039
0.6734	85408	86576	0.1117	97486	80229
0.7427	53450	03188	0.1154	09842	42554
0.8047	96126	79396	0.1193	07377	72279
0.8590	34069	81790	0.1233	55206	02390
0.9049	70875	26986	0.1273	64117	31767
0.9421	96641	28673	0.1310	90854	28518
0.9703	89031	67376	0.1342	53453	52388
0.9893	11727	28378	0.1365	66149	66189
0.9988	10853	58111	0.1377	90808	16210

$$(4.32) \quad I = \frac{2K}{\pi} \int_{-1}^1 \frac{f(\operatorname{sn}((2K/\pi)\sin^{-1}y))}{(1-y^2)^{1/2}} dy.$$

This transformation was used also in [15], although no error bound was given in [15]. We evaluate the integral I by use of n -point Chebyshev quadrature to obtain

$$(4.33) \quad I = \frac{2K}{\pi} \left[\frac{\pi}{n} \sum_{j=1}^n f \left(\operatorname{sn} \frac{(n-2j+1)K}{n} \right) + E_n(f) \right].$$

We illustrate a method of obtaining a bound on $E_n(f)$.

We use the usual notation

$$(4.34) \quad q = e^{-\pi K'/K}$$

for the nome q . The transformation $x = \operatorname{sn}[(2K/\pi)\sin^{-1}y]$ maps the ellipse \mathcal{E}_ρ in the y plane conformally [8] onto the circle $|x| \leq 1/\sqrt{k}$, where $\rho = q^{-1/4}$. Thus by use of (2.4) we have

$$(4.35) \quad |E_n(f)| < 16M^*q^{n/2},$$

where

$$(4.36) \quad M^* = \max_{|x| \leq 1/\sqrt{k}} |\operatorname{Re} f(x)|.$$

Thus, for example, for the case $|f(x)| \leq e^{\alpha|x|}$, x complex and $f(x)$ real when x is real, we have

$$(4.37) \quad |E_n(f)| < 16e^{\alpha/\sqrt{k}}q^{n/2}.$$

Comment. If we note that

$$\operatorname{sn} \left[\frac{2K}{\pi} \sin^{-1}iy \right] = \operatorname{sn} \left[\frac{2iK}{\pi} \ln r \right],$$

where $r = |y| + (|y|^2 + 1)^{1/2}$, y real, then by minimization with respect to r and with $|f(x)| \leq e^{\alpha|x|}$, as above, we get

$$(4.38) \quad |E_n(f)| < 16 \exp \left(\frac{4\pi\alpha n}{kK} \right)^{1/2} q^n,$$

a bound which is usually smaller than (4.37), although not quite as simple to obtain. This observation has the advantage that it may also be used to obtain a bound on the error of the quadrature scheme developed in the previous section. For if (4.25) is evaluated by the formula

$$(4.39) \quad \int_{-1}^1 \frac{(\alpha + \beta y^2)F(x(y)) dy}{\{(1-y^2)(1-k_0^2y^2)\}^{1/2}} = \sum_{j=1}^n w_j(\alpha + \beta y_j^2)F(x(y_j)) + E_n(F),$$

where the w_j and y_j are obtained from Figure 2, we may obtain an estimate of $E_n(F)$ as follows. We first determine ρ from Figure 1 and set $q^* = q(k^*) = 1/\rho^2$. Corresponding to k^* we find $K^* = K(k^*)$ and then minimize

$$\frac{32K_0}{\pi} \left[\alpha + \beta \left(\frac{r-r^{-1}}{2} \right)^2 \right] F^* \left[\frac{2iK^*}{\pi} \ln r \right] r^{-2n}$$

with respect to r ($1 \leq r \leq 1/q^{*1/2}$) to obtain an estimate on the bound of $E_n(F)$, where $F^*[(2iK^*/\pi)\ln r]$ bounds $F[(2K^*/\pi)\sin^{-1}y]$ in the ellipse \mathcal{E}_r ($r = |y| + (1 + |y^2|)^{1/2}$ if y is imaginary).

4.7. *A Method of Computing Elliptic Integrals and Elliptic Functions.* Two disadvantages of the method in Section 3.5 are that it requires the computation of elliptic integrals and the elliptic function sn . The method of Section 3.5 also requires the computation of sn . We suggest computing $\text{sn } u = \text{sn}(u, k)$ by use of the formula (see e.g. [9])

$$(4.40) \quad \text{sn } u = \frac{2}{\sqrt{k}} \frac{\sum_{n=0}^{\infty} (-1)^n q^{(n+1/2)^2} \sin \frac{(2n+1)\pi u}{2K}}{1 + 2\sum_{n=1}^{\infty} q^{n^2} \cos \frac{n\pi u}{2K}},$$

where K can be computed by the method of Section 4.3 for moderate values of k and by the method of Section 3.4 for k near 1. We then use (4.34) to find q and (4.40) to find $\text{sn } u$.

The methods developed in the previous sections also provide effective procedures for computing the elliptic integrals (4.21). Putting $t = ux$ in (4.21), we obtain

$$(4.41) \quad F(x, k) = \int_0^1 \frac{x \, du}{\{(1 - x^2u^2)(1 - k^2x^2u^2)\}^{1/2}}$$

and

$$(4.42) \quad E(x, k) = \int_0^1 \left(\frac{1 - k^2x^2u^2}{1 - x^2u^2} \right)^{1/2} x \, du.$$

We now make the transformation

$$(4.43) \quad \int_0^u \frac{x \, d\tau}{(1 - x^2\tau^2)^{1/2}} = \alpha \int_0^y \frac{d\tau}{(1 - \tau^2)^{1/2}}$$

choosing α so that $u = 1$ when $y = 1$. We then obtain

$$(4.43') \quad u = \frac{1}{x} \sin \left[\frac{2}{\pi} (\sin^{-1}x) \sin^{-1}y \right].$$

This transformation changes (4.41) and (4.42) into the integrals

$$(4.41') \quad F(x, k) = \frac{2}{\pi} \sin^{-1}x \int_0^1 \frac{1}{\left\{ 1 - k^2 \sin^2 \left[\left(\frac{2}{\pi} \sin^{-1}x \right) \sin^{-1}y \right] \right\}^{1/2}} \frac{dy}{(1 - y^2)^{1/2}}$$

and

$$(4.42') \quad E(x, k) = \frac{2}{\pi} \sin^{-1}x \int_0^1 \left[1 - k^2 \sin^2 \left(\frac{2}{\pi} \sin^{-1}x \right) \sin^{-1}y \right]^{1/2} \frac{dy}{(1 - y^2)^{1/2}}$$

respectively.

Both integrals (4.41') and (4.42') are now suitable for Chebyshev quadrature. On noting that each integrand in (4.41') and (4.42') is an even function of y , we may use an even number of evaluation points to obtain

$$(4.44) \quad F(x, k) = \frac{\sin^{-1} x}{n} \sum_{j=1}^n 1/M_j(x, k) + E_n(F)$$

and

$$(4.45) \quad E(x, k) = \frac{\sin^{-1} x}{n} \sum_{j=1}^n M_j(x, k) + E_n(E),$$

where

$$(4.46) \quad M_j(x, k) = \left(1 - k^2 \sin^2 \left[\frac{(2j-1)}{2n} \sin^{-1} x \right] \right)^{1/2}.$$

Proceeding similarly as in Section 3.3, we obtain

$$(4.47) \quad \left(\frac{\sqrt{(1-k^2)}}{4ne} \right)^{1/2} |E_n(F)|, \quad |E_n(E)| \leq 16 \left[\frac{k}{1 + \sqrt{(1-k^2)}} \right]^{4n},$$

bounds which are uniformly valid for all x in $-1 \leq x \leq 1$. For example, when $k = 1/\sqrt{2}$ we have the bounds

n	$E_n(F)$	$E_n(E)$,
5	2.7×10^{-6}	3.5×10^{-7} ,
6	2.6×10^{-8}	1.0×10^{-9} .

We expect that the above method compares favorably with that described in [10] and [14] or that described in [11, pp. 598–599].

The representation (4.40) converges slowly for k near 1. To find a representation of the Jacobi elliptic functions when $k \rightarrow 1$, we observe that $\operatorname{dn}(u) = \{1 - k^2 \operatorname{sn}^2(u)\}^{1/2}$ has the Fourier series representation

$$(4.48) \quad \operatorname{dn}(u) = \frac{\pi}{2K} \sum_{-\infty}^{\infty} \operatorname{sech}(\pi n \alpha) e^{int},$$

where

$$(4.49) \quad \alpha = K'/K, \quad t = u/K.$$

Let $F(t)$ be a continuous periodic function of period 2π with the representation

$$(4.50) \quad F(t) = \sum_{-\infty}^{\infty} f(t + 2\pi n),$$

where $\int_{-\infty}^{\infty} |f(t)| dt < \infty$. Then

$$(4.51) \quad \hat{f}(w) = \frac{1}{2\pi} \int_{-\infty}^{\infty} f(t) e^{-iwt} dt$$

is an interpolation of the Fourier coefficients of $F(t)$, i.e.

$$(4.52) \quad \hat{f}(n) = \frac{1}{2\pi} \int_{-\pi}^{\pi} F(t) e^{-int} dt.$$

Conversely, if $F(t)$ is a continuous periodic function of period 2π which satisfies $\int_{-\pi}^{\pi} |F(t)| dt < \infty$, and if $\hat{f}(w)$ is a function such that $\int_{-\infty}^{\infty} |\hat{f}(w)| dw < \infty$ and such that $\hat{f}(n)$ satisfies (4.52), then $F(t)$ is represented by (4.50), where

$$(4.53) \quad f(t) = \int_{-\infty}^{\infty} \hat{f}(w)e^{iwt} dw.$$

Upon setting $\operatorname{dn}(u) = F(t)$, then $\hat{f}(n) = (\pi/2K)\operatorname{sech}(n\pi\alpha)$, so that

$$(4.54) \quad \hat{f}(w) = \frac{\pi}{2K} \operatorname{sech}(w\pi\alpha)$$

is certainly an interpolation of the Fourier coefficients of $\operatorname{dn}(u)$. Upon applying the inverse Fourier transform (4.53), we get

$$(4.55) \quad f(t) = \frac{\pi}{2K'} \cdot \operatorname{sech}\left(\frac{t}{\alpha}\right).$$

This then yields the representation

$$(4.56) \quad \operatorname{dn}(u) = \frac{\pi}{2K'} \sum_{-\infty}^{\infty} \operatorname{sech}\left[\frac{1}{K'}(u + 2nK)\right],$$

which converges very rapidly when K is large, i.e., when k is near 1.

The above method of obtaining (4.56) from (4.48) is believed to be new. Note that if $|u| \leq 1$ then

$$(4.57) \quad \left| \operatorname{dn}(u) - \frac{\pi}{2K'} \sum_{-m}^m \operatorname{sech}\left[\frac{1}{K'}(u + 2nK)\right] \right| \leq \frac{\pi}{K'} (1 - e^{-2K/K'})^{-1} e^{-2(m+1)K/K'}.$$

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