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THE NUMERICAL COMPUTATION OF SPECIAL FUNCTIONS BY USE OF QUADRATURE RULES FOR SADDLE POINT INTEGRALS

I. TRAPEZOIDAL INTEGRATION RULES

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The numerical computation of special functions by use of quadrature rules for saddle point integrals

I. Trapezoidal integration rules

by

N.M. Temme

ABSTRACT

Trapezoidal integration rules are considered and representations of the error are discussed. For finite intervals the integrand is supposed to be smooth with vanishing derivatives of all order at the endpoints of the interval. For infinite intervals the function is supposed to be analytic in a strip containing the interval. In both cases the trapezoidal rule gives a small error bound. This is the first paper in a series in which quadrature rules are used for the computation of special functions.

KEY WORDS & PHRASES: *mechanical quadrature, trapezoidal integration rules, saddle point methods*

AN

PREFACE

This is the first of a set of papers dealing with uniform asymptotic methods and the computation of functions. In the main the methods are applied on special functions of mathematical physics.

The starting point of the investigations is an integral representation for the function to be approximated. Numerical approximations are not based on the asymptotic expansions of the function, but, as a rule, on suitable integral representations that are developped by methods from asymptotics. Usually, the integral will be a steepest descent contour containing one or more saddle points of the integrand. On the contour, the imaginary part of the integrand is constant or slowly varying. As a consequence, the integral can be easily evaluated by a quadrature rule.

For functions of one variable numerical methods for computation are mostly based on polynomial or rational approximations. Much material is available for the well-known special functions. See for instance HART et al. (1968), LUKE (1969) and (1975). If the functions are considered for complex argument or if additional parameters are incorporated, these approximations become useless. In these cases it is possible to construct multivariate approximants or to use expansions such as Taylor series, asymptotic series or Chebyshev series, or expansions in other functions that are simpler to compute than the original function. Often, in using expansions obtained by analytical methods, a drawback is found in the limited range of the parameters. Expanding in one variable leaves the coefficients to be functions of the remaining variables. This creates problems of effective computation, satisfactory rate of convergence, etc. An example in point is the expansion (based on Taylor series) for the Bessel function $K_\nu(z)$ of complex order and complex argument, which is treated in TEMME (1975a). In Luke's papers (1971-1972) double series of Chebyshev polynomials for Bessel functions and numerical values of the coefficients are given. The ranges of real order and real argument of the Bessel functions, however, are limited, but sometimes recursion is possible to arrive at other values of the order.

Another method for computing mathematical functions is based on mathematical tables. But to impress these tables in the memory of a computer and then program for table lookup and interpolation is not economical. A computer program requires efficient algorithms and schemes for the evaluation of functions on demand. For functions of several variables this requirement is even more appropriate.

For an excellent review for existing methods on the computation of special functions the reader is referred to GAUTSCHI (1975).

Several starting points are possible for constructing approximations of special functions. The most important are the following three possibilities

(i) Series expansions (including continued fractions and rational approximations).

(ii) Differential equations.

(iii) Integral representations.

In this series of papers we concentrate on the third category. Without discussing in full the other possibilities, some remarks on their computational aspects will be in order.

(i) If large parameters occur in the function to be approximated, one might consider asymptotic expansions of the function. For large values of the parameter (without specifying the word "large") and if realistic and strict error bounds are available, aysmptotic expansions may give excellent approximations. Sometimes, however, if more parameters are involved, the coefficients of the expansion are not easily obtained, especially in the case of uniform expansions. Moreover, asymptotic methods based on a large parameter, are not suited to highly accurate numerical approximation for small or intermediate values of the parameter. The use of converging factors may give an outlet for these cases but a lot of work has to be done in order to obtain the coefficients for the converging factor. Much progress in this field is achieved by DINGLE (1973), who collects many results on converging factors (called terminants there). Generally, Dingle's formal methods give no error bounds, and therefore his results can only be applied tentatively. OLVER (1974) also gives some examples on converging factors; only these cases are considered that enable complete discussion of the error bounds.

The use of asymptotic expansions may also be limited on behalf of additional parameters. Consider for instance the incomplete gamma function defined by

$$\Gamma(a,x) = \int_x^\infty e^{-t}\, t^{a-1}\, dt,$$

with the well-known asymptotic expansion for $x \to \infty$

$$\Gamma(a,x) = e^{-x}x^{a-1}\left[1 + \frac{a-1}{x} + \frac{(a-1)(a-2)}{x^2} + \ldots \frac{(a-1)\ldots(a-n)}{x^n} + O(x^{-n-1})\right] \tag{1}$$

with a fixed. The parameter a may depend on x, and it can easily be proved that if $a = o(x)$ then validity of (1) still holds, but if $a = O(x)$ (1) looses its asymptotic character. One way of overcoming this difficulty is using a uniform expansion, for instance the expansion given in TEMME (1975b). As a matter of fact, however, these coefficients cannot easily be obtained and moreover, the computation of them is rather difficult if $a \sim x$.

Sometimes, asymptotic series can be transformed into other expansions, such that the new expansion is more suitable for numerical approximation. We mention expansions in continued fractions, factorial series (see LAUWERIER (1974), Padé approximants, Chebyshev series or an expansion based on a transformation due to VAN WIJNGAARDEN (1964). For the above example all these types of transformations happen to be possible (see LUKE (1969) and LAUWERIER (1974)). Sometimes, the new expansions turn out to be convergent and useful for a wide range of the parameter(s), in spite of the divergence of the asymptotic expansion from which they originate. In many cases the transformed expansion can be used to develop highly accurate algorithms for the functions involved. In these papers no further attention is paid to transformation of asymptotic expansions, however, since we have a different, rather unifying method before eyes, based on integral representations.

(ii) In contrast with the other categories, in this case the function is implicitly defined. Explicit methods, however, appear to be more useful for approximating special functions, and, in addition, they are more attractive for computations. For obtaining asymptotic expansions, on the other hand, differential equations are very important in the field of special functions. For an extensive treatment see OLVER (1974), where it is shown that differential equations yield expansions with realistic and sharp error bounds for the remainder. But, again, for these expansions large parameters are essential. Other series expansions can also be obtained from differential equations. A nice example introduced by CLENSHAW (1957) is the computation of coefficients of a Chebyshev expansion. If the differential equation has polynomial coefficients, as usually is the case for the special functions of mathematical physics, Clenshaw's method gives a system of recurrence relations that is easily handled in a numerical way. For direct computation, examples are hardly found in the literature for the evaluation of special functions using differential equations. In our opinion, numerical integrating methods for differential equations are not well sutited obtaining highly accurate approximations.

(iii) For large parameters integral representations may be difficult to evaluate, especially if the integrand oscillates rapidly. By choosing special integrals or special contours of integration, these difficulties may be overcome. In forthcoming papers we give some examples of integrals for special functions of mathematical physics. In the second paper we concentrate on integrals in which large values of the parameters do not disturb the methods of computation. These disturbances are discussed in the third and fourth papers. Examples of such cases are singularities in relevant neighborhoods of the interval of integration. Functions to be discussed in the second paper are the gamma function, the modified Bessel functions and a parabolic cylinder function. We also discuss an integral (not expressible as a special function) that is considered in the literature in the theory of ionization of crystals.

Some integral representations in these papers are new, that is, they can not be found in the literature. But always they can be derived from well-known representations by transformations and by choosing special contours of integration. The integrals are derived by using methods from asymptotic analysis. But in asymptotics the integrand is expanded in a series and by termwise integration an asymptotic expansion is obtained. From a numerical point of view, much information is lost in this step, especially if the asymptotic parameter is not very large.

In this first paper we give information on quadrature rules for analytic functions. The quadrature rule is simple: it is based on the trapezoidal rule. To our opinion, this rule is easily overlooked in practice and rejected on account of false considerations. Therefore it seems worthwhile to pay attention to this rule. For easy reference in the following papers we collected the results from the literature and formulated some lemmas and theorems. The finite and infinite interval are considered separately. The algorithms for both cases are the same, and are described in the form of ALGOL-60 procedures in subsection 1.3.4.

Thanks are due to F.J. Burger who assisted in the numerical computations.

1.0. INTRODUCTION

In this paper we will discuss some aspects concerning numerical quadrature of analytic functions. Especially we pay attention to the trapezoidal rule for both finite and infinite intervals.

From elementary numerical analysis it is known that the error for a trapezoidal integration rule can be expressed in terms of the second derivative of the integrand and is generally of order $O(h^2)$, for $h \to 0$, where h is the distance between two consecutive abscissas. However, when considering analytic functions the error can be expressed in terms of the integrand function itself and, under conditions that will be specified later, the error appears to be very small, even for comparatively large values of h. In this chapter we give some representations of the error term in the trapezoidal rule and for some cases upperbounds for the error.

The integrand functions we deal with in this paper are analytic on the interval of integration with possible exception of the endpoints where the function is continuous. We consider two possibilities corresponding to the function classes H_a and $C_c^\infty([a,b])$ defined as follows.

<u>DEFINITION 1.1.</u> Let

$$(1.1) \qquad G_a = \{z = x + iy \mid x \in \mathbb{R}, |y| < a\}$$

be the strip in the complex plane of width $2a > 0$. Let H_a denote the linear space of bounded holomorphic functions $f\colon G_a \to \mathbb{C}$ for which $\lim_{x\to\pm\infty} f(x+iy) = 0$ (uniformly in $|y| \le a$) and

$$(1.2) \qquad M_{\pm a}(f) = \int_{\infty}^{\infty} |f(x\pm ia)|\,dx = \lim_{b\uparrow a} \int_{-\infty}^{\infty} |f(x\pm ib)|\,dx < \infty.$$

<u>DEFINITION 1.2.</u> Let $C_c^\infty([a,b])$ denote the class of C^∞-functions $f\colon [a,b] \to \mathbb{C}$ having compact support the real interval $[a,b]$, $-\infty < a < b < \infty$.

The functions of $C_c^\infty([a,b])$ met in this paper can often be continued analitically so as to be single valued and regular in a region $D \subset \mathbb{C}$ containing (a,b). In distribution theory elements of $C_c^\infty([a,b])$ are often referred to as test functions. We have

$$(1.3)\qquad f^{(k)}(a) = f^{(k)}(b) = 0, \quad k = 0,1,2,\dots,$$

if $f \in C_c^\infty([a,b])$.

The following lemmas are important for estimating the remainder in trapezoidal integration rules. They can be considered as special cases of the Riemann-Lebesgue lemma.

LEMMA 1.3. *Let* $f \in H_a$ *for some* $a > 0$ *and let* $\lambda \in \mathbb{R}$. *Then for* $|\lambda| \to \infty$

$$(1.4)\qquad \int_{-\infty}^{\infty} f(x)e^{i\lambda x}dx = O(|\lambda|^{-\mu})$$

for every real μ.

PROOF. Apply Cauchy's theorem and replace the integral in (1.3) by

$$\int_{-\infty}^{\infty} f(x+iy)e^{i\lambda(x+iy)}dx$$

with $0 < y < a$ if $\lambda > 0$ and $-a < y < 0$ if $\lambda < 0$, from which follows that the integral is bounded by

$$(1.5)\qquad M_{\pm a}(f)e^{-a|\lambda|}$$

where the + sign (− sign) corresponds to $\lambda > 0$ $(\lambda<0)$. □

LEMMA 1.4. *Let* $f \in C_c^\infty([a,b])$ *for some* a *and* b. *Let* $\lambda \in \mathbb{R}$. *Then for* $|\lambda| \to \infty$

$$(1.6)\qquad \int_a^b f(x)e^{i\lambda x}dx = O(|\lambda|^{-\mu})$$

for every real μ.

PROOF. Partial integration of the integral in (1.4) and use of (1.3) give a bound of the integral of the form

$$(1.7) \qquad |\lambda|^{-k} \int_a^b |f^{(k)}(x)|\,dx, \qquad k = 0,1,2,\ldots$$

from which the lemma follows. □

REMARK 1.5. The bound in (1.5) is free of derivatives. Therefore it is easier to work with (1.5) than with estimates of the form (1.7). Moreover, (1.5) gives clear information about the rate of convergence of the integral in (1.4) for $|\lambda| \to \infty$. From (1.7) it can only be learned that convergence is faster than any power of $|\lambda|^{-1}$, but, generally, more information is not available. If more information about f is given it is possible to derive sharper results. See the example in 1.2.5.

KRESS (1971), (1972), (1974) and STENGER (1973) showed recently the use of the trapezoidal integration rule and gave new error bounds for the remainders. Many papers discuss the effect of a transformation of the integration variable. Apart from Stenger's paper we mention two other important papers dealing with this aspect: RICE (1973) and TAKAHASI & MORI (1973).

Some results on the trapezoidal quadrature rule for analytic functions are obtained long time ago. In fact, all of it can be condensed to the result of Cauchy, who expresses an integral of an analytic function in terms of a single function value

$$f(z) = \frac{1}{2\pi i} \oint \frac{f(\zeta)}{\zeta - z}\, d\zeta.$$

1.1. THE INFINITE INTERVAL

The quadrature rule is applied on integrals of the type

$$(1.8) \qquad \int_{-\infty}^{\infty} f(x)\,dx$$

with $f \in H_a$ for some $a > 0$, and the trapezoidal rule can be written as

$$(1.9) \qquad \int_{-\infty}^{\infty} f(x)\,dx = h \sum_{k=-\infty}^{\infty} f(kh+d) + R_d(h)$$

where $h \in \mathbb{R}$ and $R_d(h)$ is the error term. A relevant domain of d is $0 \le d < h$ and usually $d = 0$ or $d = \frac{1}{2}h$. Information on the remainder will be given below.

1.1.2. GOODWIN (1949) showed that for infinite integrals the trapezoidal rule can be applied with excellent results.

THEOREM 1.6. *Let* $f \in H_a$ *for some* $a > 0$. *Let* $h > 0$ *and* $0 \le d < h$. *Then* $R_d(h)$ *in* (1.9) *satisfies*

$$(1.10) \qquad R_d(h) = \int_{-\infty}^{\infty} \frac{f(x+iy)\,dx}{1-\exp[-2i\pi(x+iy-d)/h]} + \int_{-\infty}^{\infty} \frac{f(x-iy)\,dx}{1-\exp[2i\pi(x-iy-d)/h]}$$

for any y with $0 < y < a$.

PROOF. The known proof is based on the method of residues for evaluating contour integrals. Remark that

$$\frac{1}{2\pi i} \int_{\partial G_y} f(z)\,\mathrm{cotg}[\pi(z-d)/h]dz = h \sum_{m=-\infty} f(mh+d),$$

where ∂G_y is the boundary of G_y defined in (1.1) and the integration is in positive direction. Furthermore,

$$\int_{-\infty}^{\infty} f(x)dx + \int_{\infty}^{-\infty} f(x+iy)dx = \int_{-\infty}^{\infty} f(x)dx + \int_{\infty}^{-\infty} f(x-iy)dx = 0.$$

Combining these results we arrive at (1.10). $\square$

COROLLARY 1.7. *Let* $f \in H_a$ *for some* $a > 0$ *and let* f *be even. Then* $R_d(h)$ *given in* (1.10) *can be bounded in the following way*

$$(1.12) \qquad |R_d(h)| \le \frac{e^{-\pi a/h}}{\sinh\,(\pi a/h)} M_a(f)$$

where $M_a(f)$ is given in (1.2).

From (1.12) it follows that the error in the trapezoidal rule for small h, $h \downarrow 0$, is $O(e^{-2\pi a/h})$. Also, large values of a result in small errors, but the influence of the quantities $M_{\pm a}(f)$ may influence the behaviour of the error if $a \to \infty$. Often it is advisable to choose a and h in such a way that the right-hand side of (1.12) is minimized. Suppose for intance that

$$(1.13) \qquad f(x) = e^{-\omega x^2} g(x), \ \omega > 0,$$

with $g \in H_a$ for some a and g an even function. (In fact Goodwin considered this type of integrals.) In this case (1.12) can be written as

$$(1.14) \qquad |R_d(h)| \le \frac{e^{-\pi a/h+\omega a^2}}{\sinh(a\pi/h)} M_a(g).$$

The function $-2\pi a/h + \omega a^2$, considered as a function of a, is minimal for

$$(1.15) \qquad a = \frac{\pi}{\omega h}.$$

From this we derive that, supposing that $M_a(g) = O(1)$, the error in the trapezoidal rule satisfies

$$(1.16) \qquad |R_d(h)| \le C\, e^{-\pi^2/\omega h^2}, \quad \text{for some } C > 0.$$

<u>REMARK 1.8</u>. A similar estimate follows from a saddle point treatment of the remainder in (1.10). With f given in (1.13) and $y = a = \pi/(\omega h)$ we obtain the aymptotic expansion

$$(1.17) \qquad R_d(h) = -2\sqrt{\pi/\omega}\; e^{-\pi^2/\omega h^2} \cos(2\pi d/h)\, g(i\pi/\omega h)\, \{1+O(h)\},$$

$h \to 0$ and $0 \le d < h$. In this formula the role of the parameter d becomes apparent. For $d = 0$ and $d = \frac{1}{2}h$ the dominant term for $R_d(h)$ has a different sign. Thus the value of the integral may be expected to lie between the sums in (1.9) with $d = 0$, $d = \frac{1}{2}h$ with the same h. This aspect is important for numerical application of (1.9), see Subsection 1.3.1.

1.1.2 Another representation for the error in the trapezoidal rule can be obtained by using Poisson's summation formula, which reads in a general

:m

$$h \sum_{n=-\infty}^{\infty} e^{ina} f(d+nh) = \sum_{m=-\infty}^{\infty} F\left(\frac{2\pi m+a}{h}\right) e^{-id(2\pi m+a)/h} \tag{.18}$$

:h

$$F(y) = \int_{-\infty}^{\infty} f(x)\, e^{iyx}\, dx.$$

e conditions of validity are given in BOCHNER (1932).

For $a = 0$ we obtain a representation as (1.9) with

$$R_d(h) = -\sum_{m\neq 0} F(2\pi m/h) e^{-id2\pi m/h}. \tag{.19}$$

r functions $f \in H_a$ the representations coincide, as follows from expanding (1.10) the intergrands in geometric series with exponential functions.

1.3. KRESS (1974) considered in a recent paper, following an idea of DAVIS 962), the remainder of the trapezoidal rule as a functional and he gives norm of this functional. In this subsection we summarize his results. the proof, which will not be given here, Hilbert space techniques are ed.

EOREM 1.9. *Let* H_a *be the normed linear space of bounded functions intro- ced in Definition* 1.1, *and let* H_a *be equipped with the norm*

$$\|f\|_a = \int_{-\infty}^{\infty} |f(x+ia) + f(x-ia)|\, dx. \tag{.20}$$

et the linear functional $E_h\colon H_a \to \mathbb{C}$ *be given by*

$$E_h(f) = \int_{-\infty}^{\infty} f(x)dx - h \sum_{n=-\infty}^{\infty} f(nh). \tag{1.21}$$

en the norm of E_h *is given by*

$$\|E_h\|_a = \sum_{m=1}^{\infty} 1/\cosh(2\pi am/h). \tag{1.22}$$

PROOF. See KRESS (1974). □

By using the estimations

$$\sum_{m=1}^{\infty} 1/\cosh(2\pi am/h) < 2 \sum_{m=1}^{\infty} e^{-2\pi am/h} = e^{-a\pi/h}/\sinh(a\pi/h)$$

we have

$$(1.23) \qquad |E_h(f)| < \frac{e^{-a\pi/h}}{\sinh a\pi/h} \|f\|_a,$$

which may be compared with (1.12). Remark that different norms for f appear in (1.12) and (1.23) and that in (1.12) f is supposed to be even.

Kress also shows that the more general rule

$$(1.24) \qquad \int_{-\infty}^{\infty} f(x)\,dx = h \sum_{m=-\infty}^{\infty} \alpha_m f(mh) + E_h(f),$$

where $\{\alpha_m\}$ is a bounded sequence such that

$$(1.25) \qquad \lim_{m\to\infty} \frac{1}{2m+1} \sum_{n=-m}^{m} \alpha_n = \alpha^0$$

exists, is optimal for constant α_m. That is, $\|E_h\|_a$ for E_h from (1.24) is as small as possible if the numbers α_m in (1.24) satisfying (1.25) are constant.

1.14. An interesting generalization of (1.9) with d = 0 is based on the idea of Hermite interpolation and is given by KRESS (1972). The result is summarized in the following theorem. For the proof the reader is referred to KRESS (1972).

THEOREM 1.10. *Let* $f \in H_a$ *for some* $a > 0$ *and let for even* $p \in \mathbb{N}$ *numbers* $a_{q,p}$ *be determined by the identity*

$$(1.26) \qquad a_{0,p} + a_{2,p}z^2 + \ldots + a_{p,p}z^p = \prod_{q=1}^{\frac{1}{2}p} [1+(z/q)^2].$$

Then for $h > 0$

$$(1.27) \qquad \int_{-\infty}^{\infty} f(x)dx = I_{p,h}(f) + E_{p,h}(f),$$

$$(1.28) \qquad I_{p,h}(f) = h \sum_{m=-\infty}^{\infty} \sum_{\substack{q=0,\\ q \text{ even}}}^{p} (h/2\pi)^q \, a_{q,p} \, f^{(q)}(mh)$$

and $E_{p,h}(f)$ *is bounded by*

$$(1.29) \qquad |E_{p,h}(f)| < \frac{e^{-\pi a/h}}{z \sinh^{p+1}(\pi a/h)} \, [M_a(f) + M_{-a}(f)].$$

The rule for $p = 0,2,4$ reads as follows

$$I_{0,h}(f) = h \sum_{m=-\infty}^{\infty} f(m,h),$$

$$(1.30) \qquad I_{2,h}(f) = I_{0,h}(f) + \frac{h^3}{4\pi^2} \sum_{m=-\infty}^{\infty} f''(mh)$$

$$I_{4,h}(f) = I_{0,h}(f) + \frac{5h^3}{16\pi^2} \sum_{m=-\infty}^{\infty} f''(mh) + \frac{h^5}{64\pi^4} \sum_{m=-\infty}^{\infty} f^{(iv)}(mh).$$

From (1.29) it follows that the accuracy can be improved by using more points of interpolation, i.e., smaller h, as well as more derivatives. Quadrature formulae involving derivatives may be useful in cases when data on the derivatives are easily available, for instance, from differential equations.

The coefficients $a_{q,p}$, of which the first few appears in (1.30), can easily be obtained as follows. By differentiation of (1.9) with respect to d and by using (1.19) for $R_d(h)$ we obtain (by taking $d = 0$ afterwards) for even functions f

$$\int_{-\infty}^{\infty} f(x)dx = h \sum_{-\infty}^{\infty} f(mh) \quad - 2 \sum_{m=1}^{\infty} F(2\pi m/h)$$

$$0 = h \sum_{-\infty}^{\infty} f^{(2)}(mh) + \frac{8\pi^2}{h^2} \sum_{m=1}^{\infty} m^2 \, F(2\pi m/h),$$

$$0 = h \sum_{-\infty}^{\infty} f^{(4)}(mh) - \frac{32\pi^4}{h^4} \sum_{m=1}^{\infty} m^4 F(2\pi m/h),$$

and so on. By taking linear combinations of these equations we can eliminate $F(2\pi/h)$, $F(4\pi/h),\ldots,$ and the coefficients for these linear combinations are the numbers $a_{p,q}$. This procedure reminds us of the Romberg method, where terms in the error representation are eliminated by taking linear combinations of the trapezoidal sums with different values of h.

1.1.5. EXAMPLES

(i) $f(x) = e^{-x^2}$. In this case $f \in H_a$ for every $a > 0$. $R_d(h)$ follows from (1.19) and is given by

$$R_d(h) = -\,2\sqrt{\pi} \sum_{m=1}^{\infty} e^{-m^2\pi^2/h^2} \cos(2\pi md/h).$$

The first term resembles (1.17) with $\omega = 1$, $g = 1$. For an accuracy of 10^{-10}, $R_d(h)$ is neglectable for h smaller than (approximately) $\pi/\sqrt{10\ln 10} = 0.65\ldots$. In (1.9), with $d = 0$, the terms are neglectable for k larger than $\sqrt{10\ln 10}/h = 7.3\ldots$ (with $h = \pi/\sqrt{10\ln 10}$). Also the error for the rule in (1.30) with $p = 2$ is easily calculated. $E_{p,h}(f)$ of (1.27) becomes

$$E_{2,h}(f) = 2\sqrt{\pi} \sum_{m=1}^{\infty} (m^2-1)\, e^{-m^2\pi^2/h^2},$$

which is neglectable if h is smaller than (approximately) $h = 2\pi/\sqrt{10\ln 10} \simeq 1.31$. In (1.30), with $p = 2$, the terms are neglectable for m larger than 3.66. Hence by using the second derivative the number of terms is halved.

(ii) $f(x) = 1/(1+x^2)$. Now, $f \in H_a$ for every $0 < a < 1$. $R_d(h)$ follows from (1.19) and is given by

$$R_d(h) = -\,2\pi \sum_{m=1}^{\infty} e^{-2\pi m/h} \cos(2\pi md/h)$$

$$= \pi \frac{e^{-2\pi/h} - \cos(2\pi d/h)}{\cosh(2\pi/h) - \cos(2\pi d/h)}$$

$$= -2\pi/(e^{2\pi/h}-1), \quad \text{if } d = 0.$$

Hence, for given ε it is possible to choose h such that $|R_0(h)| < \varepsilon$. However, for efficient use of the trapezoidal rule it is necessary that the series in (1.9) converges rapidly. In this example, the terms are neglectable for (approximately) $k > 1/\varepsilon$. Consequently, the trapezoidal rule is unattractive for functions like the one in this example.

Slowly convergent integrals can be handled by using transformation with exponential functions. For this example we use $x \to \sinh x$, which yields

$$\int_{-\infty}^{\infty} \frac{dx}{1+x^2} = \int_{-\infty}^{\infty} \frac{dx}{\cosh x} .$$

Now the integrand belongs to H_a for $0 < a < \frac{1}{2}\pi$. And $R_d(h)$ is in this case

$$R_d(h) = -2\pi \sum_{n=1}^{\infty} \frac{\cos(2\pi nd/h)}{\cosh(n\pi^2/h)}.$$

For an accuracy of 10^{-10} we need in this case (with $h = 0.43$) approximately 54 terms in the sum of (1.9). For more information on the use of transformations of the variable the reader is referred to TAKAHASI & MORI (1973).

1.1.6. SOME NUMERICAL ASPECTS

1.1.6.1. As mentioned earlier, the integrals for the infinite interval are sometimes given in the form

$$\int_{-\infty}^{\infty} e^{-x^2} g(x)dx,$$

where $g \in H_a$ for some $a > 0$.

For the trapezoidal rule function values of the integrand are needed in the points $x_n = nh$, $n = 0,1,\ldots$. With respect to numerical evaluation of the function g, the computation of the exponential function may be rather time consuming. If, from numerical experiences or from representations of the remainder, for instance, it is known how small h must be chosen for obtaining a certain accuracy, it is possible to use pretabulated values of $\exp(-x_n^2)$ in the algorithm. A different approach is using a recursion relation for these values. For $n = 0,1,\ldots$ we have, with $e_n = \exp(-n^2h^2)$, $d_n = \exp(-2nh^2)$,

$$e_{n+1} = e_1 d_n e_n, \qquad d_0 = e_0 = 1,\ e_1 = e^{-h^2},$$

$$d_{n+1} = e_1^2 d_n.$$

Fro increaisng n some accuracy is lost in using this recursion. But, large values of n, corresponding to samll values of e_n, do not contribute significantly to the sum in the trapezoidal rule.

1.1.6.2. As follows from the results in following chapters, an explicit formula for g is not always known. In some cases we have available, however, the coefficients of the Taylor series (g may be supposed to be even)

$$g(x) = g_0 + g_2x^2 + \ldots ,$$

converging for, say, $|x| < R$. If R is large enough, i.e., if

$$\int_R^\infty e^{-x^2}\, g(x)dx$$

can be ignored within the desired accuracy, it is attractive to consider the modified trapezoidal rule from Section 1.1.4 including derivatives. For, in that case, derivatives of g are also available from Taylor series.

Function values of g for arguments x away from the origin need not to be computed within full accuracy. If the desired accuracy for the computation of the integral is denoted by ε (we suppose throughout that g is suitable scaled such that absolute and relative accuracy are nearly equal) the local accuracy for the function g in the integrand at $x > 0$, say $\bar{\varepsilon}(x)$, is approximately given by

$$\bar{\varepsilon}(x) \sim \varepsilon \exp(x^2).$$

If g is to be computed by a Taylor series, or by an analoguous expansion, we can take advantage of this aspect.

1.1.6.3. If the rate of convergence of the integral

$$\int_{-\infty}^{\infty} e^{-x^2} g(x)dx$$

is determined by the exponential part of the integrand, then it is easy to assign constants u_1,u_2, $u_1 < u_2$ such that

$$\left| \int_{u_2}^{\infty} e^{-x^2} g(x)dx + \int_{-\infty}^{u_1} e^{-x^2} g(x)dx \right|$$

is smaller that the prescribed accuracy. If g is analytic in a finite domain with vertices $u_1 \pm ia$, $u_2 \pm ia$ (with some $a > 0$) a representation of the error for the trapezoidal rule can be given for a finite interval. Details will be given in the following Subsection. At the moment, it is important to notice, that singularities of g close to the real x-axis but outside the interval $[u_1,u_2]$ may have little influence upon the rate of convergence of the trapezoidal rule.

1.2. THE FINITE INTERVAL

In this section the interval of integration [a,b] is finite and the functions to be integrated belong to the linear space $C_c^\infty([a,b])$ introduced in Definition 1.2. For the integrals considered a transformation to an infinite interval is always possible and hence the case can be treated with the methods of the foregoing section. But still it is interesting to examine how the remainder in the trapezoidal rule is given and how it behaves for small values of the discretization paramter h. In the foregoing case it turned out that for a wide class of functions H_a the remainder is of order $O[\exp(-2\pi a/h)]$ and in subsection 1.1.3 we obtained $O[\exp(-\pi^2/\omega h^2)]$.

Also for the case of a finite interval we discuss some methods for obtaining estimations for the remainder. From lemma 1.4 it follows that the remainder again is exponentially small, as will be made clear in the following. The results are not as nice as in the previous section. In fact, the theory on this type of quadrature seems to be incomplete. Also, Hilbert space methods are not considered for this problem in the literature. In connection with periodic analytic function integrated over the period many examples and results can be found, however, but these results cannot be applied on the underlying case.

The quadrature rule is given by

$$(1.31)\qquad \int_a^b f(x)dx = h \sum_{m=0}^{n}{}'' f(a+mh) + R_h(f), \qquad n = 1,2,\ldots,$$

with $h = (b-a)/n$ and $\sum''$ means that the first and last terms of the sum must be halved. If $f \in C_c^\infty([a,b])$, however, the endpoints do not contribute and the primes are immaterial. In the following subsections some representations of $R_h(f)$ are given.

It is expected that generally the remainder in (1.31) for $f \in C_c^\infty([a,b])$ is not as small as for comparable cases for the infinite interval. Some examples show convergence of order $O[\exp(-\gamma/\sqrt{h})]$ for some $\gamma > 0$ not depending on h. In Remark 1.12 and the example in 1.2.5 this will be illustrated.

For $f \in C_c^\infty([a,b])$ convergence of order

$$(1.32)\qquad O[h^\mu \exp(-\gamma/h^\alpha)], \quad h \to 0, \quad \mu \in \mathbb{R}, \quad \gamma > 0, \quad \alpha \geq 1,$$

cannot be expected as follows from the following theorem, which gives a result when a Fourier transform exhibits an exponential behaviour.

THEOREM 1.11.

(i) *Let the Fourier transform*

$$\hat{f}(t) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} f(x)\, e^{-ixt} dx$$

of f *exist for* $t \in \mathbb{R}$ *and suppose*

(1.33) $$|\hat{f}(t)| \le C|t|^{\mu} \exp(-\gamma|t|^{\alpha}), \qquad t \in \mathbb{R},$$

for some positive C, γ, μ *and* α *not depending on* t, *with* $\alpha \ge 1$. *Then* f *is analytic in a strip* $|\mathrm{Im}\, x| < \gamma$.

(ii) *If* $\hat{f}$ *satisfies* (1.33) *then* f *is not a compactly supported* C^{∞}*-function.*

PROOF.

(i) The inversion for Fourier transforms gives

(1.34) $$f(x) = (2\pi)^{-\frac{1}{2}} \int_{-\infty}^{\infty} \hat{f}(t)\, e^{ixt} dt.$$

Writing $x = \xi + i\eta$, $\xi, \eta \in \mathbb{R}$, and using (1.33), we can define the integral in (1.34) for $|\eta| < \gamma$, and hence f is an analytic function for these η-values.

(ii) An analytic function cannot have a compact support. □

As in the foregoing subsection for the infinite case, the error in the trapezoidal rule can often be associated with the Fourier transform of the function to be integrated. From the above result it follows that convergence of the order indicated in (1.32) may not be expected.

REMARK 1.12. This negative statement can be supplemented with information on $R_h(f)$ if the behaviour of f is known near a and b. Take for convenience $a = 0$. If for $x \to 0$

$$f(x) \sim x^{\mu}\, e^{-\alpha/x^{\beta}}, \quad \alpha > 0, \quad \mu \in \mathbb{C}, \quad \beta > 0,$$

and a similar behaviour near b, then a reasonable (though not rigorous) estimation of $R_h(f)$ is given by

$$R_h(f) = O(\lambda^{-(\mu+1+\frac{1}{2}\beta)/(\beta+1)} \exp\{-(\alpha\beta\lambda^{\beta})^{1/(\beta+1)}(1+1/\beta).$$
$$\cos[\tfrac{1}{2}\pi\beta/(\beta+1)]\})$$

for $h \to 0$, $\lambda = 2\pi/h$.

To illustrate this, we use the result given further, see Theorem 1.14, that the behaviour of $R_h(f)$ is given by

$$\int_0^b f(x)\, e^{i\lambda x} dx, \qquad \lambda = 2\pi/h,$$

and we suppose that f can be extended to complex x-values. Near $x = 0$ we have saddle points, the most relevant one being located at

$$x_0 = (\alpha\beta\lambda^{-1} e^{\frac{1}{2}i\pi})^{1/(\beta+1)}.$$

The saddle point method gives eventually the above estimate for $R_h(f)$. This expression has to be corrected with a term governed by the remaining endpoint of integration, b. If the the β-value in the asymptotic behaviour of f at b is larger than the β-value at 0, then the contribution of the saddle point near b is neglectable.

In the applications further in this paper, the value $\beta = 1$ occurs frequently. In this case we have

$$R_h(f) = O(\lambda^{-\frac{1}{2}(\mu+3/2)} e^{-\sqrt{2\alpha\lambda}}), \qquad h \to 0.$$

Let us now turn to some representations of the error term. In all cases $R_h(f)$ is given as an integral containing the function f or its higher order derivatives. The representation containing f turns out to be useful, especially if complex variable methods can be used such as the saddle point method in Remark 1.12.

1.2.1. <u>THE EULER-MACLAURIN FORMULA</u>.

<u>THEOREM 1.13</u>. *Let* $f \in C^{(2k+1)}([a,b])$. *Then*

$$(1.35) \qquad R_h(f) = \sum_{j=1}^{k} \frac{B_{2j}}{2j} h^{2j}[f^{(2j-1)}(b) - f^{(2j-1)}(a)]$$

$$+ h^{2k+1} \int_a^b P_{2k+1}\left(n \frac{x-a}{b-a}\right) f^{(2k+1)}(x)dx.$$

where P_m *is a periodic function associated with the Bernoulli polynomials.*

PROOF. See DAVIS & RABINOWITZ (1975). □

The proof is based on integration by parts. Remark that derivatives of f appear in (1.35). If $f \in C_c^{\infty}([a,b])$, then all terms in the finite sums vanish and k may be any integer. Hence

$$(1.36) \qquad R_h(f) = O(h^{2k+1}), \quad h \to 0,$$

for any k. It is difficult to obtain further information from (1.35), but let us turn to another reprsentation of $R_n(f)$.

1.2.2. We suppose first that $a = 0$, $b = \pi$. Equally spaced quadrature rule are related with the Gauss-Chebyshev quadrature rule. The following theorem illustrates this aspect.

THEOREM 1.14. *Let* $f \in C([a,b])$ *with an absolutely and uniformly convergent Fourier series*

$$(1.37) \qquad f(x) = \sum_{k=-\infty}^{\infty} a_k e^{ikx}, \quad a_k = \frac{\omega}{2\pi} \int_a^b f(x) e^{-ik\omega x} dx,$$

(with $\omega = 2\pi/(b-a)$*). Then* $R_h(f)$ *of* (1.31) *is given by*

$$(1.38) \qquad R_h(f) = -(b-a) \sum_{\substack{m=-\infty \\ m\neq 0}}^{\infty} e^{imn\omega a} a_{mn}.$$

PROOF. We see by discrete orthogonality properties that

$$R_h(e^{ikx}) = \begin{cases} 0 & \text{if} \quad k \neq mn \\ -(b-a)\, e^{imn\omega a} & \text{if } k = mn \end{cases} \qquad m = \pm 1, \pm 2, \ldots .$$

Substitution of (1.37) in $R_h(f)$ yields (1.38). □

Remark that in (1.38) $R_h(f)$ is free of derivatives of f. For applications this aspect is very important, since, generally, data of derivatives are not available. From Lemma 1.4 it follows that if $f \in C_c^\infty([a,b])$ each term in (1.38) is of order $O(h^\mu)$, for any μ. If $f \in C_c^\infty([a,b])$ the series is often so rapidly convergent that it may be closely approximated by the terms with $m = \pm 1$. If f can be defined for complex values of its argument the integrals in (1.37) can be estimated by asymptotics (k large), for instance by deforming the contour of integration.

The vanishing of $R_h(e^{ikx})$ for $k = -n+1,\dots,n-1$ is the above-mentioned Gaussian feature.

In terms of the function f the remainder $R_h(f)$ can be written as

$$-2 \sum_{m=1}^{\infty} \int_a^b f(x) \cos mn\omega(a-x)dx.$$

1.2.3. ABEL-PLANA FORMULA. This method is described in WHITTAKER & WATSON (1972) and OLVER (1974). We give a slightly modified version of it.

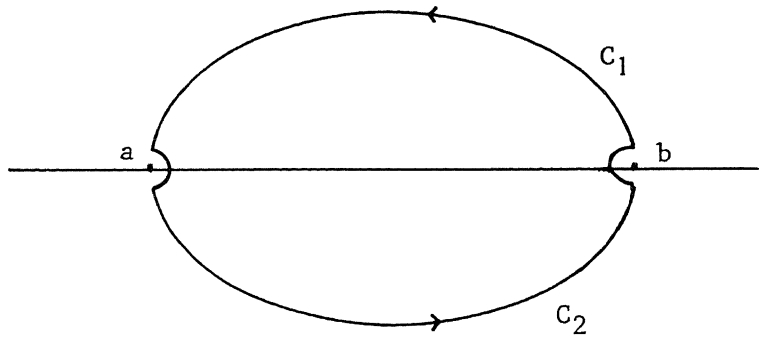

Figure 1.1

Let C be a closed contour in the complex z-plane as depicted in Figure 1.1, δ being less than $\frac{1}{2}h$, with $h = (b-a)/n$. Denote by C_1 and C_2 the upper and lower parts of C respectively. The direction of integration on C_i is indicated in the figure. Let f be continuous on C and holomorphic in the bounded domain with boundary C. Then we have by Cauchy's theorem

$$h \sum_{k=1}^{n-1} f(a+kh) = \frac{1}{2i} \int_C f(z) \operatorname{cotg}(\pi z/h)dz$$

and, furthermore,

$$h \sum_{k=1}^{n-1} f(a+kh) - \int_{a+\delta}^{b-\delta} f(x)dx =$$

$$\frac{1}{2i} \int_C f(z) \operatorname{cotg}(\pi z/h)dz + \frac{1}{2} \int_{C_1} f(z)dz - \frac{1}{2} \int_{C_2} f(z)dz =$$

$$(1.39) \qquad \int_{C_1} \frac{f(z)\, dz}{1 - \exp(-2i\pi z/h)} + \int_{C_2} \frac{f(z)\, dz}{\exp(2i\pi z/h)-1} .$$

If we suppose moreover $f \in C_c^\infty([a,b])$, then, since $f(a) = f(b) = 0$, we can take $\delta = 0$ and we write $R_h(f)$ of (1.34) as the sum of the integrals in (1.39). Hence, we have proved the following theorem.

THEOREM 1.15. *Under the conditions formulated in this subsection, we have*

$$(1.40) \qquad R_h(f) = \int_{C_1} \frac{f(z)\, dz}{1-\exp(-2i\pi z/h)} + \int_{C_2} \frac{f(z)\, dz}{\exp(2i\pi z/h)-1} .$$

REMARK 1.16. If f is holomorphic in the strip

$$(1.41) \qquad S = \{ z \mid a < \operatorname{Re} z < b \}$$

(and continuous at its boundary ∂S) and if $f(z) = o\,[\exp(2\pi|\operatorname{Im} z|)]$ as $z \to \infty$ in S, uniformly with respect to Re z, then C_1 and C_2 can be taken as parts of the lines Re z = a, Re z = b. In that case the remainder $R_h(f)$ has the form

$$(1.42) \qquad R_h(f) = i \int_0^\infty \frac{f(a+iy)-f(b+iy)-f(a-iy)+f(b-iy)}{\exp(2\pi y/h-1)} dy.$$

Again, representations in (1.40) and (1.41) are free of derivatives. Asymptotic methods may be used for obtaining esitmates of $R_h(f)$ for large values of h^{-1}. A first attempt might be applying Watson's lemma on (1.42), writing it as

$$(1.43) \qquad R_h(f) = \int_0^\infty e^{-2\pi y/h} F(y)dy,$$

but in Watson's lemma an expansion of F in positive powers of y is needed. For the functions considered here such an expansion is not available, owing to the essential singularities of f at a and b (and hence that of F at y = 0). In fact, due to these singularities, the asymptotic behaviour is much more intricate. For special cases it is possible to choose contours C_1 and C_2 in (1.40) such that they correspond to steepest descent contours on which the phase of the integrand is constant. For small values of h^{-1} these contours h are situated close to the interval [a,b], for $h^{-1} = 0$ they coincide with [a,b]. (We assume that f does not change sign in [a,b]). If h^{-1} becomes larger, C_i leave the interval [a,b], but the endpoints are still at a and b. In some cases both contours may split up in several contours extending to infinity. The example in Subsection 1.2.5 will show these phenomena.

1.2.4. In 1.1.4 results are given on a quadrature rule including derivatives of the integrand. For the finite case such a generalization can be given also. We summarize some results of KRESS (1971), where periodic functions are considered that are analytic in a strip containing the real line. The quadrature rule reads as follows. Let $f \in C^p([0,2\pi])$, with p even, then

$$\int_0^{2\pi} f(x)dx = I_{p,n}(f) + E_{p,n}(f),$$

$$I_{p,n}(f) = \sum_{\substack{q=0 \\ q \text{ even}}}^{p} \frac{a_{q,p}}{(2n)^q}\, h \sum_{m=0}^{2n-1} f^{(q)}(mh), \qquad h = \pi/n,$$

where the $a_{q,p}$ are given via (1.26). For periodic analytic functions the remainder can be estimated as in (1.29) (with some modifications). For 2π-periodic functions $f\colon \mathbb{R} \to \mathbb{C}$ which have continuous q-th derivatives, $q \geq p + 2$, the remainder is bounded as follows

$$|E_{p,n}(f)| \le \frac{2\pi M_q}{(q-p-1)(\frac{1}{2}p!)^2 2^p p^{q-p-1} n^q},$$

where M_q is the maximum of $|f^{(q)}(x)|$ in $\mathbb{R}$. If $f \in C_c^\infty[0,2\pi]$, f can be considered as a 2π-periodic function on $\mathbb{R}$ and q can be taken arbitrarily.

We list below the first three integration formulas for $p = 0,2,4$, respectively.

For $f \in C_c^\infty([-a,a])$, $a > 0$, $h = a/n$ we have

$$I_{0,n}(f) = h \sum_{m=-n}^{n} f(mh),$$

(1.44)
$$I_{2,n}(f) = I_{0,n}(f) + \frac{h^3}{4\pi^2} \sum_{m=-n}^{n} f^{(2)}(mh),$$

$$I_{4,n}(f) = I_{0,n}(f) + \frac{5h^3}{16\pi^2} \sum_{m=-n}^{n} f^{(2)}(mh) + \frac{h^5}{64\pi^4} \sum_{m=-n}^{n} f^{(4)}(mh).$$

The coefficients $a_{q,p}$ of which the first are contained in (1.44) can easily be obtained by an elimination procedure as in 1.1.4. Representing the even function $f \in C_c^\infty([-a,a])$ by its Fourier series given in (1.37) and applying the quadrature rule on f and its even derivatives we have

$$\int_{-a}^{a} f(x)dx = h \sum_{m=-n}^{n} f(mh) - \pi \sum_{k=1}^{\infty} a_{2kn},$$

$$\int_{-a}^{a} f^{(2)}(x)dx = h \sum_{m=-n}^{n} f^{(2)}(mh) + \pi \sum_{k=1}^{\infty} (2kn)^2 a_{2kn},$$

$$\int_{-a}^{a} f^{(4)}(x)dx = h \sum_{m=-n}^{n} f^{(4)}(mh) - \pi \sum_{k=1}^{\infty} (2kn)^4 a_{2kn},$$

and so on. By taking linear combinations of these equations and using the property that the integrals of the derivatives vanish we can eliminate the first coefficients a_{2kn} at the right-hand sides.

1.2.5. EXAMPLE. Consider the function f defined as follows

$$f(x) = \begin{cases} \exp(-\omega/\cos x), & |x| < \tfrac{1}{2}\pi, \\ 0 \quad , & |x| \geq \tfrac{1}{2}\pi, \end{cases}$$

where $\omega \geq 0$. The integral

$$(1.45) \qquad F(\omega) = \int_{-\frac{1}{2}\pi}^{\frac{1}{2}\pi} f(x)dx$$

can be expresses as an integral of a Bessel function, but this aspect will not further used here. In fact we have

$$(1.46) \qquad F(\omega) = 2\int_{\omega}^{\infty} K_0(x)dx,$$

where $K_0(x)$ is the modified Bessel function. The function f of (1.45) is even and its definition can be extended to the complex varaibles, $z = x+iy$ giving an analytic function in the strip $|\mathrm{Re}\ z| < \frac{1}{2}\pi$. By using symmetric contours in (1.40) it can easily be seen that he two integrals equal each other; (1.42) reduces in this example to

$$(1.47) \qquad R_h(f) = -4\int_0^{\infty} \sin(\omega/\sinh y)\,\frac{dy}{\exp(2\pi y/h)-1}\ .$$

Since $F(\omega)$ is exponentially small for large positive ω we consider henceforth $e^{\omega}F(\omega)$. An estimate of $e^{\omega}R_h(f)$ will be obtained by considering h^{-1} as a large parameter in (1.40), which is modified for this example into

$$(1.48) \qquad e^{\omega}R_h(f) = 2\int_{C_1} \frac{e^{\varphi(z)}}{\exp(2i\pi z/h)-1}\, dz,$$

where

$$(1.49) \qquad \varphi(z) = \omega - \omega/\cos z + 2i\pi z/h,$$

and C_1 is a contour in the upper half plane Im $z \geq 0$ joining the points $\pm \frac{1}{2}\pi$. For the present analysis the function in the denominator will not be taken into account since it is of no importance in $I_m\ z > 0$.

We use saddle point methods for estimating (1.49). In this simple example, the calculations are rather complicated already, especially if we are allowing small and large values of ω ("small" and "large" specified further on, but with respect to h). For convenience we write

$$(1.49) \qquad \lambda = 2\pi/h (= 2n).$$

Saddle points are solutions of the equation

$$(1.50) \qquad \omega \frac{\sin z}{\cos^2 z} = i\lambda.$$

In order to solve this equation it is convenient to consider three distinct cases in which $2\lambda/\omega$ is less than, greater than, or equal to 1, respectively. We consider these three cases in turn.

(i) If $\omega > 2\lambda$, we define $\mu = \omega/(2\lambda) > 1$. In the strip $|\mathrm{Re}\ z| < \frac{1}{2}\pi$ the saddle points are situated at the positive imaginary axis at

$$(1.51) \qquad z^{\pm} = i \operatorname{arcsinh} (\mu \pm \sqrt{\mu^2-1}).$$

A further analysis shows that of these saddle points the one closest to the origin (i.e., z^-) can be used for a steepest descent path joining $\pm \frac{1}{2}\pi$. At z^- the exponential function in the numerator of the integrand in (1.48) has the value $\exp[\varphi(z^-)]$, with

$$(1.52) \qquad \varphi(z^-) = \omega\{1 - [(1 + \sqrt{1-1/\mu^2})/2]^{\frac{1}{2}} - \frac{1}{2\mu} \operatorname{arcsinh}(\mu - \sqrt{\mu^2-1})\}.$$

From asymptotic analysis it follows that $\exp[\varphi(z^-)]$ gives a measure for the smallness of $|e^{\omega} R_h(f)|$. For large μ (i.e., $\omega >> 2\lambda$), $\varphi(z^-)$ behaves as

$$(1.53) \qquad \varphi(z^-) = -\frac{\omega}{8\mu^2}(1+0(\mu^{-1})), \quad \mu \to \infty$$

(considering ω fixed). Hence, if both $\frac{\omega}{8\mu^2} = \frac{\lambda^2}{2\omega}$ and $\omega/2\lambda$ are large, then $|R_h(f)|$ may be expected to be small. In subsection 1.2.5.1 some numerical results based on (1.52) will be discussed together with the corresponding results for the remaining cases.

It is not difficult to give an explicit expression for the path of steepest descent through z^-. It follows from the equation Im $\varphi(z) = 0$. But details will not be given here.

(ii) If $\omega < 2\lambda$, we can find a real number α such that

(1.54) $\quad \omega = 2\lambda \sin\alpha, \qquad 0 \le \alpha < \frac{1}{2}\pi.$

Then, equation (1.50) is reduced to the two equations

(1.55) $\quad \sin z = e^{i\alpha}$

(1.56) $\quad \sin z = -e^{-i\alpha}$

First we remark that if $z = x + iy$ is a solution of one of these equations, then $\zeta = -x + iy$ is a solution of the other one. In the strip $|\mathrm{Re}\, z| < \frac{1}{2}\pi$ the solution of (1.55) is given by $z(\mu) = x(\mu) + iy(\mu)$ with

$$x(\mu) = \arccos(\sqrt{\mu}),$$

$$y(\mu) = \operatorname{arc\,sinh}(\sqrt{\mu}),$$

$$\mu = \omega/(2\lambda),$$

where the square root is positive and arc cos en arc sinh have their principle values. Hence, the solution of (1.55) lies on the curve defined by $y = \ln(\cos x + \sqrt{1+\cos^2 x})$ $(0 < x < \frac{1}{2}\pi)$, and that of (1.56) on the curve defined by the same equations, but with $-\frac{1}{2}\pi < x < 0$.

The steepest descent contour, into which C_1 from (1.48) can be deformed, consists of two parts: one part from $-\frac{1}{2}\pi$ through $-x(\mu) + iy(\mu)$, and the other part from $\frac{1}{2}\pi$ through $x(\mu) + iy(\mu)$, both parts extending to $y \to +\infty$.

Again, an equation for the steepest descent paths can be given, but it gives no relevant information.

An indication for the smallness of $|e^{\omega} R_h(f)|$ is obtained from $\exp\{\operatorname{Re}\varphi[z(\mu)]\}$, with

$$\varphi[z(\mu)] = \lambda[2\mu - \sqrt{\mu(1+\mu)} - \ln(\sqrt{\mu} + \sqrt{1+\mu})]. \tag{1.57}$$

For small μ (i.e., $\omega << 2\lambda$), $\varphi[z(\mu)]$ behaves as

$$\varphi[z(\mu)] \sim -\sqrt{2\lambda\omega} = -2\sqrt{\pi\omega/h}, \qquad \mu \to 0.$$

Hence for $h \to 0$, ω fixed, we have

$$e^{\omega} R_h(f) = O[\exp(-2\sqrt{\pi\omega/h})].$$

Remark that for small μ the saddle points are close to the singular points $\pm \frac{1}{2}\pi$. In fact we have

$$z(\mu) = \tfrac{1}{2}\pi - \sqrt{\mu} + i\sqrt{\mu} + O(\mu\sqrt{\mu}), \ \mu \to 0.$$

Numerical results based on (1.57) will be discussed in subsection 1.2.5.1.

(iii) If $\omega = 2\lambda$, the two saddle points of the foregoing case coincide. It is possible to give an estimate for $e^{\omega} R_h(f)$ which describes the transition of case (i) into case (ii) uniformly by using Airy functions. Taking (1.52) with $\mu = 1$ or (1.57) with $\mu = \frac{1}{2}\pi$ gives the dominant part in the asymptotic behaviour, viz.

$$\varphi[z(\tfrac{1}{2}\pi)] = \lambda[2-\sqrt{2} - \ln(1+\sqrt{2})] \simeq -0.30\lambda. \tag{1.58}$$

<u>REMARK 1.17</u>. This last result seems to contradict an aspect discussed earlier. With Theorem 1.11 it was concluded that convergence of order as indicated in (1.31) is not possible. But in our example we are allowing large values of ω ("large" with respect to h) resulting in a different qualitative behaviour of $R_h(f)$. We emphasize the dependence on ω in this example, since in the applications the quadrature rule is used for functions with large and small values of the parameters.

1.2.5.1. Numerical computations based on the estimated accuracy.

For several values of ω the equation

$$(1.59) \qquad e^{\varphi} = \varepsilon$$

will be approximately solved, where φ is given in (1.52), (1.57) and (1.58) and ε is a parameter indicating the accuracy. In this way we obtain a value of n, the number of function evaluations, or a value of h, the discretization parameter. In this example we have $h = \pi/n$. This value of n is not a correct indication of the number of function evaluations. First, the function to be integrated is even. Owing to this symmetry the value of n must be halved for obtaining the correct number of function evaluations. In the second place, some terms in the finite sum (1.34) do not contribute to the total sum (within a certain accuracy). Namely, since $f \in C_c^{\infty}([-\frac{1}{2}\pi,\frac{1}{2}\pi])$, f equals zero (within a certain accuracy) in neighborhoods containing as endpoints $\pm \frac{1}{2}\pi$. We suppose in this example, that fumction values smaller than ε (of (1.59)) do not contribute to the finite sum in the trapezoidal rule. In order to obtain the number of relevant function evaluations, denoted by n_0, we proceed as follows. We use the number $x_0(\omega,\varepsilon)$, defined by

$$e^{\omega - \omega/\cos x_0(\omega,\varepsilon)} = \varepsilon,$$

and we put

$$n_0 = 1 + [\tfrac{1}{2}n\, x_0(\omega,\varepsilon)/(\tfrac{1}{2}\pi)],$$

where the $\frac{1}{2}$ before n is due to the symmetry of the integrand and [ ] denotes the entier function.

For some values of ε we list the results, in Table I. More digits for h follows from $h = \pi/n$. For the meaning of ε_0 see Remark 1.18.

TABLE I

ω	$\varepsilon = 10^{-4}$				$\varepsilon = 10^{-8}$				$\varepsilon = 10^{-12}$			
	n	n_0	h	ε_0	n	n_0	h	ε_0	n	n_0	h	ε_0
1	26	13	0.12	$1.3_{10}-5$	95	46	0.03	$3.2_{10}-10$	205	101	0.02	$7.1_{10}-15$
3	13	6	0.24	$3.1_{10}-5$	38	18	0.08	$3.2_{10}-9$	78	37	0.04	$1.9_{10}-13$
5	10	4	0.31	$7.0_{10}-5$	28	13	0.11	$3.1_{10}-9$	53	24	0.06	$1.8_{10}-13$
10	9	3	0.35	$7.7_{10}-5$	20	8	0.16	$4.4_{10}-9$	35	15	0.09	$3.8_{10}-13$
15	9	3	0.35	$8.1_{10}-5$	18	7	0.18	$9.5_{10}-10$	30	12	0.11	$8.2_{10}-14$
25	10	3	0.31	$9.6_{10}-5$	17	6	0.19	$3.4_{10}-9$	26	9	0.12	$5.8_{10}-13$
50	14	3	0.22	$1.0_{10}-4$	20	5	0.16	$5.2_{10}-9$	27	8	0.12	$2.3_{10}-13$
75	18	3	0.18	$4.9_{10}-5$	24	5	0.13	$2.8_{10}-9$	30	8	0.11	$2.8_{10}-13$
100	21	3	0.15	$4.3_{10}-5$	28	6	0.11	$3.3_{10}-9$	35	8	0.10	$3.6_{10}-15$
250	34	3	0.09	$2.5_{10}-5$	47	6	0.07	$2.3_{10}-9$	56	9	0.06	$3.2_{10}-13$
500	48	3	0.07	$2.0_{10}-5$	67	6	0.05	$2.2_{10}-9$	82	9	0.04	$1.4_{10}-13$
750	59	3	0.05	$1.6_{10}-5$	83	6	0.04	$1.4_{10}-9$	101	9	0.03	$1.3_{10}-13$
1000	68	3	0.05	$1.5_{10}-5$	96	6	0.03	$1.2_{10}-9$	117	9	0.03	$1.1_{10}-13$

REMARK 1.18. The values of h in Table I are computed by using (1.52), (1.57) and (1.58). At yet it is not clear if indeed $R_h(f)$ is smaller than the corresponding values of ε. A verification will be given by computing the function $e^{\omega}F(\omega)$, with F given in (1.45), with high accuracy and compare these values againts those obtained with the trapezoidal rule with $h = \pi/n$ and n_0 (n and n_0 from Table I). The computed errors are given in Table I in the columns with heading ε_0.

Since the derivatives of the integrand of (1.45) are easily obtained, it is interesting to compare the trapezoidal rule with the extended rule including derivatives, as given in 1.2.4. For $p = 0,2,4$ and $n = 2,4, \ldots$ we comptuted $I_{p,n}(f)$ and $E_{p,n}(f)$ as defined in 1.2.4. The first value of n

that made $e^{\omega} E_{p,n}(f)$ smaller than ε is given in Table II, together with n_0, the number of relevant function evaluations; n_0 is taken as the largest value of m in the sums of (1.44) for which the terms are larger than $\frac{1}{2}\varepsilon$. The corresponding values of h are not given in the table, but they follow from $h = \pi/n$.

TABLE II

ε		$p = 0$		$p = 2$		$p = 4$	
10^{-4}	ω	n	n_0	n	n_0	n	n_0
	1	22	12	12	7	12	7
	3	12	7	4	3	6	4
	5	10	5	6	4	6	4
	10	10	5	6	4	4	3
	15	10	4	6	3	4	3
	25	10	4	6	3	4	3
	50	16	4	8	3	6	3
	75	18	4	10	3	8	3
	100	22	4	12	3	8	3
	250	32	4	18	3	12	3
	500	44	4	24	3	18	3
	750	54	4	30	3	22	3
	1000	62	4	34	3	24	3

ε		$p = 0$		$p = 2$		$p = 4$	
10^{-8}	ω	n	n_0	n	n_0	n	n_0
	1	42	22	44	23	30	16
	3	32	16	20	11	14	8
	5	26	13	14	8	12	7
	10	20	9	12	6	8	5
	15	18	8	10	5	8	5
	25	18	7	10	5	8	4
	50	20	6	12	5	8	4
	75	24	6	12	4	10	4
	100	28	7	14	4	10	4
	250	46	7	24	5	16	4
	500	66	7	34	5	24	4
	750	80	7	42	5	28	4
	1000	92	7	48	5	34	4

ε		$p = 0$		$p = 2$		$p = 4$	
10^{-12}	ω	n	n_0	n	n_0	n	n_0
	1	160	80	82	42	66	34
	3	68	33	34	18	28	15
	5	50	24	26	13	20	11
	10	32	15	18	9	14	7
	15	30	13	16	8	10	6
	25	26	10	14	6	10	5
	50	26	9	14	6	10	4
	75	30	9	16	5	12	5
	100	34	9	18	6	12	4
	250	56	10	28	6	20	5
	500	80	10	42	6	28	5
	750	98	10	50	6	34	5
	1000	114	10	58	6	40	5

REMARK 1.19. From Table I it follows that the estimates for h and n based on the asymptotic formulas are in good agreement with the correct values. A striking phenomenon in Table I is the slowly varying value of n_0 : the number of relevant function evaluations does not change much for increasing ω. From Table II it follows that the difference between $p = 0$ and $p = 2$ is more significant than that between $p = 2$ and $p = 4$.

It should be noted that, we cannot conclude that for all n larger than that of the table $|E_{p,n}(f)|$ is smaller than ε. For, $|E_{p,n}(f)|$ is not necessarily monotone with respect to n.

1.3. NUMERICAL ALGORITHMS

1.3.1. ON THE DISCRETIZATION ERROR

In the foregoing sections much attention was paid to the representation of the error in the trapezoidal rule. It turned out that for the infinite interval information from this representation can be obtained for estimating the error, while for the finite interval no good estimates can be given. The functions met in the subsequent sections are more complicated than that of the example in Subsection 1.2.5. Therefore it cannot be expected that for these cases asymptotic methods can be applied as was outlined in the simple case.

For numerical purposes, however, it is not important to have detailed information about the error terms. In the algorithm discussed below, the choice of h (discretization parameter) or the number of function evaluations can be easily corrected, since we use an iterative procedure. In such a procedure function values of the integrand are added to previous results over the entire range of integration in contrast to adaptive procedures where additional points are taken only in regions where the integrand varies rapidly.

1.3.1. Before discussing the details of the algorithms, it is worthwhile to make some remarks on the role of the parameter d introduced in Section 1.1, especially in (1.9). Let us recall this expression written as follows

$$\int_{-\infty}^{\infty} f(x)dx = T_d(h) + R_d(h), \tag{1.60}$$

with

$$(1.61) \qquad T_d(h) = h \sum_{k=-\infty}^{\infty} f(kh+d).$$

Considered as a function of d, $T_d(h)$ is a periodic function with period h. Therefore, $R_d(h)$ is periodic with the same period. If we have an even function f (which is not a restriction) then it is clear from (1.61) that $\partial T_d(h)/\partial d$ is zero when $d = 0$ and $d = \frac{1}{2}h$. Since $T_d(h)$ is a periodic function it will usually happen that one of these is a maximum amd the other a minimum. The left-hand side of (1.60) does not depend on h. Consequently, the same remarks apply on $R_d(h)$.

Combining terms with positive and negative m-values in (1.19), we obtain the Fourier series of $R_d(h)$ (considered as a function of d)

$$(1.62) \qquad R_d(h) = -\tfrac{1}{2} \sum_{m=1}^{\infty} F(2\pi m/h)\cos(2\pi md/h).$$

which describes the above mentioned periodicity with respect to d. If $f \in H_a$ (see Definition 1.1) the series is so rapidly convergent that the first term closely approximates $R_d(h)$. Hence $R_d(h)$ vanishes in neighborhoods of $d = \frac{1}{4}h$ and $d = \frac{3}{4}h$. (There must be at least one zero of $R_d(h)$ in $[0,h]$ since the integral of $R_d(h)$ with respect to d over a period h vanishes).

This suggests the choice $d = \frac{1}{4}h$ or $d = \frac{3}{4}h$. But, since f is even, these choices correspond to the case (h^*,d^*), with $h^* = \frac{1}{2}h$, $d^* = \frac{1}{2}h^*$. Therefore, it is sufficient to consider the choice $d = \frac{1}{2}h$, but we combine it with $d = 0$. The reason for this is obvious. When computing $T_0(h)$ and $T_{\frac{1}{2}h}(h)$ the value of $T_0(\frac{1}{2}h)$ follows immediately from

$$(1.63) \qquad T_0(\tfrac{1}{2}h) = \tfrac{1}{2}[T_0(h) + T_{\frac{1}{2}h}(h)],$$

giving an iterative procedure for the computation of the integral. An important feature is, that it is very plausible to assume that $R_0(h)$ and $R_{\frac{1}{2}h}(h)$ have a different sign, when f is real and even. Consequently, we expect that one of the following cases applies

$$T_0(h) < \int_{-\infty}^{\infty} f(x)dx < T_{\frac{1}{2}}(h)$$

or

$$T_{\frac{1}{2}h}(h) < \int_{-\infty}^{\infty} f(x)dx < T_0(h).$$

An important consequence is that the value of

$$(1.64) \qquad \varepsilon_h = |T_0(h) - T_{\frac{1}{2}h}(h)|$$

is a useful indication of the accuracy in our approximations process. If ε_h is smaller than the desired accuracy, the value of $T_0(\frac{1}{2}h)$, eventually computed by using (1.63), will be much more accurate than both members at the right of this formula. From the above discussion it also follows that the initial choise of h is rather immaterial, since all earlier computed function values are used in the final answer. Of course, too small starting values of h must be avoided.

Although the stop criterion based on the testing of ε_h is reliable, it may give an algorithm which is not very economical. In fact, if ε_h is small enough, both $T_0(h)$ and $T_{\frac{1}{2}h}(h)$ are good approximations for the integral. Hence one of them, say $T_{\frac{1}{2}h}(h)$, is computed only for the stop criterion, but it is not needed in the final answer. The computation of $T_{\frac{1}{2}h}(h)$, however, requires as many function evaluations as that of $T_0(h)$. The effort in computer time required in the computation of $T_0(h)$ is slightly greater than the effort required in all the previous stages of the iterative procedure added together. Consequently, if we fail to terminate the process when sufficient accuracy has been achieved, but carry out a single unnecessary iteration, the effort required for the whole calculation is doubled. (Incidentally, the effect on the accuracy of the result is that the number of correct significant figures is also approximately doubled.) It is important to have available a criterion for gauging the the accuracy at any stage, so that the iteration may be terminated appropriately. For instance, we might consider the sequences

$$T_0(h_0),\ T_0(h_1),\ T_0(_2),\dots,T_0(h_n)$$

(1.65)

$$T_{\frac{1}{2}h_0}(h_0),\ T_{\frac{1}{2}h_1}(h_1),\ T_{\frac{1}{2}h_2}(h_2),\ldots,T_{\frac{1}{2}h_n}(h_n),$$

with h_0 as the initial choice and $h_{i+1} = \frac{1}{2}h_i$, $i = 0,\ldots,n-1$. Some extrapolation device must be used in order to predict if it is necessary to compute the next terms in the sequence, or that it is sufficient to use $\frac{1}{2}[T_0(h_n) + T_{\frac{1}{2}h_n}(h_n)]$. Since it is not necessary to extrapolate for obtaining accurate values of $T_0(h_{n+1})$ and $T_{\frac{1}{2}h_{n+1}}(h_{n+1})$, but rather for the order of smallness of ε_{h_n}, we expect that it is possible to construct an algorithm being both reliable and efficient. After computing $T_0(h_{n+1})$ by using (1.63) it is possible to extrapolate on the sequence for $T_0(h_i)$ in (1.65), but this aspect is not examined in this paper.

In the case of a finite interval we have not introduced the shift parameter d. This can easily be done and the conclusions on the role of d are as above for the infinite interval. Since in the algorithms the role of d is explored in the iterative procedure, it is not necessary to give formulas in which d explictly occurs.

1.3.2. ON THE TERMINATION ERROR

In addition to the discretization error $R_d(h)$ a termination error must be considered for the series in (1.9), since in practice the summation is limited to a finite number of terms. The smallest integer number n_0, such that in

$$\int_{-\infty}^{\infty} f(x)dx = h[f(0) + 2\sum_{j=1}^{n_0} f(jh) + S_{n_0}(h;f)$$

(where f is even) $|S_{n_0}(h;f)|$ is smaller than the desired accuracy, is called the number of relevant function evaluations corresponding to h. Of course we suppose that h is so small that such a number n_0 exists.

Also in the finite case we can use n_0, as mentioned already in Subsection 1.2.5.1. Since we suppose throughout this paper that for a finite interval $f \in C_c^{\infty}([a,b])$, f equals zero (within a certain accuracy) in neighborhoods containing as endpoints a and b. For even f and $a = -b$ we write the quadrature rule as

$$\int_{-a}^{a} f(x)dx = h[f(0) + 2 \sum_{j=1}^{n_0} f(jh)] + S_{n_0}(h;f)$$

with $0 < n_0 \le n$, $n = a/h$. Again, the smallest integer n_0, such that $|S_{n_0}(h;f)|$ is smaller than the desired accuracy, is called the number of relevant function evaluations. If f is not even or $a \neq -b$ the concept is introduced equivalently. For an algorithm the user must supply constants α and β such that terms in the series (1.34) with function-arguments in $[a,\alpha]$ and $[\beta,b]$ do not contribute (within desired accuracy) to the sum.

1.3.3. ALGORITHMS

For a reliable algorithm h must be small enough, for an efficient algorithm n_0 must be small enough. For an optimal algorithm combining reliability and efficiency we should like to have a pair (h_0,n_0), where h_0 is the largest h for which the discretization error is small enough and n_0 is the number of relevant function evaluations (corresponding to h_0). If good estimates of the discretization error are available, as in the examples of Subsection 1.1.5, first h_0 can be computed and with this h_0 we compute n_0. In general an optimal pair (h_0,n_0) is not available and the algorithm will run with a pair (h,n) with $h < h_0$ and $n > n_0$.

The algorithm is already discussed in Subsection 1.3.1. Summarizing we list the several steps, as was done by STENGER (1973), for approximating $\int_{-\infty}^{\infty} f(x)dx$ to within ε, where $\varepsilon > 0$ and f even.

1. Pick $h = h_0$ and a real number x_0 such that

$$|h \sum_{hj \ge x_0} f(hj)| < \tfrac{1}{2}\varepsilon.$$

2. Set

$$T_0(h) = h \sum_{jh\in(-x_0,x_0)} f(hj)$$

(*) $$T_{\frac{1}{2}h}(h) = h \sum_{(j+\frac{1}{2})h \in (-x_0, x_0)} f[h(j+\tfrac{1}{2})]$$

3. Set

$$\varepsilon_h = |T_0(h) - T_{\frac{1}{2}h}(h)|,$$

$$T_0(\tfrac{1}{2}h) = \tfrac{1}{2}[T_0(h) + T_{\frac{1}{2}}h(h)].$$

4. If

$$\varepsilon_h < \tfrac{1}{2}\,\varepsilon$$

then roughly

$$\left| \int_{-\infty}^{\infty} f(x)dx - T_0(\tfrac{1}{2}h) \right| < \varepsilon.$$

5. If $\varepsilon_h \geq \frac{1}{2}\,\varepsilon$, then we replace h by $\frac{1}{2}h$ and return to (*).

The test criterion in 4. can be replaced by a criterion based on extrapolating of the sequence ε_{h_0}, $\varepsilon_{\frac{1}{2}h_0}$, ...

For a finite interval the algorithm is similar.

1.3.4. ALGOL-60 PROCEDURES

We describe the algorithms of the trapezoidal rule in terms of ALGOL-60 procedures, for the finite case. The simplest algorithm evaluates one of the sums

$$h \sum_{j=0}^{n-1} f(a+d+jh), \quad h \sum_{j=0}^{n}{}'' f(a+jh),$$

$0 < d < h$, $h = (b-a)/n$, $n = 1,2,\ldots$, as an approximation for the integral

$$\int_a^b f(x)dx.$$

It is given by

```
real procedure trap sum (a,b,x,fx,h,d,sym);
value a,b,h,d,sym; real a,b,x,fx,h,d; Boolean sym;
if sym then
trap sum:= 2* trap sum ((a+b)/2,b,x,fx,h,d,false) else
begin real s; s:= 0;
      if d = 0 then
      begin for x:= a,b do s:= s + fx/2;
            a:= a + h; b:= b - h/2
      end else a:= a + d;
      for x:= a step h until b do s:= s + fx;
      trap sum:= s * h
end trap sum;
```

The meaning of the formal parameters is

a,b: < variable >;
endpoints of the interval of integration; $a \leq b$;

x: < variable >;
integration variable; x can be used as Jensen-parameter for fx;

fx: < arithmetic expression >;
the integrand f(x);

h: < variable >;
discretization parameter; $0 < h < b-a$;

d: < variable >;
shift parameter; $0 \leq d < h$;

sym: < Boolean expression >;
if $f((a+b)/2+x) = f((a+b)/2-x)$
then sym should be true else false;

This procedure can be used for a fixed value of h. For an iterative algorithm we can use the procedure

```
real procedure trap (a,b,x,fx,h,d,sym,n);
value a,b,h,d,sym,n; real a,b,x,fx,h,d; Boolean sym; integer n;
begin real e,p,q,v;
     if d> h/2 then d:= h - d; e:= .5 * 10↑(-n);
     p:= trap sum (a,b,x,fx,h,d,sym);
     for h:= h, h/2 while v > e do
     begin q:= trap sum (a,b,x,fx,h,d+h/2,sym);
          v:= abs (p-q); p:= (p+q)/2
     end;
     trap:= p
end trap;
```

The meaning of the parameters a,b,x,fx,h,d and sym is as in trap sum; further we have

n: < variable >;
 the number of correct significant digits desired.

REMARK 1.20.

(i) The supplied value of n must not be too large: $\frac{1}{2}\ 10^{-n}$ must be larger than the machine accuracy. The value of n corresponds to the relative accuracy. It is indeed supposed that the integrals can be computed with relative precision and that (for intance by scaling f) relative and absolute accuracy are nearly equal. When this condition is satisfied, the procedure trap can also be used for less smooth functions than those of $C_c^\infty([a,b])$.

(ii) The procedure trap is not protected againts a too large number of iterations. The user can settle this for instance by replacing the statement $v > e$ by $v > e \wedge (b-a)/h < 1000$.

(iii) Fortran programs for related integrals are found in SQUIRE (1975) and (1976).

1.4. SOME CONCLUDING REMARKS

The methods of the Sections 1.1 and 1.2 on the trapezoidal rule for infinite and finite interval respectively resulted in a numerical algorithm in Section 1.3. It turned out that for both cases the same ALGOL-60 procedure can be used. Indeed, from a numerical point of view, there is not much distinction between the functions in the corresponding classes. In both cases the functions are smooth and they vanish (numerically) outside a finite interval. The representation for the discretization error, however, is quite different and, as mentioned earlier, the rate of convergence with respect to $h \to 0$ is more favourable in the infinite case.

In the following papers both cases will be demonstated for the computation of certain special functions. It will turn out that both cases have their own charm. The integrands will be constructed by methods from asymptotics and the integrand in the finite case is usually explicitly given, while that of the infinite case is defined by an implicit relation. From this phenomenon it might be concluded that the finite interval is more attractive for numerical purposes. It requires more function evaluations but these require not as much computing time as in the infinite case.

Although the function for the infinite interval is usually implicitly given, it is sometimes worthwhile to pay special attention to this case. It may happen, for instance, that an approximation for the integrand can easily be given in the form of a Taylor series. The coefficients in this series follow from asymptotic expansion, for instance from recurrence relations defining the coefficients. In that case it is also attractive to use derivatives of the integrand by which the rate of convergence is increased significantly.

Therefore both methods are presented. If efficiency is not the main point in the program and the ease of programming is preferred, the finite case should be considered. With some extra effort of the programmer, the infinite case may yield very efficient algorithms. As a rule, in both cases the reliability of the method is definitely established.

For easy reference we formulate a theorem for the connection between the coefficients of the Taylor series of an integrand and the coefficients of the asymptotic expansion of the integral and a condition for the validity of this connection.

THEOREM 1.21. *Let the function* $f(\omega)$ *have an asymptotic expansion for* $\omega \to \infty$

$$f(\omega) \sim \frac{1}{\sqrt{\omega}} [f_0 + \frac{f_1}{\omega} + \frac{f_2}{\omega^2} + \dots]$$

where the coefficients f_i *do not depend on* ω *and suppose that* f *for positive* ω *can be written as*

$$f(\omega) = \int_{-\infty}^{\infty} e^{-\omega u^2} g(u)du,$$

with g *holomorphic in a stirp containing the real* u-*axis*, $g(u) = O(e^{\sigma u^2})$ *as* $u \to +\infty$, *where* σ *is an assignable constant, and* g *does not depend on* ω. *Then*

$$f_k = \frac{\Gamma(k+\frac{1}{2})}{\Gamma(2k+1)} g^{(2k)}(0), \qquad k = 0,1,\dots .$$

PROOF. Follows from Watson's lemma and the uniqueness property of asymptotic expansions; see OLVER (1974). □

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