FINAL REPORT NGR 15-005-039

Work under this grant has resulted in the following papers which are currently in the process of publication:

Sent previously

[1] W. Gautschi and B. J. Klein, Recursive computation of certain derivatives - a study of error propagation, submitted to Comm. ACM.

[2] " and ", Remark on Algorithm 282, to appear in Comm. ACM.

[3] W. Gautschi, Efficient computation of the complex error function, to appear in SIAM J. Mathem. Anal.

[4] ", Algorithm-Complex error function, to appear in Comm. ACM.

In addition, R. V. M. Zahar, who received support from this grant, has completed the following thesis:

[5] R. V. M. Zahar, Computational algorithms for linear difference equation, Purdue University Ph.D. thesis, January, 1968.

Completion of a second Ph.D. thesis (by B. J. Klein) is pending.

Walter Gautschi
Computer Sciences Department
Purdue University
Lafayette, Indiana 47907

July 25, 1969

ALGORITHM...

COMPLEX ERROR FUNCTION*

Walter Gautschi (Recd.

Computer Sciences Department, Purdue University, Lafayette, Indiana 47907

*Work supported, in part, by the National Aeronautics and Space Administration (NASA) under grant NGR 15-005-039 and, in part, by Argonne National Laboratory.

KEY WORDS AND PHRASES: error function for complex argument, Voigt function, Laplace continued fraction, Gauss-Hermite quadrature, recursive computation

CR CATEGORIES: 5.12

```
procedure  wofz(x,y,re,im); value x,y; real x,y,re,im;
comment  This procedure evaluates the real and imaginary part of the function
   w(z) = exp(-z^2)erfc(-iz) for arguments z = x+iy in the first quadrant of
   the complex plane.  The accuracy is 10 decimal places after the decimal
   point, or better.  For the underlying analysis, see W. Gautschi, "Efficient
   computation of the complex error function," submitted to (to appear in) SIAM J. Math.
   Anal.;
begin integer  capn, nu, n, npl; real h, h2, lambda, r1, r2, s, s1, s2, t1,
   t2, c; Boolean b;
   if y < 4.29 ∧ x < 5.33 then
   begin
      s := (1-y/4.29) × sqrt(1-x × x/28.41);
      h := 1.6 × s; h2 := 2 × h;
      capn := 6 + 23 × s; nu := 9 + 21 × s
   end else begin h := 0; capn := 0; nu := 8 end;
   if h > 0 then lambda := h2 ↑ capn;
```

```
    b := h = 0 ∨ lambda = 0;
    r1 := r2 := s1 := s2 := 0;
    for n := nu step -1 until 0 do
    begin
      np1 := n+1;
      t1 := y+h+np1 × r1; t2 := x-np1 × r2; c := .5/(t1 × t1 + t2 × t2);
      r1 := c × t1; r2 := c × t2;
      if h > 0 ∧ n ≤ capn then
      begin
        t1 := lambda + s1; s1 := r1 × t1 - r2 × s2; s2 := r2 × t1 + r1 × s2;
        lambda := lambda/h2
      end
    end;
    re := if y = 0 then exp(-x × x) else
            1.12837916709551 × (if b then r1 else s1);
    im := 1.12837916709551 × (if b then r2 else s2)
  end wofz
```

NGR-15-005-039

MANUSCRIPT DOCUMENTATION SHEET

Title: Efficient computation of the complex error function

Author: Walter Gautschi, Department of Computer Sciences, Purdue University, Lafayette, Indiana 47907

Abstract: The paper is concerned with the computation of $w(z) = \exp(-z^2)\operatorname{erfc}(-iz)$ for complex $z = x+iy$ in the first quadrant Q_1: $x \geq 0$, $y \geq 0$. Using Stieltjes' theory of continued fractions it is first observed that the Laplace continued fraction for $w(z)$, although divergent on the real line, represents $w(z)$ asymptotically for large z in the sector S: $-\pi/4 < \arg z < 5\pi/4$. Specifically, the n-th convergent approximates $w(z)$ to within an error of $O(z^{-2n-1})$ as $z \to \infty$ in S. A recursive procedure is then developed which permits evaluating $w(z)$ to a prescribed accuracy for any $z \in Q_1$. The procedure has the property that as $|z|$ becomes sufficiently large, it automatically reduces to the evaluation of the Laplace continued fraction, or, equivalently, to Gauss-Hermite quadrature of $(i/\pi)\int_{-\infty}^{\infty} \exp(-t^2)\,dt/(z-t)$.

Key words and key phrases: error function for complex argument, Voigt function, Laplace continued fraction, Gauss-Hermite quadrature, recursive computation

EFFICIENT COMPUTATION OF THE COMPLEX ERROR FUNCTION*

By Walter Gautschi[1]

Introduction. The error function of a complex variable, in more or less disguised forms, occurs in many branches of science and technology. Properties of this function, and computational methods, have been studied extensively. A useful survey, as of 1966, may be found in [1], and more recent work in [2], [11], [14]. In many applications the function must be evaluated a large number of times. It is therefore important to search for methods which are as efficient as possible. Current practice attempts to achieve the desired economy by adopting different methods in different regions of the complex plane. In this paper, instead, we propose a single algorithm which is uniformly effective for all complex arguments. A corresponding ALGOL procedure is to appear in [8].

In section 1 we review some relevant mathematical properties of the complex error function. Although much of this material is known, a few remarks are made which do not seem to be common knowledge. Among these is the observation that a certain continued fraction, known as the Laplace continued fraction, while divergent on the real line, approximates the error function asymptotically in the sense of Poincaré. The computational algorithm is developed in section 2. Basically, it consists of evaluating a truncated Taylor expansion. The increment, h, as well as the number of terms, N, are made to depend on the argument z at which the function is evaluated. As $|z|$ increases, h and N decrease, until eventually both

*Work supported, in part, by the National Aeronautics and Space Administration (NASA) under grant NGR 15-005-039 and, in part, by Argonne National Laboratory.

[1]Department of Computer Sciences, Purdue University, Lafayette, Indiana 47907.

become zero, at which time the algorithm reduces to that of evaluating the Laplace continued fraction. Some performance characteristics, and data on testing the algorithm, are included in section 3.

1. Mathematical preliminaries. The function

$$w(z) = e^{-z^2} \operatorname{erfc}(-iz), \tag{1.1}$$

where $\operatorname{erfc} \zeta = (2/\sqrt{\pi}) \int_{\zeta}^{\infty} e^{-t^2}\, dt$ denotes the complementary error function, was first introduced (and tabulated) by Faddeeva and Terent'ev [4]. As a function of the complex variable z, w(z) represents an entire function, and has the property that both its real and imaginary parts are between zero and one for z in the first quadrant of the complex plane. This property may well have been one of the motivations for considering (1.1) as the basic form of the error function for complex argument.

Closely related to (1.1) is the integral

$$f(z) = \int_{-\infty}^{\infty} \frac{e^{-t^2}}{z-t}\, dt. \tag{1.2}$$

We have in fact

$$w(z) = \begin{cases} \frac{i}{\pi} f(z) & (\operatorname{Im} z > 0) \\ \frac{i}{\pi} f(z) + 2e^{-z^2} & (\operatorname{Im} z < 0). \end{cases} \tag{1.3}$$

While w(z) is an entire function, f(z) is analytic for all z not on the real line, and represents two analytic functions, one in the upper, another

in the lower half-plane, neither of which is the analytic continuation of the other. For real z, the integral in (1.2) is meaningful only in the sense of a Cauchy principal value integral.

We note that (1.2) is a special case of a Stieltjes transform $\int_{-\infty}^{\infty} d\alpha(t)/(z-t)$. Most of the properties to be described below follow from Stieltjes' classical theory [12], [10] concerning integrals of this type, and are therefore applicable in other situations as well (e.g., in the computation of the complex exponential integral).

Expanding the integrand in (1.2) in descending powers of z, and integrating term by term, one obtains the asymptotic expansion

$$f(z) \sim \sum_{s=0}^{\infty} \frac{\mu_s}{z^{s+1}} \qquad (z \to \infty \text{ in } |\operatorname{Im} z| \geq a, \quad a > 0 \text{ arbitrary}), \tag{1.4}$$

where

$$\mu_s = \int_{-\infty}^{\infty} t^s e^{-t^2} dt = \begin{cases} 0 & (s \text{ odd}), \\ \Gamma((s+1)/2) & (s \text{ even}) \end{cases} \tag{1.5}$$

are the moments of e^{-t^2}. Since e^{-z^2} has the zero asymptotic expansion in $-\pi/4 < \arg z < 5\pi/4$ and $3\pi/4 < \arg z < 5\pi/4$, it is not surprising, in view of (1.3), that

$$w(z) \sim \frac{i}{\pi} \sum_{s=0}^{\infty} \frac{\mu_s}{z^{s+1}} \qquad (z \to \infty \text{ in } -\pi/4 < \arg z < 5\pi/4). \tag{1.6}$$

With the (formal) expansion (1.4) is associated the continued fraction

$$\frac{\mu_0}{z-} \; \frac{1/2}{z-} \; \frac{1}{z-} \; \frac{3/2}{z-} \; \cdots, \tag{1.7}$$

known as the Laplace continued fraction. More precisely, (1.7) is associated with (1.4) in the following sense. Let

$$(1.8)\qquad \frac{\mu_o}{z-}\ \frac{1/2}{z-}\ \frac{1}{z-}\ \frac{3/2}{z-}\ \cdots\ \frac{(n-1)/2}{z} = \frac{q_n(z)}{p_n(z)}$$

denote the n-th convergent of the continued fraction (1.7). It is easily verified that $q_n(z)$ is a polynomial of degree n-1, while $p_n(z)$ is a monic polynomial of degree n. Then the quotient in (1.8), if expanded in descending powers of z,

$$(1.9)\qquad \frac{q_n(z)}{p_n(z)} = \sum_{s=o}^{\infty} \frac{\nu_s^{(n)}}{z^{s+1}}\ ,$$

yields a power series which agrees with that in (1.4) up to and including the term with z^{-2n}, i.e.

$$(1.10)\qquad \nu_s^{(n)} = \mu_s \qquad \text{for} \qquad s = 0,1,2,\ldots,2n-1.$$

It is also known [13] that the continued fraction (1.7) in fact converges to f(z) for every nonreal z.

Another remarkable connection of the continued fraction (1.7) with the integral in (1.2) is obtained if the rational function (1.8) is decomposed into partial fractions,

$$(1.11)\qquad \frac{q_n(z)}{p_n(z)} = \sum_{k=1}^{n} \frac{\lambda_k^{(n)}}{z - t_k^{(n)}}\ .$$

Expanding both sides of this equation in descending powers of z, and comparing coefficients of like powers, one finds that

$$\nu_s^{(n)} = \sum_{k=1}^{n} \lambda_k^{(n)} [t_k^{(n)}]^s \qquad (s = 0,1,2,\ldots).$$

In view of (1.10) it follows that

$$\mu_s = \sum_{k=1}^{n} \lambda_k^{(n)} [t_k^{(n)}]^s \qquad \text{for} \qquad s = 0,1,2,\ldots,2n-1,$$

which, on account of (1.5), implies that $\lambda_k^{(n)}$ and $t_k^{(n)}$ are the weights and nodes, respectively, of n-point Gauss-Hermite quadrature. Consequently,

$$\lim_{n\to\infty} \sum_{k=1}^{n} \frac{\lambda_k^{(n)}}{z-t_k^{(n)}} = \int_{-\infty}^{\infty} \frac{e^{-t^2}}{z-t}\, dt \qquad (\text{Im } z \neq 0), \tag{1.12}$$

i.e., Gauss-Hermite quadrature, applied to the integral in (1.2), converges for every z not on the real line.

Using the well-known remainder term of Gauss-Hermite quadrature it also follows that

$$\mu_{2n} - \nu_{2n}^{(n)} = \int_{-\infty}^{\infty} t^{2n} e^{-t^2}\, dt - \sum_{k=1}^{n} \lambda_k^{(n)} [t_k^{(n)}]^{2n} = \frac{\sqrt{\pi}\, n!}{2^n}\,. \tag{1.13}$$

It is interesting to observe that, although (1.12) does not converge if $z = x$ is real, the Gauss-Hermite quadrature sum (1.11) for fixed n and $z = x \to \infty$ nevertheless approximates $-i\pi\, w(x)$ to within an error of $O(x^{-2n-1})$. In fact, this is true as $z \to \infty$ in the sector $-\pi/4 < \arg z < 5\pi/4$. In other words, the quadrature sums (1.11), and thus *the convergents of the Laplace continued fraction* (1.7) *approximate* $-i\pi\, w(z)$ *asymptotically as* $z \to \infty$ *in* $-\pi/4 < \arg z < 5\pi/4$. This follows by combining (1.6) and (1.9)-(1.11),

$$w(z) - \frac{i}{\pi}\sum_{k=1}^{n}\frac{\lambda_k^{(n)}}{z-t_k^{(n)}} = \frac{i}{\pi}\sum_{s=0}^{2n}\frac{\mu_s}{z^{s+1}} + O\left(\frac{1}{z^{2n+3}}\right) - \frac{i}{\pi}\sum_{s=0}^{\infty}\frac{\nu_s^{(n)}}{z^{s+1}}$$

$$= \frac{i}{\pi}\frac{\mu_{2n} - \nu_{2n}^{(n)}}{z^{2n+1}} + O\left(\frac{1}{z^{2n+3}}\right) \quad (z \to \infty \text{ in } -\tfrac{\pi}{4} < \arg z < \tfrac{5\pi}{4}).$$

We have used here the symmetry of the Gauss-Hermite weights and nodes, which implies that (1.11) is an odd function of z, and therefore $\nu_s^{(n)} = 0$ for s an odd integer. Also, the series in (1.9), in view of (1.11), obviously converges for $|z| > \max_k t_k^{(n)}$. By virtue of (1.13) we thus have

$$w(z) - \frac{i}{\pi}\sum_{k=1}^{n}\frac{\lambda_k^{(n)}}{z-t_k^{(n)}} = \frac{i}{\sqrt{\pi}}\frac{n!}{2^n}\frac{1}{z^{2n+1}} + O\left(\frac{1}{z^{2n+3}}\right)$$

(1.14)

$$(z \to \infty \text{ in } -\tfrac{\pi}{4} < \arg z < \tfrac{5\pi}{4}).$$

If this is compared with the asymptotic expansion (1.6), i.e.

$$w(z) - \frac{i}{\pi}\sum_{s=0}^{2n-2}\frac{\mu_s}{z^{s+1}} = \frac{i}{\pi}\frac{\mu_{2n}}{z^{2n+1}} + O\left(\frac{1}{z^{2n+3}}\right), \tag{1.15}$$

one notes that the leading term on the right in (1.14) is smaller than the corresponding term in (1.15) by a factor of

$$\frac{\sqrt{\pi}\, n!}{2^n \Gamma(n+\frac{1}{2})} \sim \sqrt{\pi}\, n^{\frac{1}{2}} 2^{-n} \qquad (n \to \infty).$$

This is why Gauss-Hermite quadrature is so much more effective for computation than straightforward asymptotic expansion.

There is yet another approach to the continued fraction in (1.7), which involves the repeated integrals of the complementary error function. Consider (see [6] for notations)

$$(1.16)\qquad w_n(z) = e^{-z^2}\, i^n\mathrm{erfc}(-iz) \qquad (n = 0,1,2,\ldots), \qquad w_{-1}(z) = \frac{2}{\sqrt{\pi}},$$

so that in particular

$$(1.17)\qquad w_0(z) = w(z).$$

If $\mathrm{Im}\, z > 0$, the sequence $\{w_n(z)\}_{n=-1}^{\infty}$ is known to be a "minimal" solution of the linear second-order difference equation

$$(1.18)\qquad y_{n+1} - \frac{iz}{n+1}\, y_n - \frac{1}{2(n+1)}\, y_{n-1} = 0 \qquad (n = 0,1,2,\ldots).$$

(For terminology, and subsequent development, see [7].) For any integer $N \geq 0$, and $\nu > N$, define

$$(1.19)\qquad \begin{cases} r_\nu = 0, \quad r_{n-1} = \dfrac{1/2}{-iz + (n+1)r_n} & (n = \nu,\nu-1,\ldots,0), \\ \\ v_{-1} = \dfrac{2}{\sqrt{\pi}}, \quad v_n = r_{n-1}v_{n-1} & (n = 0,1,2,\ldots,N). \end{cases}$$

We shall write $r_{n-1}^{[\nu]}(z)$, $v_n^{[\nu]}(z)$ for r_{n-1}, v_n, if we wish to indicate their dependency on ν and z. It can then be shown that

$$(1.20)\qquad \lim_{\nu\to\infty} v_n^{[\nu]}(z) = w_n(z) \qquad (\mathrm{Im}\, z > 0,\ n = -1,0,1,2,\ldots),$$

and consequently,

$$\lim_{\nu\to\infty} r_{n-1}^{[\nu]}(z) = w_n(z)/w_{n-1}(z) \qquad (\text{Im } z > 0,\ n = 0,1,2,\ldots).$$

In particular, by (1.17),

$$(1.21) \qquad w(z) = \lim_{\nu\to\infty} v_o^{[\nu]}(z) = \frac{2}{\sqrt{\pi}} \lim_{\nu\to\infty} r_{-1}^{[\nu]}(z) \qquad (\text{Im } z > 0).$$

To see the connection with the Laplace continued fraction, let n = 0 in the second line of (1.19), and then in turn n = 0,1,2,...,ν in the first line of (1.19). One obtains

$$v_o^{[\nu]}(z) = \frac{1}{\sqrt{\pi}} \; \frac{1}{(-iz)+} \; \frac{1/2}{(-iz)+} \; \frac{1}{(-iz)+} \; \frac{3/2}{(-iz)+} \cdots \frac{\nu/2}{(-iz)}$$

$$= \frac{i}{\pi} \; \frac{\mu_o}{z-} \; \frac{1/2}{z-} \; \frac{1}{z-} \; \frac{3/2}{z-} \; \cdots \; \frac{\nu/2}{z} \; ,$$

where the second expression follows from the first by an obvious equivalence transformation. Comparison with (1.8) shows that

$$(1.22) \qquad v_o^{[\nu]}(z) = \frac{i}{\pi} \; \frac{q_{\nu+1}(z)}{p_{\nu+1}(z)} \; .$$

Curiously, the function $w_n(z)$ defined in (1.16) is related to the n-th derivative of w(z) by

$$(1.23) \qquad w^{(n)}(z) = (2i)^n \, n! \, w_n(z) \qquad (n = 0,1,2,\ldots),$$

a result apparently first observed in [5, p. 223].

2. Computational procedure. Our objective is to devise an efficient procedure for computing the function w(z) defined in (1.1) to a given number d of correct decimal digits after the decimal point, i.e., to within an (absolute) error of $\frac{1}{2}\,10^{-d}$. We shall assume z to lie in the first quadrant Q_1 of the complex plane. This is no restriction of generality, since

$$w(-z) = 2\,e^{-z^2} - w(z), \qquad w(\bar{z}) = \overline{w(-z)} \tag{2.1}$$

can be used to continue w into the remaining quadrants.

As shown in (1.12), (1.14), Gauss-Hermite quadrature, or equivalently, the Laplace continued fraction (1.7), provides an effective means of computing w(z) for $z \in Q_1$ and $|z|$ large. To obtain a more concrete idea as to the errors involved, we construct the altitude map of the meromorphic function

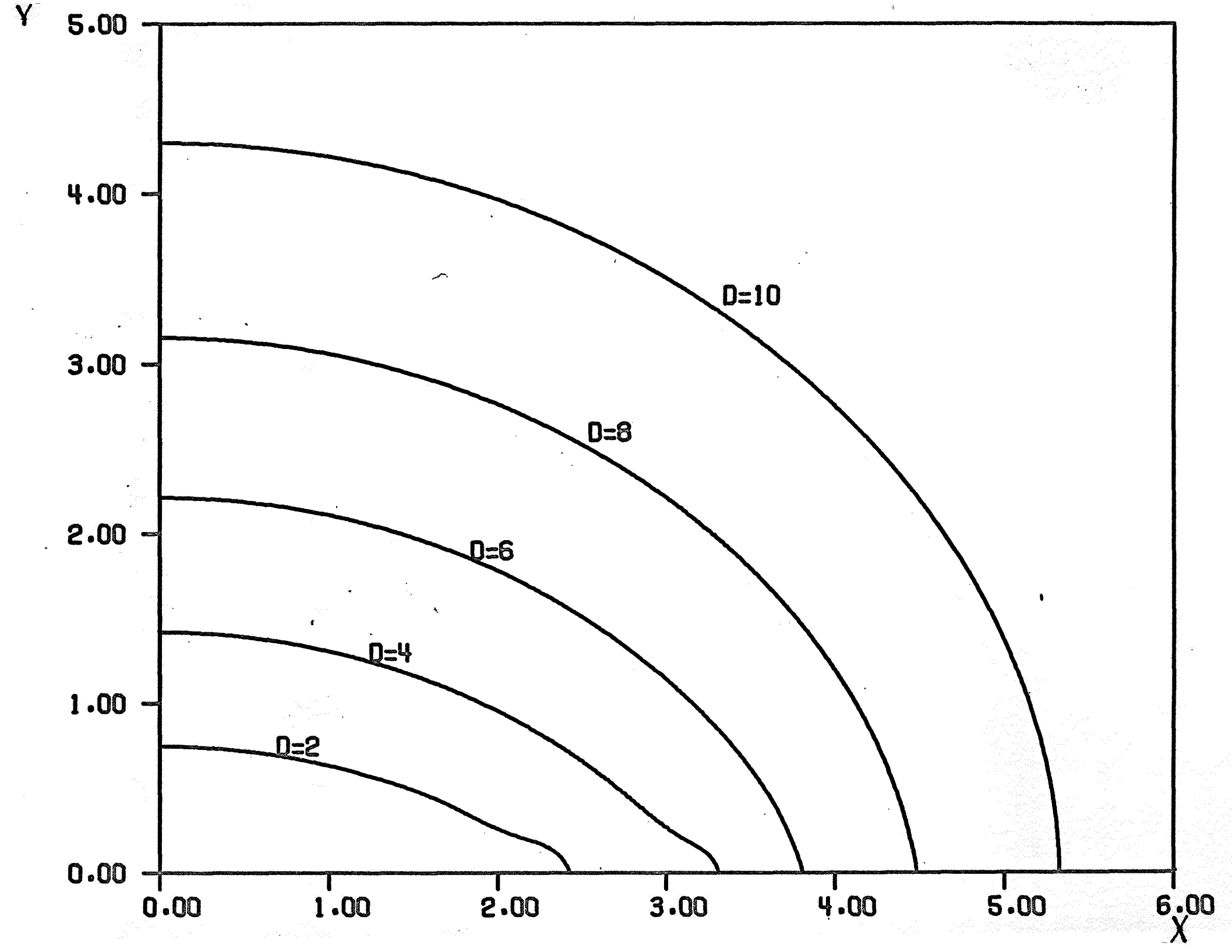
$$e_n(z) = w(z) - \frac{i}{\pi} \sum_{k=1}^{n} \frac{\lambda_k^{(n)}}{z - t_k^{(n)}},$$

i.e., the curves of constant modulus $|e_n(z)| = r$. These may be obtained by numerical integration of the differential equations

$$\frac{dx}{d\phi} = -\mathrm{Im}\left[\frac{e_n(z)}{e_n'(z)}\right], \qquad \frac{dy}{d\phi} = \mathrm{Re}\left[\frac{e_n(z)}{e_n'(z)}\right] \qquad (z = x+iy),$$

subject to the initial conditions

$$x(0) = 0, \qquad y(0) = \eta,$$


Y
5.00
4.00
3.00
2.00
1.00
0.00
D=10
D=8
D=6
D=4
D=2
0.00
1.00
2.00
3.00
4.00
5.00
6.00
X

where η is the root of $|e_n(iy)| = r$. Selected results are shown in Fig. 1, where $n = 9$, and $r = \frac{1}{2}\,10^{-d}$, $d = 2(2)10$.

Given any d, it is obviously possible to construct a rectangular region

$$(2.2) \qquad R: \quad 0 \le x \le x_o, \qquad 0 \le y \le y_o$$

outside of which 9-point Gauss-Hermite quadrature yields an accuracy of d decimal places. For $d = 10$, e.g., Fig. 1 suggests the choice $x_o = 5.33$, $y_o = 4.29$. Larger values of n would result in a smaller rectangle R, whereas smaller values of n would require a larger rectangle R for the same accuracy. It is not possible, in general, to arrive at an optimal choice of n, as such a choice would depend on the relative frequency with which the procedure is used in various regions of the complex plane. The choice $n = 9$ appears to be a reasonable compromise, and we shall fix this value for what follows.

To compute w(z) outside of R, we thus apply (1.19) with $\nu = 8$ and $N = 0$. In view of (1.22), (1.11), this is indeed equivalent to evaluating w(z) from the integral representation (1.2), (1.3) by a 9-point Gauss-Hermite quadrature rule.

It remains to consider the case where $z \in R$. If $y = \mathrm{Im}\, z$ is relatively small, a common procedure consists of computing w(z) from a Taylor expansion about $z_o = \mathrm{Re}z$, or alternatively, to write

$$w(z) = e^{-z^2} + \frac{2i}{\sqrt{\pi}} F(z), \qquad F(z) = e^{-z^2} \int_o^z e^{t^2} dt,$$

and to expand F(z) about $z_o = \mathrm{Re}z$. There are two disadvantages to this approach:

(1) it requires the computation of Dawson's integral, F(x), for $x = z_o$. Although good rational approximations are available for F(x) (see, e.g., [3]), the necessity of computing F(x) is apt to increase both the length of the program, and the total machine time, for computing w(z);

(2) the recursive computation of the expansion coefficients is subject to considerable loss of accuracy, particularly for large $x > 0$.

Interestingly enough, both these defects are removed if one expands "downward" rather than "upward", i.e., if one computes w(z) from the Taylor expansion

$$w(z) = \sum_{n=o}^{\infty} \frac{w^{(n)}(z+ih)}{n!} (-ih)^n, \tag{2.3}$$

where $h > 0$ is suitably chosen. This approach has the further advantage of being related to the Laplace continued fraction approach, and in fact gives rise to an algorithm which generalizes algorithm (1.19) (used outside of R).

We observe from (1.23) that (2.3) can be written in the form

$$w(z) = \sum_{n=o}^{\infty} (2h)^n w_n(z+ih). \tag{2.4}$$

Approximating w_n by $v_n^{[\nu]}$ [cf. (1.20)], and truncating the infinite series, we are led to define

$$\sigma_N^{[\nu]}(z,h) = \sum_{n=o}^{N} (2h)^n v_n^{[\nu]}(z+ih). \tag{2.5}$$

Letting $t_n = (2h)^n v_n^{[\nu]}(z+ih)$, one obtains from (1.19) the following algorithm to compute (2.5),

$$(2.6)\qquad \begin{cases} r_\nu = 0, \quad r_{n-1} = \dfrac{1/2}{h - iz + (n+1)r_n} \quad (n = \nu, \nu-1, \ldots, 0), \\ t_0 = \sigma_0 = \dfrac{2}{\sqrt{\pi}} r_{-1}, \\ t_n = 2h\, r_{n-1}\, t_{n-1}, \quad \sigma_n = \sigma_{n-1} + t_n \qquad (n = 1,2,\ldots,N). \end{cases}$$

We note that for $h = 0$, $N = 0$, algorithm (2.6) reduces to algorithm (1.19).

Given $\varepsilon = \frac{1}{2} 10^{-d}$, it is clearly possible to determine N and ν (both depending on z, h, and ε) such that

$$(2.7)\qquad |\sigma_N^{[\nu]}(z,h) - w(z)| \leq \varepsilon.$$

Since the series in (2.4) converges for every z and h, we can indeed find N such that $|\sigma_N^{[\infty]}(z,h) - w(z)| \leq \varepsilon/2$, and with N so determined, find $\nu > N$ such that $|\sigma_N^{[\nu]}(z,h) - \sigma_N^{[\infty]}(z,h)| \leq \varepsilon/2$. The triangular inequality then yields the desired result (2.7).

Efficiency being one of our major concerns, we propose to

(i) let h, N, and ν depend on z in such a way that $h = N = 0$, $\nu = 8$ for z outside of R, the rectangle introduced in (2.2);

(ii) empirically determine the smallest integers N and ν, subject to (i) and compatible with (2.7), for each $z \in R$.

The motivation behind the first of these objectives is to arrive at a *single* algorithm for computing w(z) in all of Q_1, viz. algorithm (2.6), which, as was already observed, automatically reduces to the Laplace

continued fraction algorithm (1.19) when $h = N = 0$. The objective can be attained in many different ways. Exploratory computations led us to set up h, N, ν tentatively in the form[2]

$$h = h_o\, s(z), \qquad N = \{N_o + N_1 s(z)\}, \qquad \nu = \{\nu_o + \nu_1 s(z)\} \quad \text{if } z \in R,$$
$$h = N = 0, \qquad \nu = 8 \quad \text{if} \quad z \in Q_1 \setminus R, \tag{2.8}$$

where

$$s(z) = (1 - \frac{y}{y_o}) \sqrt{1 - (\frac{x}{x_o})^2} \qquad (z = x+iy),$$

and h_o, N_o, N_1, ν_o, ν_1 are parameters which remain to be determined. Our second objective (ii) will serve to determine the last four of these parameters, while the first, h_o, will be chosen so as to minimize machine time.

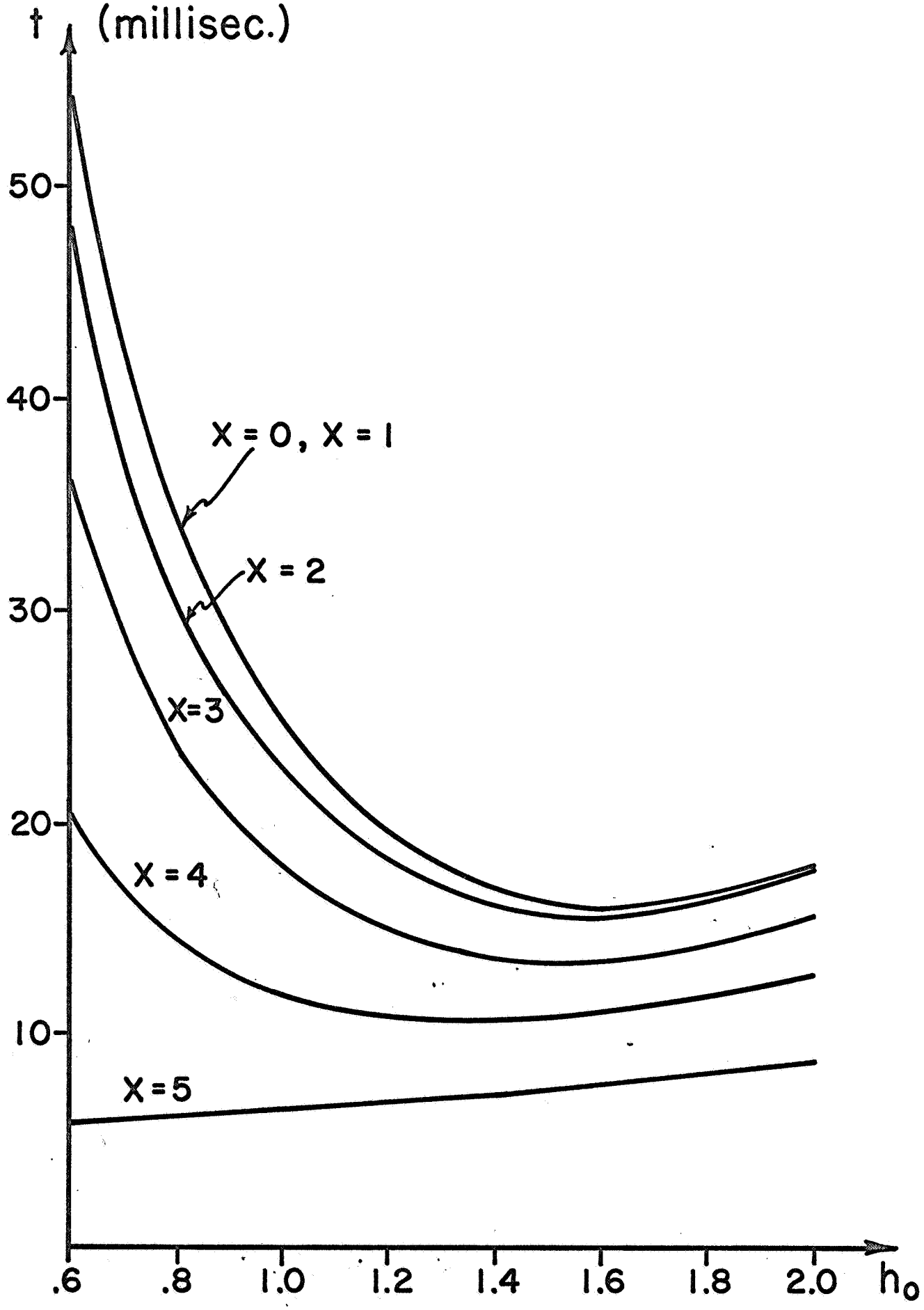
A basic aid in this parameter study is a gauging routine Γ, which does the following: given $z = x+iy$, h, and ε, it returns nearly optimal values $N = N_\Gamma$, $\nu = \nu_\Gamma$ compatible with (2.7). The detailed steps involved in Γ are as follows:

(1) Select $N = \hat{N}$ sufficiently large (say, $\hat{N} = 40$).

(2) Determine $\check{\nu}$, the smallest integer $\nu > \hat{N}$ such that $\max_{0 \le N \le \hat{N}} |\sigma_N^{[\nu+10]}(z,h) - \sigma_N^{[\nu]}(z,h)| \le \varepsilon/100$. The quantities $\sigma_N^{[\check{\nu}]}(z,h)$, $N = 0,1,\ldots,\hat{N}$, are considered sufficiently accurate to represent true partial sums of the Taylor series (2.4).

---

[2] $\{u\}$ denotes the integer closest to u, i.e., the largest integer contained in $u+1/2$.


t (millisec.)
50
40
30
20
10
X = 0, X = 1
X = 2
X=3
X = 4
X=5
.6
.8
1.0
1.2
1.4
1.6
1.8
2.0
h_0

(3) Find N_Γ as the smallest integer $N \le \hat{N} - 3$ satisfying $|\sigma_{N+3}^{[\check{\nu}]}(z,h) - \sigma_N^{[\check{\nu}]}(z,h)| \le \varepsilon$. If there is no such integer N, increase $\hat{N}$ by 10, and repeat steps (1)-(3).

(4) Determine ν_Γ as the smallest integer ν satisfying $|\sigma_{N_\Gamma}^{[\nu+1]}(z,h) - \sigma_{N_\Gamma}^{[\nu]}(z,h)| \le \varepsilon$.

A first application of the gauging routine Γ is made in determining the parameter h_o. The choice of h_o affects both the convergence of $\sigma_N^{[\nu]}(z,h)$, as $\nu \to \infty$, and the convergence of the Taylor expansion (2.4). In fact, large values of h_o give rise to fast convergence of $\sigma_N^{[\nu]}(z,h)$, but slow convergence in (2.4), while small values of h_o yield slow convergence of $\sigma_N^{[\nu]}(z,h)$ (particularly if $y = \mathrm{Im}\, z$ is small), but fast convergence in (2.4). A good choice of h_o is therefore one which strikes a balance between these two opposing effects. In order to search for such a value, we let $y = 0$ (where these effects are most pronounced) and apply Γ with input parameters $z = x$, $h = h_o\, s(x)$, ε, for selected values of x and h_o. After each application of Γ we measure the machine time required to compute $\sigma_N^{[\nu]}(x,h)$ by algorithm (2.6), where $\nu = \nu_\Gamma$, $N = N_\Gamma$ are the integers returned by Γ. With $x_o = 5.33$, $\varepsilon = \frac{1}{2}10^{-10}$, the results are shown in Fig. 2, where machine time (in milliseconds) is plotted versus h_o for $x = 0(1)5$. It is seen from these graphs that a good choice of h_o is $h_o = 1.6$.

We next apply Γ to determine the parameters N_o, N_1, ν_o, ν_1 in (2.8). A first pair of constraints is obtained by letting $z = 0$ and requiring that

$$(2.9) \qquad N_o + N_1 = \overset{o}{N}_\Gamma, \qquad \nu_o + \nu_1 = \overset{o}{\nu}_\Gamma,$$

where $\overset{o}{N}_\Gamma$, $\overset{o}{\nu}_\Gamma$ are the results returned by Γ with input parameters $z = 0$, $h = h_o$, ε. A narrow band near the separation line $y = y_o$ is then examined more carefully, since our preliminary computations indicated that N_Γ and ν_Γ approach limits larger than 0 and 8, respectively, as $y \uparrow y_o$. With $\hat{N}_\Gamma$ the largest N_Γ, and $\hat{\nu}_\Gamma$ the largest ν_Γ returned by Γ for input parameters z(near the line $y = y_o$), $h = h_o s(z)$, ε, we let

$$(2.10) \qquad N_o = \hat{N}_\Gamma \quad , \quad \nu_o = \hat{\nu}_\Gamma,$$

which, together with (2.9), determines the desired parameters uniquely. In our case of interest ($x_o = 5.33$, $y_o = 4.29$, $h_o = 1.6$, $\varepsilon = \frac{1}{2}10^{-10}$), the results are $\overset{o}{N}_\Gamma = 29$, $\overset{o}{\nu}_\Gamma = 30$, $\hat{N}_\Gamma = 6$, $\hat{\nu}_\Gamma = 9$, giving

$$(2.11) \qquad h = 1.6\ s(z), \qquad N = \{6+23\ s(z)\}, \qquad \nu = \{9+21\ s(z)\} \quad \text{if } z \in R.$$

Note that $\nu > N$ for all z, as required in algorithm (2.6).

It remains to examine whether this choice of parameters is indeed compatible with (2.7). This is done by applying Γ with input parameters $z = x+iy$, $h = h_o\ s(z)$, ε over a grid of points $z \in R$, and by checking the inequalities

$$\{N_o + N_1\ s(z)\} \geq N_\Gamma(z) \quad , \quad \{\nu_o + \nu_1\ s(z)\} \geq \nu_\Gamma(z),$$

where $N_\Gamma(z)$ and $\nu_\Gamma(z)$ are the output values of Γ at the point z. Using the grid $x = 0(.5)5(.05)5.4$, $y = 0(.2)4(.05)4.4$, and $\varepsilon = \frac{1}{2}10^{-10}$, it was found that both inequalities are consistently satisfied.

With the values of h, N, ν, defined in (2.8), (2.11), the desired function w(z) is thus approximated by $\sigma_N^{[\nu]}(z,h)$ in (2.5), which in turn can be calculated by algorithm (2.6). The result is essentially the Algorithm in [8], except that in this procedure the sum $\sigma_N^{[\nu]}(z,h)$ is evaluated somewhat differently. Letting $s_n = [v_n^{[\nu]}(z+ih)]^{-1} \sum_{k=n+1}^{N} (2h)^k v_k^{[\nu]}(z+ih)$, $s_N = 0$, one can write indeed

$$(2.12)\qquad \left\{ \begin{array}{ll} r_\nu = 0, & s_N = 0, \\ r_{n-1} = \dfrac{1/2}{h-iz+(n+1)r_n} & \\ s_{n-1} = r_{n-1}[(2h)^n + s_n] & (\text{if } n \leq N) \end{array} \right\} n = \nu,\nu-1,\ldots,0,$$

and then has

$$(2.13)\qquad \sigma_N^{[\nu]}(z,h) = \left\{ \begin{array}{ll} \dfrac{2}{\sqrt{\pi}}\, s_{-1} & (h > 0), \\ \dfrac{2}{\sqrt{\pi}}\, r_{-1} & (h = 0). \end{array} \right.$$

The advantage of this algorithm over algorithm (2.6) is its increased speed on a digital computer [cf. section 3] together with the fact that no array of storage must be provided to hold the quantities $r_{n-1}(n = 1,2,\ldots,N)$.

3. Performance characteristics and tests. We begin by comparing the computing times of the algorithm in [8] (referred to below as Algorithm...) with those of a similar algorithm, in which (2.12), (2.13) is replaced by (2.6). Both algorithms are compiled and executed on the CDC 6500 computer.

We select five layers S_n (n = 0,1,...,4) in R, defined by

$$S_n: \quad 0 \leq x \leq x_o, \quad ny_o/5 \leq y \leq (n+1)y_o/5 \quad (x_o = 5.33,\ y_o = 4.29),$$

and time the algorithms on each S_n. The average time on S_n is obtained by measuring the computing time of evaluating w(z) for 1000 values of z, distributed uniformly in S_n, and by dividing the measured time by 1000. Both algorithms are timed similarly in the region outside of R (where computing time is independent of z). The results[3] are shown in Table 1. It is seen that the second algorithm is slower than the first by a factor of 1.6-2.2.

z in	Computing time (in millisec.)	
	Algorithm...	(2.6) replacing (2.12),(2.13)
S_0	6.7	14.5
S_1	6.0	12.6
S_2	5.2	10.7
S_3	4.4	8.7
S_4	3.6	6.8
$Q_1 \setminus R$	2.2	3.6

Table 1. Timing of Algorithm... and a related algorithm.

[3] Such timings are subject to slight variations, even on the same computer, due to such incidental factors as compiler, executive system, clock reading routine, etc.

For comparison we also timed the library subroutine for the exponential function e^x for selected values of x in the interval $1 \leq x \leq 20$. The time observed was rather consistently .315 milliseconds. The computation of w(z) (both real and imaginary part) by Algorithm... thus takes about as long as 7-21 exponentiations, depending on the location of the argument z.

In order to gain further confidence in the accuracy claimed, Algorithm... is run for x = 0(.02)5.32(.005)5.35, 5.4(.2)6, y = 0(.02)4.28(.005)4.31, 4.4(.2)5, the results being compared with those obtained by the same algorithm, where h is replaced by 1.6, N by 33, and ν by 36. (This combination of parameter values yields 14 correct decimal digits for z near the origin.) The largest absolute deviation is found to be 5.18×10^{-11} in the real part, and 4.91×10^{-11} in the imaginary part. For the maximum relative deviation the figures are 1.18×10^{-8} and 6.64×10^{-9}, respectively.

The region very close along the real axis is known to be a difficult region in which to compute w(z), particularly its real part. To see how well our algorithm does in this region, it is used to compute $\frac{1}{\sqrt{\pi}}$ Re w(x+iy) for x = 0(1)10 and $y = s \cdot 10^{-r}$ (s = 1,2,3,5,7; r = 4,3,2). The results are compared with those in Hummer's table [9]. Remarkably enough, although some of the answers (for large x and small y) have order of magnitude 10^{-7}, there is agreement to 8 significant digits (the precision in [9]), excepting occasional end figure errors of 1-7 units.

Acknowledgments. The author is indebted to Professor Henry C. Thacher, Jr., for stimulating conversations, and to Mr. Thomas J. Aird for writing the program to produce the altitude map of Fig. 1.

References

[1] B. H. Armstrong, Spectrum line profiles: the Voigt function, J. Quant. Spectrosc. Radiat. Transfer 7 (1967), 61-88.

[2] C. Chiarella and A. Reichel, On the evaluation of integrals related to the error function, Math. Comput. 22 (1968), 137-143.

[3] W. J. Cody, K. A. Paciorek, and H. C. Thacher, Jr., Chebyshev approximations for Dawson's integral, to appear in Math. Comput.

[4] V. N. Faddeeva and N. N. Terent'ev, Tables of values of the function $w(z) = e^{-z^2}(1 + \frac{2i}{\sqrt{\pi}}\int_0^z e^{t^2}\,dt)$ for complex argument (Russian), Gosud. Izdat. Teh.-Teor. Lit., Moscow, 1954. {English translation by D. G. Fry, Pergamon Press, New York, 1961.}

[5] A. Fletcher, J. C. P. Miller, and L. Rosenhead, An Index of Mathematical Tables, Scientific Computing Service Limited, London, 1946.

[6] W. Gautschi, Error function and Fresnel integrals, Ch. 7, Handbook of Mathematical Functions (M. Abramowitz and I. A. Stegun, Eds.), Nat. Bur. Standards Appl. Math. Ser. 55 (1964), 295-329.

[7] _____, Computational aspects of three-term recurrence relations, SIAM Rev. 9 (1967), 24-82.

[8] _____, Algorithm... - Complex error function, submitted to Comm. ACM.

[9] D. G. Hummer, The Voigt function: An eight-significant-figure table and generating procedure, Mem. Roy. Astronom. Soc. 70 (1965), 1-31.

[10] O. Perron, Die Lehre von den Kettenbrüchen, 3rd ed., Vol. II, Teubner, Stuttgart, 1957.

[11] A. Reichel, Error estimates in simple quadrature with Voigt functions, Math. Comput. 21 (1967), 647-651.

[12] T. J. Stieltjes, Reserches sur les fractions continues, Ann. Fac. Sci. Toulouse 8 (1894), 1-122; 9 (1895), 1-47. {Oevres Complètes de Thomas Jan Stieltjes, Vol. II, 402-566.}

[13] O. Szász, Bemerkungen zu Herrn Perrons Erweiterung eines Markoffschen Satzes über die Konvergenz gewisser Kettenbrüche, Math. Ann. 76 (1915), 301-314.

[14] H. C. Thacher, Jr., Computation of the complex error function by continued fractions, Blanch Anniversary Volume, 315-337, Aerospace Research Lab., U. S. Air Force, Washington, D. C., 1967.