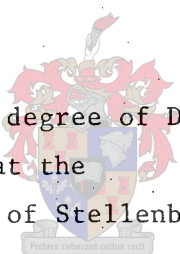


ON THE NUMERICAL EVALUATION OF FINITE-PART INTEGRALS INVOLVING
AN ALGEBRAIC SINGULARITY

by

H.R. Kutt

Thesis presented for the degree of Doctor of Philosophy
at the
University of Stellenbosch

The crest of the University of Stellenbosch is centered behind the text. It features a shield with a red and white design, topped with a crown and a banner. The banner contains the Latin motto "Fides subleuat culmen sapientiae".

Promoter: Prof. S.R.F. Göldner

Co-Promoter: Dr. R. Rösel

August, 1975

A B S T R A C T

Some problems of applied mathematics, for instance in the fields of aerodynamics or electron optics, involve certain singular integrals which do not exist classically. The problems can, however, be solved provided that such integrals are interpreted as finite-part integrals.

Although the concept of a finite-part integral has existed for about fifty years, it was possible to define it rigorously only by means of distribution theory, developed about twenty-five years ago. But, to the best of our knowledge, no quadrature formula for the numerical evaluation of finite-part integrals has been given in the literature.

The main concern of this thesis is the study and discussion of two kinds of quadrature formulae for evaluating finite-part integrals involving an algebraic singularity.

Apart from a historical introduction, the first chapter contains some physical examples of finite-part integrals and their definition based on distribution theory. The second chapter treats the most important properties of finite-part integrals; in particular we study their behaviour under the most common rules for ordinary integrals. In chapters three and four we derive a quadrature formula for equispaced stations and one which is optimal in the sense of the Gauss-type quadrature. In connection with the latter formula, we also study a new class of orthogonal polynomials. In the fifth and last chapter we give a derivative-free error bound for the equispaced quadrature formula. The error quantities which are independent of the integrand were computed for the equispaced quadrature formula and are also given. In the case of some examples, we compare the computed error bounds with the actual errors.

Besides this theoretical investigation of finite-part integrals, we also computed - for several orders of the algebraic singularity - the coefficients for both of the aforesaid quadrature formulae, in which the number of stations ranges from three up to twenty. In the case of the equispaced quadrature formula, we give the weights and - for integer order of the singularity - the coefficients for a numerical derivative of the integrand function. For the Gauss-type quadrature, we give the stations, the corresponding weights and the coefficients of the orthogonal polynomials.

These data are being published in a separate report [18] which also contains detailed instructions on the use of the tables.

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C O N T E N T S

ABSTRACT	i
ACKNOWLEDGEMENTS	iii
NOTATION	vi
<u>Chapter I</u> THE DEFINITION OF A FINITE-PART INTEGRAL	1
1.1 Historical introduction	1
1.2 Physical examples of finite-part integrals ...	22
1.3 Direct definition of finite-part integrals within the framework of distribution theory ..	26
1.4 The general case	37
<u>Chapter II</u> PROPERTIES OF FINITE-PART INTEGRALS	45
2.1 The basic rules of classic integration applied to finite-part integrals	45
2.2 Basic transformations of a finite integration interval	48
2.3 Transformation of an infinite integration interval	52
2.4 The continuity of the finite-part integral as a functional	55
<u>Chapter III</u> AN INTERPOLATORY QUADRATURE FORMULA	66
3.1 Derivation of the formula	66
3.2 Computation of the coefficients w_i and c_i	71
3.3 General properties of the w_i and c_i	75

<u>Chapter IV</u>	THE OPTIMAL QUADRATURE FORMULA	77
	4.1 The orthogonal polynomials associated with the optimal quadrature formula	77
	4.2 Theory of the optimal quadrature	105
	4.3 Quadrature formulae containing preassigned stations	118
	4.4 Computation of the stations and weights for the optimal quadrature formula	125
	4.5 Properties of the stations and weights	127
<u>Chapter V</u>	A. DERIVATIVE-FREE ERROR BOUND	130
	5.1 Error estimates for finite-part integrals in general	130
	5.2 The first method of obtaining the error quantities	134
	5.3 The second method of obtaining the error quantities	145
	5.4 General remarks	159
CONCLUSION	166
REFERENCES	167

NOTATION

$\delta(x - x_0)$	Dirac's delta function
$\theta(x - x_0)$	step function
$\int \dots, \text{f.p.} \int \dots, \int$	finite-part integrals
φ	a test function as a mapping
\mathcal{D}	the set of all test functions
$\langle d$	a distribution
$\langle d, \varphi \rangle$	the value of $\langle d$ for a specific φ
$f(x), g(y), h(t), F(x), \dots$	real valued functions
x, y, t, \dots	real variables
\ln	natural logarithm
$C^n [s, r]$	space of functions which are n times continuously differentiable in $[s, r]$
$\text{Re}(\lambda)$	real part of the complex magnitude λ
$R_n(x)$	remainder of Taylor's series
s, r	a singular, a regular point of an integrand
c, τ, χ	real vectors
$A, B, a, b, \alpha, \beta,$	real coefficients

x_i, w_i	stations, weights of a quadrature formula
$w(x)$	weight function
$\lambda_i^{m_i}$	monomial or moment
$P_n(x), p_n(x)$	orthogonal polynomials
$P_n^*(x), p_n^*(x)$	orthonormal polynomials
G_n	Gram determinant
\mathcal{H}	pseudo-Euclidean space
l_0, l_1, l_2, l_3	light vectors
$E_n(f)$	error of a quadrature formula
$\sigma_{n,p}$	error quantity independent of the integrand

CHAPTER ITHE DEFINITION OF A FINITE-PART INTEGRAL1.1 Historical introduction

1.1.1 The concept "finite-part integral" (f.p. integral) was first introduced by the French mathematician JACQUES HADAMARD in 1923. In his book "Lectures on Cauchy's Problem in Linear Partial Differential Equations" [9] he defined a certain class of f.p. integrals and also stated some of their main properties. The study of non-parabolic linear partial differential equations of second order with an odd number of variables had prompted him to introduce this new type of integral.

In the following we give a brief survey of his reflections on a specific example.

Given the equation for cylindrical waves (hyperbolic type)

$$F(u) \equiv \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - \frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} = f(x, y, t) \quad (1.1.1a)$$

where $u(x, y, t)$ is an unknown function (e.g. the velocity potential) and c a constant (the velocity of sound in the gas), the determination of u can be completed by the Cauchy-type conditions

$$u(x, y, 0) = u_0(x, y), \quad \frac{\partial u}{\partial t}(x, y, 0) = u_1(x, y), \quad (1.1.1b)$$

where u_0 and u_1 are also assumed given.

The value of the solution function u at a given point (x_0, y_0, t_0) may be calculated by first finding the Green's function $v = v(x, y, t; x_0, y_0, t_0)$ which is the solution of the adjoint equation $G(v) =$ (because F is self-adjoint) $F(v) = \delta(x-x_0)\delta(y-y_0)\delta(t-t_0)$ (in modern notation) and then substituting v into the generalized Green's formula

$$\iiint_T [vF(u) - uG(v)] dx dy dt = \iint_S \left[u \frac{dv}{dn} - v \frac{du}{dn} \right] dS, \quad (S = \partial T). \quad (1.1.1c)$$

HADAMARD assumed that if we draw the characteristic conoid from the point (x_0, y_0, t_0) as vertex, one of its sheets will cut out a certain (finite) portion S_0 of S , and, together with S_0 , be the boundary of the portion T of our space (x, y, t) . This geometric condition is expressed by saying that we have to deal with the interior problem. Under these assumptions it is well known that for linear hyperbolic equations the integral on the right-hand side of (1.1.1c) has to be taken only over the base S_0 and not over the mantle of T .

In the particular example, he assumed that S_0 is in the plane $t=0$.

The significant feature of HADAMARD's method for solving (1.1.1a) - where for the sake of simplicity he assumed $c=1$ - consists in directly substituting the Green's function

$$v = \frac{1}{\sqrt{\Gamma}}, \quad \text{where } \Gamma = (t_0 - t)^2 - (x - x_0)^2 - (y - y_0)^2 \quad (1.1.2)$$

and $\Gamma = 0$ represents the equation of the characteristic conoid with vertex (x_0, y_0, t_0) ,

into (1.1.1c). Doing so, he at first found a meaningless improper integral since the quantity under the integration signs becomes infinite in an impermissible manner. This fact had also been previously recognized by other mathematicians. However, they were able to - and in fact forced to - solve the Cauchy problem for the cylindrical wave equation by using other kinds of functions for v . But such methods have one decisive drawback: not the solution itself is obtained direct as by HADAMARD's method, but only an integral of the solution function.

We shall now show what actually happens when applying this method.

Inserting the Green's function (1.1.2) together with the initial conditions (1.1.1b) in formula (1.1.1c) and then integrating the left-hand side, we obtain, due to

$$G(v) = \delta(x-x_0)\delta(y-y_0)\delta(t-t_0),$$

$$2\pi u(x_0, y_0, t_0) = \iiint_T \frac{f}{\sqrt{\Gamma}} dx dy dt + \iint_{S_0} \left[\frac{u_1}{\sqrt{\Gamma}} - u_0 \frac{d}{dn} \frac{1}{\sqrt{\Gamma}} \right] dx dy. \quad (1.1.3a)$$

Since $\frac{d}{dn} = \epsilon \frac{\partial}{\partial t}$, where ϵ has the value +1 if the useful half-conoid is directed towards the decreasing t 's (the case of $t_0 > 0$) and -1 in the contrary case, we have

$$\frac{d}{dn} \frac{1}{\sqrt{\Gamma}} = \frac{|t_0|}{\Gamma^{3/2}}, \quad (1.1.3b)$$

irrespective of the sign of t_0 . We see immediately that this expression yields a meaningless integral if it is inserted in (1.1.3a). Nevertheless, HADAMARD was convinced he could find the correct solution by this method, provided he could give meaning to such "improper" integrals. This idea led him to conceive f.p. integrals. In [9], he says: "I thought it is worth while to attain this, though we cannot do so without introducing a rather paradoxical notation which I shall now speak of".

Introducing his new kind of "improper" integrals, he starts with a simple example corresponding to the previous Green's function, viz.

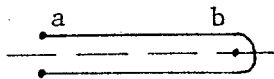
$$\int_a^b \frac{A(x)}{\sqrt{b-x}} dx. \quad (1.1.4a)$$

Direct differentiation of this integral with respect to b yields the absurd expression

$$-\frac{1}{2} \int_a^b \frac{A(x)}{(b-x)^{3/2}} dx + \left[\frac{A(x)}{\sqrt{b-x}} \right]_{x=b}, \quad (1.1.4b)$$

a sum of two terms, the first of which has no meaning as containing an infinity of order $3/2$ under the integral sign and the second being evidently meaningless. HADAMARD remarks that there are nevertheless two approaches for evaluating the derivative of (1.1.4a).

- (1) Direct differentiation (i.e. differentiation without any transformation) would consist in replacing the real integral (1.1.4a) by half the complex integral taken along a circuit consisting of two lines along a, b , connected by a small circle around b^1 (see fig. below);



- (2) In order to avoid complex quantities, he notices that (replacing b by x in the upper limit) not the integral in (1.1.4b) but the algebraic sum

$$\int_a^x \frac{A(y)}{(b-y)^{3/2}} dy - 2 \frac{A(x)}{\sqrt{b-x}}$$

approaches a perfectly definite limit when x approaches b . Moreover, he says, the same takes place for

$$\int_a^x \frac{A(y)}{(b-y)^{3/2}} dy + \frac{B(x)}{\sqrt{b-x}} \quad (1.1.5)$$

if B is any function of x , provided it is differentiable (or at least satisfies Lipschitz's condition

$|B(x_2) - B(x_1)| < K|x_2 - x_1|$, $x_1, x_2 \in [a, b]$), and such that

$B(b) = -2A(b)$.

¹ Here $A(x)$ is supposed to be analytic: a hypothesis which is easily avoided since it is sufficient to suppose that $A(x)$ has a derivative.

Indeed, if we integrate the integral in (1.1.5) by parts and form the limit, we obtain

$$- 2A(a)(b-a)^{-\frac{1}{2}} - 2 \lim_{x \rightarrow b} \int_a^x \frac{A'(y)}{\sqrt{b-y}} dy \quad (1.1.6)$$

under the above conditions on $B(x)$.

Furthermore, we notice the important property that the result (1.1.6) is independent of the choice of this function B . This is owing to the above assumptions made in regard to B and the fact that the denominator is of a fractional order, while a change of the function B (under our hypothesis) would alter it by terms containing as factor $(b-x)$ to at least the first power, so that the corresponding terms in the fraction would necessarily vanish for $x=b$. Therefore, in order to calculate the limit of (1.1.5), we do not even need to indicate what special function B we choose.

HADAMARD denoted that limit by "the finite part" of the integral in (1.1.4b) and wrote it

$$\left[\int_a^b \frac{A(x)}{(b-x)^{3/2}} dx \right]$$

The sign $\left[\right]$ being read "finite part of".

If A is analytic, this expression can equally well be defined as half of the corresponding integral taken along the circuit mentioned previously.

The same symbol was similarly defined by HADAMARD for higher orders of infinity, provided they always are fractional. The integral

$$\int_a^b \frac{A(x)}{(b-x)^{p+\frac{1}{2}}} dx, \quad p=1,2,3,\dots$$

is meaningless, but he defined the quantity

$$I = \sqrt{\int_a^b \frac{A(x)}{(b-x)^{p+\frac{1}{2}}} dx} \quad (1.1.7)$$

(the finite part of the integral in question):

- (i) if A is analytic, as half of the corresponding integral taken along the above-mentioned circuit;
- (ii) if A is supposed to have only p derivatives in the vicinity of b, as the limit for $x=b$, of the sum

$$\int_a^x \frac{A(y)}{(b-y)^{p+\frac{1}{2}}} dy + \frac{B(x)}{(b-x)^{p-\frac{1}{2}}},$$

B(x) being again any function bound by the conditions:

- (a) that the limit in question must exist;
- (b) that B must be differentiable p times, at least in the vicinity of $x=b$.

Again, the arbitrary choice of B has no influence on the value of the limit obtained. We may say briefly that HADAMARD gave a meaning to those "improper" integrals by removing "fractional infinities" at b .

Of course, his concept may also be introduced for the integral

$$\int_a^b \frac{A(x)}{(b-x)^{p+\mu}} dx, \quad p=1,2,3,\dots \quad (1.1.8)$$

μ being no longer necessarily equal to $\frac{1}{2}$, but still being necessarily contained in $(0,1)$. He also remarks that such considerations would even hold good to a certain extent for

$$\int_a^b \frac{A(x)}{(b-x)^p} dx \quad (1.1.9)$$

with p an integer. This integral could be reduced to a finite value by adding the terms

$$\frac{B(x)}{(b-x)^{p-1}} + B_1(x) \ln(b-x). \quad (1.1.10)$$

But then, he says, for $p > 1$ we could, by adding to $B(x)$ terms in $(b-x)^{p-1}$, modify the result in an arbitrary manner. Therefore this result is not determined when we merely know the integral (1.1.9), but requires the additive terms (1.1.10) to be given as well.

HADAMARD also gave a simple method for calculating the actual value of his f.p. integrals. This method consists in first finding

$$\int_a^b \frac{dx}{(b-x)^{3/2}} = \frac{-2}{\sqrt{b-a}}, \quad (1.1.11)$$

which is easily deduced from (1.1.6). If we now want to calculate, for instance, the quantity

$$\int_a^b \frac{A(x)}{(b-x)^{p+1/2}} dx$$

we subtract from $A(x)$ its expansion in powers of $(b-x)$ by Taylor's formula up to the term in $(b-x)^{p-1}$, which changes our expression into an ordinary integral; then we have to integrate (according to our meaning) such terms as

$$\int_a^b \frac{dx}{(b-x)^{q+1/2}},$$

the value of which is $\frac{-1}{(q-1/2)(b-a)^{q-1/2}}$, so that finally

$$I = \int_a^b \frac{A(x)}{(b-x)^{p+1/2}} dx = -\frac{A(b)}{(p-1/2)(b-a)^{p-1/2}} + \dots - \frac{(-1)^{p-1} A^{(p-1)}(b)}{(p-1)! (b-a)^{1/2}} + \int_a^b \frac{A_1(x)}{(b-x)^{p+1/2}} dx, \quad (1.1.12)$$

where

$$A_1(x) = A(x) - [A(b) - A'(b)(b-x) + \dots + (-1)^{p-1} \frac{A^{(p-1)}(b)}{(p-1)!} (b-x)^{p-1}].$$

This is equivalent to using the former definition and taking, for $B(x)$,

$$B(x) = \frac{A(b)}{(p-\frac{1}{2})(b-x)^{p-\frac{1}{2}}} - \frac{A'(b)}{(p-\frac{3}{2})(b-x)^{p-\frac{3}{2}}} + \dots + \frac{(-1)^{p-1} A^{(p-1)}(b)}{(p-1)! \frac{1}{2}(b-x)^{\frac{1}{2}}}.$$

Besides introducing this method of actually evaluating f.p. integrals, HADAMARD also stated some of their principal properties.

The rules for calculating a symbol such as (1.1.7) are generally identical to the rules applicable to ordinary integrals, as far

as equalities are concerned, for instance $\int_a^b = \int_a^c + \int_c^b$ and so on.

Changing the variable is also permissible, provided the variable is regular in b , i.e. one variable has with respect to the other a derivative, finite and different from zero, such that the order of infinitesimals around b is not changed.

Any property implying an inequality also requires due precaution since we cannot conclude anything as to the sign of a f.p. integral from the knowledge of the sign of the function, as the example of (1.1.11) immediately shows. We shall return to such properties in the next chapter.

Replacing the function A by another \tilde{A} in (1.1.12), whereby I is changed into \tilde{I} , and finding an upper limit for the difference $|\tilde{I}-I|$, we can write (on account of the well-known expression for the remainder of Taylor's series)

$$|\tilde{I}-I| \leq \frac{|\tilde{A}(b)-A(b)|}{\alpha_0} + \frac{|\tilde{A}'(b)-A'(b)|}{\alpha_1} + \dots + \frac{|\tilde{A}^{(p-1)}(b)-A^{(p-1)}(b)|}{\alpha_{p-1}} - \frac{|\tilde{A}_p - A_p|}{\alpha_p},$$

where $\alpha_i = 1/[i!(p-i-\frac{1}{2})(b-a)^{p-i-\frac{1}{2}}]$ ($i=0,1,\dots,p$) and A_p is an upper limit for the modulus of the p -th derivative of A in (a,b) .

If, for all $\varepsilon > 0$, there exists a set $\{\delta_0, \delta_1, \dots, \delta_p\}$ ($\delta_i > 0$ for $i=0,1,\dots,p$) and a function \tilde{A} (under our hypothesis (i) or (ii)) such that $|\tilde{I}-I| < \varepsilon$ when $\max_{x \in [a,b]} |\tilde{A}^{(i)}(x)-A^{(i)}(x)| < \delta_i$

($i=0,1,\dots,p$), we call the value of our f.p. integral (1.1.7) continuous with respect to the function A .

HADAMARD also extended his concept of f.p. integrals to multiple integrals, using arguments similar to the above. In this thesis we are, however, restricting ourselves to one-dimensional f.p. integrals.

With HADAMARD's concept of f.p. integrals in mind, we return to his method for solving the cylindrical wave equation.

Substituting (1.1.3b) into the right-hand side of (1.1.3a), we obtain

$$2\pi u(x_0, y_0, t_0) = \iiint_T \frac{f}{\sqrt{\Gamma}} dx dy dt + \iint_{S_0} \frac{u_1}{\sqrt{\Gamma}} dx dy - |t_0| \sqrt{\iint_{S_0} \frac{u_0}{\Gamma^{3/2}} dx dy}.$$

Introducing the polar coordinates $x = x_0 + r \cos \varphi$, $y = y_0 + r \sin \varphi$

($r = \sqrt{(x-x_0)^2 + (y-y_0)^2}$), the latter f.p. integral can be written

as

$$\int_0^{2\pi} d\varphi \sqrt{\int_0^{|t_0|} \frac{u_0 r dr}{(t_0^2 - r^2)^{3/2}}}.$$

As previously explained (see formula (1.1.12)), we have

$$\sqrt{\int_0^{|t_0|} \frac{u_0 r dr}{(t_0^2 - r^2)^{3/2}}} = \int_0^{|t_0|} \frac{(u_0 - \bar{u}) r}{(t_0^2 - r^2)^{3/2}} dr - \frac{\bar{u}}{|t_0|},$$

where \bar{u} stands for the value of u_0 at the extremity of the corresponding radius, i.e.

$$\bar{u} = u_0(x_0 + |t_0| \cos \varphi, y_0 + |t_0| \sin \varphi).$$

Thus we finally obtain

$$2\pi u(x_0, y_0, t_0) = \iiint_T \frac{f}{\sqrt{\Gamma}} dx dy dt + \iint_{S_0} \left[\frac{u_1}{\sqrt{\Gamma}} - \frac{|t_0|}{\Gamma^{3/2}} (u_0 - \bar{u}) \right] r dr d\varphi + \int_0^{2\pi} \bar{u} d\varphi,$$

which is indeed the correct solution of our Cauchy problem for the cylindrical wave equation (see e.g. [24]).

We remark that HADAMARD succeeded in dealing with the equation for damped cylindrical waves in a very similar way.

Before we conclude this brief survey of his new type of "improper" integrals, we consider a remarkable example of a f.p. integral given by him in [9].

It is well known that the integral representation of the Beta function $B(w, z)$, w and z complex, viz

$$\int_0^1 (1-t)^{w-1} t^{z-1} dt,$$

is valid for all w, z with $\text{Re}(w) > -1$ and $\text{Re}(z) > -1$. HADAMARD demonstrated the existence of a very similar integral representation which is valid even for certain real arguments ≤ -1 .

He considered

$$\int_{-\sqrt{\alpha}}^{+\sqrt{\alpha}} x^{q-1} (\alpha-x^2)^{m-\frac{1}{2}} dx = \alpha^{\frac{m+q-1}{2}} \int_0^1 t^{\frac{q-2}{2}} (1-t)^{m-\frac{1}{2}} dt = \alpha^{\frac{m+q-1}{2}} B(m+\frac{1}{2}, \frac{q}{2}), \tag{1.1.13}$$

where q is any positive integer and m any integer ≥ 0 . Starting from $m=0$, we obtain f.p. integrals containing $(1-t)^{n+\frac{1}{2}}$ or $(\alpha-x^2)^{n+\frac{1}{2}}$ (n a positive integer) in the denominator by differentiation with respect to α (or by a classic integration by parts, with respect to t , applied to the second form of the integral). Doing so, we see that

$$(i) \int_{-\sqrt{\alpha}}^{+\sqrt{\alpha}} \frac{x^{q-1}}{(\alpha-x^2)^{n+\frac{1}{2}}} dx \quad \text{or} \quad \int_0^1 \frac{t^{\frac{q-2}{2}}}{(1-t)^{n+\frac{1}{2}}} dt$$

is zero when q is odd and $n > \frac{q-1}{2}$;

(ii) otherwise

$$\int_{-\sqrt{\alpha}}^{+\sqrt{\alpha}} \frac{x^{q-1}}{(\alpha-x^2)^{n+\frac{1}{2}}} dx = \alpha^{\frac{q-1}{2}-n} \frac{\Gamma(\frac{q+1}{2})\Gamma(\frac{1}{2}-n)}{\Gamma(\frac{q-1}{2}-n)\Gamma(\frac{1}{2})} B(\frac{1}{2}, \frac{q}{2}). \quad (1.1.14)$$

By expressing the Beta function of (1.1.14) in terms of Γ -functions, it is possible to verify that the numerical factor will be the same as in (1.1.13), except that m is changed into $-n$, i.e. the factor is $B(\frac{1}{2}-n, \frac{q}{2})$. If we set $\alpha = 1$, we obtain in particular the relationship

$$\int_{-1}^{1} \frac{x^{q-1}}{(1-x^2)^{n+\frac{1}{2}}} dx = \int_0^1 \frac{t^{\frac{q}{2}-1}}{(1-t)^{n+\frac{1}{2}}} dt = B(\frac{1}{2}-n, \frac{q}{2}),$$

n any positive integer.

This means that, for certain real arguments not greater than -1 , the value of the Beta function is given by the f.p. of the usual integral definition.

1.1.2 When the theory of distributions had been established by LAURENT SCHWARTZ, who first presented this theory in a course of lectures given in the Seminar of the Canadian Mathematical Congress in 1949, it became possible to study f.p. integrals in a more general way than HADAMARD did. This study led to quite a new interpretation of those integrals.

L. SCHWARTZ published his theory of distributions in [28]. We shall here briefly repeat the results of that section of [28]

where he treats f.p. integrals from the point of view of distributions, and we assume the basic concept of the theory of distributions to be well known. Before going further, we explain the notation which will be used.

We choose DIRAC's "bra" and "ket" notation for distributions and test functions. Accordingly, we denote a typical test function as a whole (i.e. as a mapping, not as a set of values) by φ (the symbol φ is read "ket"), and the set of all test functions by \mathcal{D} . We denote a typical distribution (i.e. any linear continuous functional on \mathcal{D}) by $\langle d$ (the symbol \langle is read "bra") and denote the number which is the value of $\langle d$ for a specific φ by $\langle d, \varphi \rangle$ ("bra-c-ket"; hence bra and ket). If this number is ≥ 0 for all $\varphi \in \mathcal{D}$ such that $\varphi(x) \geq 0$ for all x , we call the distribution $\langle d$ positive. If $f(x)$ is an integrable function, we may define the distribution $\langle f$ "generated" by $f(x)$ by $\langle f, \varphi \rangle = \int_{-\infty}^{\infty} f(x)\varphi(x)dx$ for all $\varphi \in \mathcal{D}$. Such a distribution is called regular.

We shall now see how f.p. integrals arose in L. SCHWARTZ's theory of distributions.

He considered the function

$$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1/\sqrt{x} & \text{for } x > 0 \end{cases}$$

which is not defined at $x=0$. The derivative of this function exists and is continuous in the open intervals $(-\infty, 0)$ and $(0, +\infty)$. Differentiation, in the sense of distribution theory, of the

distribution $\langle f, \varphi \rangle$ generated by $f(x)$ yields

$$\begin{aligned} \langle f', \varphi \rangle &= - \langle f, \varphi' \rangle = - \int_0^{\infty} \varphi'(x) x^{-\frac{1}{2}} dx \\ &= - \lim_{\varepsilon \rightarrow 0} \int_{\varepsilon}^{\infty} \varphi'(x) x^{-\frac{1}{2}} dx, \end{aligned}$$

and applying integration by parts we obtain

$$\langle f', \varphi \rangle = \lim_{\varepsilon \rightarrow 0} \left[\frac{\varphi(\varepsilon)}{\sqrt{\varepsilon}} + \int_{\varepsilon}^{\infty} \varphi(x) \left(-\frac{1}{2} x^{-\frac{3}{2}}\right) dx \right].$$

Since $\varphi(\varepsilon) = \varphi(0) + o(\varepsilon)$ for $\varepsilon \rightarrow 0$, we have finally

$$\langle f', \varphi \rangle = \lim_{\varepsilon \rightarrow 0} \left[\int_{\varepsilon}^{\infty} \varphi(x) \left(-\frac{1}{2} x^{-\frac{3}{2}}\right) dx + \varphi(0) \varepsilon^{-\frac{1}{2}} \right]. \quad (1.1.15)$$

It is not difficult to see that the right-hand side of (1.1.15)

is exactly HADAMARD's definition for the f.p. of

$\int_0^{\infty} \varphi(x) \left(-\frac{1}{2} x^{-\frac{3}{2}}\right) dx$; i.e. the value of this f.p. integral is equal

to the value of the derivative of $\langle f$ on the test function $\varphi \rangle$.

This fact rendered it possible for L. SCHWARTZ to study f.p. integrals from the point of view of distributions. He generalized this concept of a f.p. integral in the following way.

Let $g(x)$ be a function which is integrable in the closed interval $[a+\varepsilon, b]$, $\varepsilon > 0$, but not in $[a, b]$. It could be that

$g(x)$ is the sum of a polynomial of $1/(x-a)$ and a function $h(x)$ which is integrable in $[a, b]$:

$$g(x) = P[1/(x-a)] + h(x) = \sum \frac{A_r}{(x-a)^{\lambda_r}} + h(x).$$

By a polynomial, he meant a sum of powers of monomials, in which the exponents λ_r may be complex, $\text{Re}(\lambda_r) \geq 1$, but not integers.

Under this assumption, we can write

$$\int_{a+\epsilon}^b g(x) dx = I(\epsilon) + F(\epsilon).$$

$I(\epsilon)$, the "infinite part" of the integral, is a polynomial in $\frac{1}{\epsilon}$ and has the form

$$I(\epsilon) = \sum \frac{A_r}{\lambda_r - 1} \left(\frac{1}{\epsilon}\right)^{\lambda_r - 1},$$

whereas $F(\epsilon)$ has a finite limit F for $\epsilon \rightarrow 0$. This quantity F is the one which HADAMARD calls the f.p. of the integral

$\int_a^b g(x) dx$ and L. SCHWARTZ writes for it:

$$F = \text{f.p.} \int_a^b g(x) dx = - \sum \frac{A_r}{\lambda_r - 1} \left(\frac{1}{b-a}\right)^{\lambda_r - 1} + \int_a^b h(x) dx.$$

His idea of generalizing the f.p. integral which still contains a non-integer exponent is based on the following fact: since φ is indefinitely differentiable, the function

$g(x)\varphi(x)$ has the same properties on $[a,b]$ as $g(x)$; in particular it is not integrable at $x=a$, and thus we may define the

$$\text{f.p.} \int_a^b g(x)\varphi(x)dx.$$

But, since $g(x)$ is integrable everywhere on $[a,b]$ except at $x=a$, $g(x)$ defines a distribution² $\langle g, \varphi \rangle$ the value of which is given by

$$\langle g, \varphi \rangle = \text{f.p.} \int_a^b g(x)\varphi(x)dx.$$

If we assume the function $g(x)$ to be zero outside a finite interval $[a,b]$ and to be not integrable at a finite number of points $a_i \in [a,b]$, we can write in a more general way

$$\langle g, \varphi \rangle = \text{f.p.} \int_{-\infty}^{\infty} g(x)\varphi(x)dx.$$

Replacing $g(x)$ by our above-mentioned function $f'(x)$, we see that the derivative of $\langle f$ in the sense of distributions is nothing else but the distribution generated by f' , viz

$$\langle f', \varphi \rangle = \text{f.p.} \int_0^{\infty} \varphi(x) \left(-\frac{1}{2} x^{-\frac{3}{2}}\right) dx.$$

At this point, we also refer to the footnote 1 of chapter IV (page 78).

² L. SCHWARTZ calls such a distribution a pseudo-function.

We now come to his most important statement about f.p. integrals. We calculate, still with the aforesaid function $g(x)$, the integral $\int_a^b g(x)(x-a)^\lambda dx$. If we assume λ to be complex, $\text{Re}(\lambda) > 0$ and sufficiently large, $g(x)(x-a)^\lambda$ is integrable on $[a, b]$ and thus that integral is an ordinary one.

We consider the (complex-valued) function F of the complex parameter λ as independent variable,

$$\begin{aligned}
 F(\lambda) &= \int_a^b g(x)(x-a)^\lambda dx \\
 &= - \sum \frac{A_r}{\lambda_r - \lambda - 1} \left(\frac{1}{b-a}\right)^{\lambda_r - \lambda - 1} + \int_a^b h(x)(x-a)^\lambda dx. \quad (1.1.16)
 \end{aligned}$$

The first term in (1.1.16) is analytically continuable; it is a meromorphic function of λ in the whole complex plane with a finite number of poles at the points $\lambda = \lambda_r - 1$. The second term in (1.1.16) is holomorphic for $\text{Re}(\lambda) > 0$ and continuous for $\lambda \rightarrow 0$. Thus, $F(\lambda)$ is meromorphic for $\text{Re}(\lambda) > 0$, since the λ_r 's are not integers, and it is continuous for $\lambda \rightarrow 0$. Forming this limit, we obtain

$$F(0) = - \sum \frac{A_r}{\lambda_r - 1} \left(\frac{1}{b-a}\right)^{\lambda_r - 1} + \int_a^b h(x) dx = \text{f.p.} \int_a^b g(x) dx.$$

L. SCHWARTZ therefore found that a f.p. integral involving a non-integer exponent can be considered as the analytic continuation of the function defined by an ordinary integral.

This is a quite new interpretation of a f.p. integral.

But we remember that HADAMARD had previously given an example, in connection with the Beta function, where such an interpretation is easily verified.

L. SCHWARTZ also made a very important remark which corresponds to that of HADAMARD concerning the signs of a f.p. integral and of the integrand involved. The previously mentioned function $f'(x) \leq 0$ in its whole domain whereas the distribution $\langle f' \rangle$ is not necessarily ≤ 0 for $\varphi \geq 0$. But this means that the signs of $\langle f', \varphi \rangle$ (value of f.p. integral) and $f'\varphi$ (integrand) may, in general, differ.

The fact that the behaviour of f.p. integrals involving an integer exponent is completely different, was also recognized. We now assume some λ_r 's to be integers and such that we can write the previous function $g(x)$ in the form

$$g(x) = \sum_{r \neq 1} \frac{A_r}{(x-a)^{\lambda_r}} + \frac{A_1}{x-a} + h(x).$$

The quantity $I(\varepsilon)$ in this case is therefore

$$I(\varepsilon) = \sum_{r \neq 1} \frac{A_r}{\lambda_r - 1} \left(\frac{1}{\varepsilon}\right)^{\lambda_r - 1} + A_1 \ln \frac{1}{\varepsilon}$$

and thus

$$\begin{aligned} F &= \text{f.p.} \int_a^b g(x) dx \\ &= - \sum_{r \neq 1} \frac{A_r}{\lambda_r - 1} \left(\frac{1}{b-a}\right)^{\lambda_r - 1} + A_1 \ln(b-a) + \int_a^b h(x) dx. \end{aligned}$$

Apart from the logarithmic term, the two most significant properties of f.p. integrals involving an integer exponent are the following:

- (i) They are no longer invariant with respect to a change of the variable. We shall return to this property in the second section of the next chapter and here consider only a simple example given by L. SCHWARTZ. It is clear from the above definition that

$$\text{f.p.} \int_0^1 \frac{dx}{x} = 0.$$

Transforming x by $t = \frac{x}{2}$, we obtain

$$\text{f.p.} \int_0^{\frac{1}{2}} \frac{dt}{t} = -\ln 2.$$

- (ii) F is not an analytic continuation of $F(\lambda)$ till $\lambda = 0$.

It is immediately seen that $F(\lambda)$ tends to ∞ if λ tends to

zero, whereas the f.p. $\int_a^b g(x)dx$ is the limit of $F(\lambda) - A_1/\lambda$ for $\lambda \rightarrow 0$.

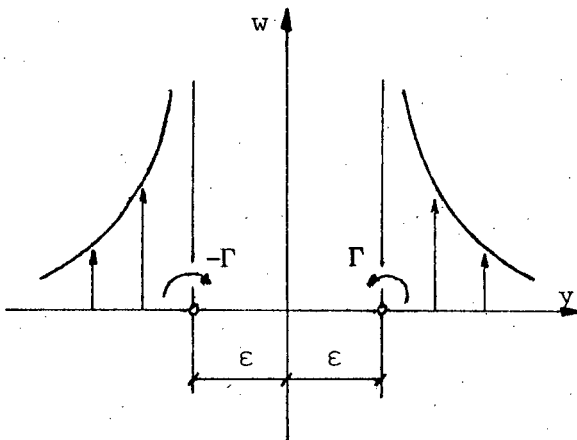
Concerning the last property, we remark that it is, nevertheless, possible to represent such f.p. integrals as an analytic continuation by means of the concept of regularization and by taking the residue at the pole of that continuation.

Before we come to our basic formula defining f.p. integrals, we shall illustrate the occurrence of such integrals in practice.

1.2 Physical examples of finite part integrals

To give a first example, we consider a simplified calculation of the velocity potential of a wing. Here one usually separates the thickness effects from the incidence effects by introducing the concept of a very thin wing at incidence and adding the thickness effects afterwards. The thin wing is then replaced by a distribution of horseshoe vortices in the plane $z = 0$.

The cross section through the tail of such a horseshoe vortex is given in the figure below.



We have thus a pair of vortices, each vortex with an absolute strength Γ , inducing a velocity distribution. The total linear momentum B of the two vortices is equal $2\epsilon\Gamma$. The component of the velocity in the z -direction (called downwash) is given by

$$w = \frac{1}{2\pi} \left(\frac{\Gamma}{y-\epsilon} - \frac{\Gamma}{y+\epsilon} \right).$$

Now, we ask for w if ϵ tends to zero, i.e. the two vortices coincide. Thereby, we require the total linear momentum B to remain constant, which means that as $\epsilon \rightarrow 0$ the vortex strength must tend to infinity. Forming that limit process, we obtain for the downwash

$$\lim_{\epsilon \rightarrow 0^+} w = \frac{B}{2\pi} \lim_{\epsilon \rightarrow 0^+} \left[\frac{1}{2\epsilon} \left(\frac{1}{y-\epsilon} - \frac{1}{y+\epsilon} \right) \right] = \frac{-B}{2\pi} \frac{d}{dy} \left(\frac{1}{y} \right) = \frac{B}{2\pi y^2}.$$

In this case, w becomes infinite at the origin.

Since the wing is idealized by a distribution of horseshoe vortices, the downwash at any point η of the wing is given by

$$w(\eta) = \frac{1}{2\pi} \text{f.p.} \int_{-s}^s \frac{B(y)}{(y-\eta)^2} dy,$$

where the integral is taken over the span length $2s$ of the wing.

In order to obtain the correct value for $w(\eta)$, we have to take the f.p. of the singular integral involved. But this fact was not always recognized in the literature. TRUCKENBRODT, for instance, evaluates such singular integrals in [32] in such a way that he obtained the correct result; however, his method is intuitive rather than mathematically founded. On the other hand, MANGLER applied the concept of f.p. integrals for the calculation of the downwash in [21], but he did not define them properly.

As a second example, we consider the Newtonian potential of a continuous mass distribution.

Let there be given a simple, piecewise smooth, space curve C : $x = x(s)$, $y = y(s)$, $z = z(s)$, s the arc length, and furthermore let a continuous mass distribution $\gamma(s)$ be defined on C (such a distribution is called line density). Then

$$U(P) = U(x,y,z) = - \int_C \frac{\gamma(s)}{r} ds,$$

represents the Newtonian potential of that distribution given on C ; r is the distance from the space point $P(x,y,z)$ to the current point of C . Thus, the above integral does not only depend on the integration variable s , but also on the coordinates of P , and is as a function of the latter continuous and arbitrarily often continuously differentiable, provided that the point P does not lie on C . Then, we can differentiate under the integral and obtain the field vector

$$\delta_i(x,y,z) = \partial_i U = \int_C \gamma(s) \frac{\kappa_i}{r^3} ds, \quad i=1,2,3,$$

where κ_i denotes the i -th component of the vector κ .

Now, we assume the point P to be on the curve C . Both integrals above become then improper. If the singularity is removable or integrable, i.e. $\gamma(P)$ vanishes in a neighbourhood of P , then the limits of the integrals are still considered to define the potential and the field vector respectively. Of course, this will essentially depend on the behaviour of the given dis=

tribution density γ . But since in general $\gamma(P) \neq 0$, these integrals will not exist and then they must be interpreted as f.p. integrals. We see that in this case the integrand for the potential becomes singular as x^{-1} and that for the field vector as x^{-2} .

In practice, it can also be that higher order derivatives of U (they form tensors) have to be calculated. Thus, the order of the singularity of the integrand involved increases.

As last example we calculate the potential at any space point $P(x,y,h)$ induced by a constant charge density σ on the (x,y) plane.

Introducing polar coordinates such that the origin coincides with the x,y coordinates of P , the potential would be given by

$$U(P) = 2\pi\sigma \int_0^{\infty} \frac{r}{\sqrt{r^2+h^2}} dr = 2\pi\sigma \sqrt{r^2+h^2} \Big|_0^{\infty} = \text{"}\infty\text{"} - 2\pi\sigma|h|,$$

which is meaningless since the above integral does not exist classically. We know that $U(P)$ is equal $-2\pi\sigma|h|$, thus in order to remove the infinite term the singular integral must be interpreted in the sense of an f.p. integral. To calculate this f.p. integral we first write the potential in the form

$$U = 2\pi\sigma|h| \text{ f.p. } \int_0^{\infty} \frac{x dx}{\sqrt{x^2+1}}, \quad \text{where } x = r/|h|,$$

and then substitute $1/y = \sqrt{x^2+1}$ into the latter f.p. integral. This yields, since $d(\sqrt{x^2+1}) = x dx/\sqrt{x^2+1} = -dy/y^2$,

$$U = 2\pi\sigma|h| \text{ f.p. } \int_1^0 \frac{-dy}{y^2} = 2\pi\sigma|h| \text{ f.p. } \int_0^1 \frac{dy}{y^2} = -2\pi\sigma|h|,$$

which is indeed the correct value of the potential at P.

1.3 Direct definition of f.p. integrals within the framework of distribution theory

Among the function with non-summable singularities at isolated points, the most important in practice are those with algebraic singularities. These are functions which, as x approaches the singular point x_0 , increase according to some power of $1/|x-x_0|$. In this thesis we shall consider only f.p. integrals which involve such functions.

So far we have seen how f.p. integrals involving an algebraic singularity of non-integer order were defined. In this section, we shall give two general formulae defining f.p. integrals by means of the concept of regularization (see e.g. [7]); one formula each for the cases of an integer and a non-integer exponent.

Since regularization is the main concern of this section, we repeat its definition fully. Let $f(x)$ be a function locally integrable in some neighbourhood of any $x \neq x_0$, x_0 a fixed, given point. A *regularization* of $f(x)$ is any continuous linear functional $\langle d$ over \mathcal{D} such that

$$\langle d, \varphi \rangle = \int_{[I]} f(x)\varphi(x)dx$$

whenever the closed interval $[I]$ does not contain x_0 and for all test functions φ whose support - the closure of the set on which they are not zero - is contained in the open interval I .

By means of any such regularization, we define a f.p. integral as follows. Let the function $f(x)$ be locally integrable over some neighbourhood of any $x \neq x_0$, and let $\langle f$ be any regularization of it. Then we define, for any interval $[a, b]$ with $a < x_0 < b$, the f.p. integral of $f(x)\varphi(x)$ over $[a, b]$ as

$$\int_a^b f(x)\varphi(x)dx \equiv \langle f, \varphi \rangle - \int_{-\infty}^a f(x)\varphi(x)dx - \int_b^{\infty} f(x)\varphi(x)dx. \quad (1.3.1)$$

The symbol \int here denotes the f.p. integral and we shall use it from now on throughout the thesis. The integrals on the right-hand side of (1.3.1) are ordinary ones (since $\varphi(x) \equiv 0$ outside a finite interval); one or both of them may vanish. Whereas a regularization is a distribution, i.e. a functional, the f.p. is a number, the value of the corresponding functional on a specific function. We remark that this latter function need not be a test function; it is sufficient if it can be uniformly approximated by test functions over a finite interval, and this is certainly possible if, for instance, the function is continuous. We should then take the limit of a sequence in (1.3.1).

Finally, we observe that, so far, our definition is not unique (since the regularization is not unique). It is known from distribution theory (see e.g. [7]) that two different regularizations of the same function differ by some finite linear combination of $\langle \delta^{(k)} \rangle$, $k=0,1,\dots$, i.e. by distributions concentrated at the singularity. If the order of the singularity is non-integer, uniqueness can be achieved by requiring the (distributional) derivative of the regularization of $f(x)$ to be equal to the regularization of the (ordinary) derivative of $f(x)$. The regularization defined in such a way commutes with differentiation and is uniquely characterized by this property.

As a typical example of a function with the type of singularity under discussion, consider

$$x_+^{-3/2} = \begin{cases} x^{-3/2} & \text{for } x > 0 \\ 0 & \text{for } x \leq 0. \end{cases} \quad (1.3.2)$$

The distribution generated by this function is not regular, since

$$\int_0^{\infty} x^{-3/2} \varphi(x) dx$$

will, in general, diverge. However, the function $x_+^{-3/2}$ can be regularized by the following method. We form the distributional derivative of the (regular) distribution generated by the function

$$x_+^{-1/2} = \begin{cases} x^{-1/2} & \text{for } x > 0 \\ 0 & \text{for } x \leq 0 \end{cases}$$

and obtain

$$\langle (x_+^{-1/2})', \varphi \rangle = - \langle x_+^{-1/2}, \varphi' \rangle = - \int_0^{\infty} x^{-1/2} \varphi'(x) dx.$$

Integrating the last expression by parts, whereby we introduce a limit process for the lower boundary, we have

$$\langle (x_+^{-1/2})', \varphi \rangle = - \frac{1}{2} \int_0^{\infty} \frac{\varphi(x) - \varphi(0)}{x^{3/2}} dx.$$

It is easily seen that the latter integral now converges. In view of the requirement regarding the derivative, stated above, we can also write

$$\langle x_+^{-3/2}, \varphi \rangle = \int_0^{\infty} \frac{\varphi(x) - \varphi(0)}{x^{3/2}} dx \quad (1.3.3)$$

and it is easily verified that the right-hand side of (1.3.3) represents a regularization of the function $x_+^{-3/2}$.

This same process of (distributional) differentiation can be continued, yielding a regularization for $x_+^{-1/2-n}$ after n steps. But we do not apply this process here in order to obtain our definition formulae for f.p. integrals since, if the order of singularity were integer, it would yield a formula valid only for integration intervals symmetric about the singularity.

Another method of obtaining the result of (1.3.3) is by analytic continuation, and it is essentially this method we shall use for finding our definition formulae. Before explaining the underlying principle of the method, we introduce the following definition. Consider a distribution $\langle f_\lambda \rangle$ depending on a parameter λ running over some open region Λ in the complex plane. Then $\langle f_\lambda \rangle$ is called an analytic functional of λ in Λ if $\langle f_\lambda, \varphi \rangle$ is an analytic function of λ for all $\varphi \in \mathcal{D}$.

The analytic continuation method is the following. Let $f_\lambda(x)$ be a function (of x) locally integrable when λ is in some region Λ of the complex plane, but not in general integrable otherwise. Further, for $\lambda \in \Lambda$ let $\langle f_\lambda, \varphi \rangle$ be analytic for every $\varphi \in \mathcal{D}$, and assume that it can be extended analytically to a wider region Λ_1 independent of φ . Then with the function $f_{\lambda_0}(x)$ for $\lambda_0 \in \Lambda_1 - \Lambda$ we may associate the functional $\langle f_{\lambda_0}, \varphi \rangle$ obtained by analytic continuation of $\langle f_\lambda, \varphi \rangle$ out of Λ . In other words we shall write

$$\int f_{\lambda_0}(x)\varphi(x)dx = \text{a.c.} \int_{\lambda \rightarrow \lambda_0} f_\lambda(x)\varphi(x)dx.$$

For instance, to define the distribution generated by the function (1.3.2) we shall consider the function

$$x_+^\lambda = \begin{cases} x^\lambda & \text{for } x > 0 \\ 0 & \text{for } x \leq 0. \end{cases}$$

For $\text{Re}(\lambda) > -1$ this is the regular functional given by

$$\langle x_+^\lambda, \varphi \rangle = \int_0^\infty x^\lambda \varphi(x) dx. \quad (1.3.4)$$

Now (1.3.4) is a function which is obviously analytic in λ , for its derivative with respect to λ is

$$\int_0^\infty x^\lambda \ln x \varphi(x) dx.$$

Let us rewrite the right-hand side of (1.3.4) in the form

$$\int_0^1 x^\lambda [\varphi(x) - \varphi(0)] dx + \int_1^\infty x^\lambda \varphi(x) dx + \frac{\varphi(0)}{\lambda+1}.$$

Here the first term is defined for $\text{Re}(\lambda) > -2$, the second for all λ , and the third for $\lambda \neq -1$. Thus the functional defined in (1.3.4) can be analytically continued to $\text{Re}(\lambda) > -2$, $\lambda \neq -1$, i.e. the function $\langle x_+^\lambda, \varphi \rangle$ itself is, for every $\varphi \in \mathcal{D}$, analytic for $\text{Re}(\lambda) > -2$, except for $\lambda = -1$ where it has a simple pole, the residue there being $\varphi(0)$.

In particular, for $\lambda = -3/2$ we have

$$\langle x_+^{-3/2}, \varphi \rangle = \int_0^1 x^{-3/2} [\varphi(x) - \varphi(0)] dx + \int_1^\infty x^{-3/2} \varphi(x) dx - 2\varphi(0). \quad (1.3.5)$$

The right-hand side of (1.3.5) agrees with that of (1.3.3),

since $2 = \int_0^{\infty} x^{-3/2} dx$. The extension of the definition to complex

values of λ was thus performed in a manner consistent with the previous definition for real λ .

We may proceed similarly and continue $\langle x_+^\lambda \rangle$ into the region $\text{Re}(\lambda) > -n-1$, $\lambda \neq -1, -2, \dots, -n$ to obtain

$$\begin{aligned} \langle x_+^\lambda, \varphi \rangle &= \int_0^{\infty} x^\lambda \varphi(x) dx = \int_0^1 x^\lambda [\varphi(x) - \varphi(0) - x\varphi'(0) - \dots - \\ &\quad - \frac{x^{n-1}}{(n-1)!} \varphi^{(n-1)}(0)] dx + \int_1^{\infty} x^\lambda \varphi(x) dx + \\ &\quad + \sum_{k=1}^n \frac{\varphi^{(k-1)}(0)}{(k-1)! (\lambda+k)}. \end{aligned} \quad (1.3.6)$$

Here again the right-hand side regularizes the integral on the left. This defines the distribution $\langle x_+^\lambda \rangle$ for all $\lambda \neq -1, -2, \dots, -n$.

In any strip of the form $-n-1 < \text{Re}(\lambda) < -n$, the equation (1.3.6) can be written in the simpler form

$$\langle x_+^\lambda, \varphi \rangle = \int_0^{\infty} x^\lambda [\varphi(x) - \varphi(0) - x\varphi'(0) - \dots - \frac{x^{n-1}}{(n-1)!} \varphi^{(n-1)}(0)] dx, \quad (1.3.7)$$

as follows from the fact that for $1 \leq k \leq n$

$$\int_1^{\infty} x^{\lambda+k-1} dx = \frac{-1}{\lambda+k}.$$

Equation (1.3.6) shows that when we treat $\langle x_+^{\lambda}, \varphi \rangle$ as a function of λ , it has simple poles at $\lambda = -1, -2, \dots, -n$, and its residue at $\lambda = -k$ is $\varphi^{(k-1)}(0)/(k-1)!$, $k=1, 2, \dots, n$.

It is shown in [7] that the regularization (1.3.6) commutes with differentiation, i.e. $\langle (x_+^{\lambda})', \varphi \rangle = \lambda \langle x_+^{\lambda-1}, \varphi \rangle$ if $\lambda \neq -1, -2, \dots, -n$. Thus it gives exactly the f.p. required by our definition based on regularization.

The regularization given by (1.3.7) enables us to evaluate any f.p. integral of the form $\int_a^b x^{\lambda} \varphi(x) dx$ provided that λ is not a negative integer.

We now come to the problem of finding a regularization of x_+^{-n} with $n=1, 2, 3, \dots$. The method of arriving at such a regularization is given in [7, page 85] and therefore it is here described only briefly.

In the neighbourhood of the pole $\lambda = -n$, the previous function $\langle x_+^{\lambda}, \varphi \rangle$ can be expanded in a Laurent series. To obtain this expansion explicitly, we isolate the term that fails

to converge at $\lambda = -n$, viz $\varphi^{(n-1)}(0)/[(n-1)!(\lambda+n)]$. The remaining (regular) part of this Laurent expansion is then an analytic function of λ in the strip $|\operatorname{Re}(\lambda) + n| > 1$. In particular, we are interested in the value of this regular part at $\lambda = -n$ which we shall denote by $\langle x_+^{-n}, \varphi \rangle$; so that by definition

$$\langle x_+^{-n}, \varphi \rangle \equiv \lim_{\lambda \rightarrow -n} \{ \langle x_+^{\lambda}, \varphi \rangle - \varphi^{(n-1)}(0)/[(n-1)!(\lambda+n)] \}.$$

It follows then that

$$\begin{aligned} \langle x_+^{-n}, \varphi \rangle &= \int_0^{\infty} x^{-n} [\varphi(x) - \varphi(0) - x\varphi'(0) - \dots - \\ &\quad - \theta(1-x) \frac{x^{n-1}}{(n-1)!} \varphi^{(n-1)}(0)] dx \end{aligned} \tag{1.3.8}$$

where $\theta(1-x)$ is equal to zero for $x > 1$ and equal to one for $x < 1$. We emphasize that $\langle x_+^{-n}$ is not the value of $\langle x_+^{\lambda}$ at $\lambda = -n$, as $\langle x_+^{\lambda}$ there has a pole and thus does not exist at this point.

Purely formally, all we have to do when setting $\lambda = -n$ in $\langle x_+^\lambda \rangle$ is to multiply the last term of the subtracted Taylor series by $\theta(1-x)$, so that it is set to zero when $x > 1$. The essential thing is that the integral in (1.3.8) does converge and that it does represent a regularization of the function x^{-n} (as is seen by considering a $\varphi(x)$ which vanishes in a neighbourhood of $x = 0$). However, the question as to whether the regularization (1.3.8) commutes with differentiation must be answered in the negative (see [7], page 87). Although we were able to establish a correspondence between the ordinary function x_+^{-n} and a distribution, we had to sacrifice the ordinary formula for the derivative. It is shown in [27] however, that it is possible to define another regularization which commutes with differentiation, but at the expense of losing the analytic connection to $\langle x_+^\lambda \rangle$. Since in view of problems of physics we prefer this latter property, we shall retain the above-mentioned definition.

By means of the regularizations (1.3.7) and (1.3.8) we can now derive two definition formulae for f.p. integrals; one formula each for the cases of an integer and non-integer exponent.

For practical purposes we introduce a notation for the remainder of Taylor's series. Explicitly, we shall use the form of Lagrange:

$$R_n(x) \equiv \varphi(x) - [\varphi(0) + \dots + x^n \varphi^{(n)}(0)/n!] = \frac{1}{n!} \int_0^x (x-y)^n \varphi^{(n+1)}(y) dy.$$

Thus we can write, for instance,

$$\langle x_+^{\lambda-n}, \varphi \rangle = \int_0^{\infty} x^{\lambda-n} R_{n-1}(x) dx; \quad -1 < \lambda < 0, \quad n=1, 2, \dots$$

For the f.p. integral, according to (1.3.1), we have the expression

$$\begin{aligned} \int_0^r x^{\lambda-n} \varphi(x) dx &\equiv \langle x_+^{\lambda-n}, \varphi \rangle - \int_r^{\infty} x^{\lambda-n} \varphi(x) dx = \\ &= \int_0^r x^{\lambda-n} R_{n-1}(x) dx - \sum_{k=0}^{n-1} [\varphi^{(k)}(0)/k!] \int_r^{\infty} x^{\lambda-n+k} dx = \\ &= \int_0^r x^{\lambda-n} R_{n-1}(x) dx + \sum_{k=0}^{n-1} \varphi^{(k)}(0) r^{\lambda-n+k+1} / [(\lambda-n+k+1)k!]. \end{aligned} \quad (1.3.9)$$

Proceeding in the same manner with the f.p. of $\langle x_+^{-n} \rangle$ we get one additional term,

$$\begin{aligned} \int_0^r x^{-n} \varphi(x) dx &= \int_0^r x^{-n} R_{n-1}(x) dx - \sum_{k=0}^{n-2} [\varphi^{(k)}(0)/k!] \int_r^{\infty} x^{-n+k} dx + \\ &\quad + [\varphi^{(n-1)}(0)/(n-1)!] \int_1^r x^{-1} dx = \\ &= \int_0^r x^{-n} R_{n-1}(x) dx + \sum_{k=0}^{n-2} \varphi^{(k)}(0) r^{-n+k+1} / [(-n+k+1)k!] + \\ &\quad + \ln r \varphi^{(n-1)}(0)/(n-1)! . \end{aligned} \quad (1.3.10)$$

Obviously, the sum over k drops out in (1.3.10) if $n = 1$.

1.4 The general case

So far we have assumed the singularity to be at the origin, but this is of course not necessary. In the following, we assume the singular point to be at $x_0 = s$, and consider the function.

$$(x-s)_+^\lambda = \begin{cases} (x-s)^\lambda & \text{for } x > s \\ 0 & \text{for } x \leq s. \end{cases}$$

For $\text{Re}(\lambda) > -1$, this function generates a regular distribution of the form

$$\langle (x-s)_+^\lambda, \varphi \rangle = \int_s^\infty (x-s)^\lambda \varphi(x) dx, \quad (1.4.1)$$

which is analytic in λ . It is easy to see that the same method of analytic continuation as before may be applied to (1.4.1). Instead of the equations (1.3.7) and (1.3.8) we here have the regularizations

$$\langle (x-s)_+^\lambda, \varphi \rangle = \int_s^\infty (x-s)^\lambda [\varphi(x) - \varphi(s) - (x-s)\varphi'(s) - \dots - \frac{(x-s)^{n-1}}{(n-1)!} \varphi^{(n-1)}(s)] dx,$$

$$\text{if } -n-1 < \text{Re}(\lambda) < -n$$

and

$$\langle (x-s)_+^{-n}, \varphi \rangle = \int_s^\infty (x-s)^{-n} [\varphi(x) - \varphi(s) - (x-s)\varphi'(s) - \dots - \theta(s+1-x) \frac{(x-s)^{n-1}}{(n-1)!} \varphi^{(n-1)}(s)] dx,$$

where $\theta(s+1-x)$ is equal to zero for $x > s+1$ and equal to one for $x < s+1$.

If we set

$$\begin{aligned} R_n(x,s) &\equiv \varphi(x) - [\varphi(s) + \dots + (x-s)^n \varphi^{(n)}(s)/n!] = \\ &= \frac{1}{n!} \int_s^x (x-y)^n \varphi^{(n+1)}(y) dy, \end{aligned}$$

the equations corresponding to (1.3.9) and (1.3.10) are here

$$\begin{aligned} \int_s^r (x-s)^{\lambda-n} \varphi(x) dx &= \int_s^r (x-s)^{\lambda-n} R_{n-1}(x,s) dx + \\ &+ \sum_{k=0}^{n-1} \varphi^{(k)}(s) (r-s)^{\lambda-n+k+1} / [(\lambda-n+k+1)k!] \end{aligned}$$

(1.4.2)

$$\begin{aligned}
\int_s^r (x-s)^{-n} \varphi(x) dx &= \int_s^r (x-s)^{-n} R_{n-1}(x,s) dx + \\
&+ \sum_{k=0}^{n-2} \varphi^{(k)}(s) (r-s)^{-n+k+1} / [(-n+k+1)k!] + \\
&+ \ln (r-s) \varphi^{(n-1)}(s) / (n-1)! \quad (1.4.3)
\end{aligned}$$

$$s < r.$$

(1.4.2) and (1.4.3) represent our definition formulae for the more general case of a f.p. integral involving an algebraic singularity at any point $x_0 = s$.

We now come to a generalization of f.p. integrals which concerns the integrand function. If we consider only the definition formulae (1.4.2) and (1.4.3) it is no longer necessary to assume $\varphi(x)$ to be a test function. Indeed, it is sufficient to take instead of $\varphi(x)$ any real function $f(x)$ of the real variable x satisfying the conditions

- (i) $f(x) \in C$ in an interval I containing $[s, r]$
- (ii) $f(x) \in C^n$ in a neighbourhood U of $x = s \in I$.

Under these conditions, the function $f(x)$ can be represented for any $x \in U$ by

$$f(x) = \sum_{k=0}^{n-1} (x-s)^k f^{(k)}(s) / k! + R_n(x,s),$$

where R_n denotes the remainder of the Taylor series.

We see that it is thus possible to define the f.p. integrals

$$\int_s^r (x-s)^{\lambda-n} f(x) dx \quad \text{and} \quad \int_s^r (x-s)^{-n} f(x) dx$$

by means of our definition formulae (1.4.2) and (1.4.3).

From now on, we shall consider exclusively f.p. integrals which involve an integrand function $f(x) \in C^n [s, r]$.

We now apply the above definition formulae to such f.p. integrals.

Since we introduced a specific form of the remainder $R_{n-1}(x, s)$, i.e. the form of Lagrange, we can go further. Indeed, changing the order of integration, for $-1 < \lambda \leq 0$, yields

$$\int_s^r (x-s)^{\lambda-n} R_{n-1}(x, s) dx = [1/(n-1)!] \int_s^r f^{(n)}(y) \int_y^r (x-s)^{\lambda-n} (x-y)^{n-1} dx dy.$$

We shall now show that the latter double integral can be almost completely integrated elementarily. In order to do so we must separate the cases $\lambda = 0$ and $-1 < \lambda < 0$. We start with the former case and set

$$I = [1/(n-1)!] \int_s^r f^{(n)}(y) \tilde{I} dy,$$

where

$$\tilde{I} = \int_y^r \left(\frac{x-y}{x-s} \right)^{n-1} \frac{dx}{x-s}.$$

The integral \tilde{I} can easily be evaluated by means of the substitution $t = (x-y)/(x-s)$. Thus we obtain

$$\tilde{I} = - \left[\sum_{k=0}^{n-2} \frac{1}{k+1} \left(\frac{r-y}{r-s} \right)^{k+1} + \ell n \frac{y-s}{r-s} \right]. \quad (1.4.4)$$

Inserting (1.4.4) in the equation for I yields

$$\begin{aligned} I = [-1/(n-1)!] \{ & \sum_{k=0}^{n-2} \frac{1}{(k+1)(r-s)^{k+1}} \int_s^r (r-y)^{k+1} f^{(n)}(y) dy + \\ & + \int_s^r \ell n (y-s) f^{(n)}(y) dy - \\ & - \ell n (r-s) \int_s^r f^{(n)}(y) dy \}. \quad (1.4.5) \end{aligned}$$

If we evaluate the first integral on the right-hand side of (1.4.5) sufficiently often by parts, the second one by the substitution $t = (y-s)/(r-s)$, the third one directly and insert I in (1.4.3) we finally obtain the formula

$$\begin{aligned}
 \int_s^r \frac{f(x)}{(x-s)^n} dx &= \frac{f^{(n-1)}(s)}{(n-1)!} \ln(r-s) + \sum_{k=0}^{n-2} \left[\frac{(r-s)^{-n+k+1}}{k!(-n+k+1)} f^{(k)}(s) - \right. \\
 &\quad \left. - \frac{k!}{(n-1)!(r-s)^{k+1}} f^{(n-k-2)}(r) + \right. \\
 &\quad \left. + \frac{k!}{(n-1)!} \sum_{m=0}^{k+1} \frac{1}{(k+1-m)!(r-s)^m} f^{(n-1-m)}(s) \right] + \\
 &\quad + \frac{r-s}{(n-1)!} \int_0^1 f^{(n)}[(r-s)t+s] \ln(1/t) dt.
 \end{aligned} \tag{1.4.6}$$

The remaining integral can, in general, not be integrated elementarily but, if $f^{(n)}$ is known, the integral can be evaluated numerically in a convenient way by a Gauss-type quadrature formula (given e.g. in [30]).

For the case $-1 < \lambda < 0$, we again set

$$\hat{I} = [1/(n-1)!] \int_s^r f^{(n)}(y) \hat{I} dy,$$

where

$$\hat{I} = \int_s^r (x-s)^{\lambda-n} (x-y)^{n-1} dx.$$

Integrating this integral $(n-1)$ times by parts yields

$$\hat{I} = \sum_{k=0}^{n-1} \frac{(-1)^k (n-1)! (r-s)^{\lambda-n+k+1} (r-y)^{n-1-k}}{(n-1-k)! \prod_{m=0}^k (m+1+\lambda-n)} + \frac{(-1)^n (n-1)! (y-s)^\lambda}{\prod_{m=0}^{n-1} (m+1+\lambda-n)}. \quad (1.4.7)$$

We insert the right-hand side of (1.4.7) in the above expression for I and obtain

$$I = \sum_{k=0}^{n-1} \frac{(-1)^k (r-s)^{\lambda-n+k+1}}{(n-1-k)! \prod_{m=0}^k (m+1+\lambda-n)} \int_s^r (r-y)^{n-1-k} f^{(n)}(y) dy + \frac{(-1)^n}{\prod_{m=0}^{n-1} (m+1+\lambda-n)} \int_s^r (y-s)^\lambda f^{(n)}(y) dy. \quad (1.4.8)$$

If we integrate the first integral in (1.4.8) $(n-k-1)$ times by parts and insert I in (1.4.2) we finally obtain the formula

$$\int_s^r \frac{f(x)}{(x-s)^{n-\lambda}} dx = \sum_{k=0}^{n-1} \left\{ \frac{(-1)^k (r-s)^{\lambda-n+k+1}}{(n-1-k)! \prod_{m=0}^k (m+1+\lambda-n)} \left[\sum_{m=1}^{n-k} \frac{(-1)^m (n-k-1)! (r-s)^{n-k-m}}{(n-k-m)!} f^{(n-m)}(s) + (-1)^{n-k} (n-k-1)! f^{(k)}(r) \right] + \frac{(r-s)^{\lambda-n+k+1}}{k! (\lambda-n+k+1)} f^{(k)}(s) \right\} + \frac{(-1)^n (r-s)^{\lambda+1}}{\prod_{m=0}^{n-1} (m+1+\lambda-n)} \int_0^1 t^\lambda f^{(n)}[(r-s)t+s] dt.$$

$$-1 < \lambda < 0$$

Owing to the structure of the formulae (1.4.6) and (1.4.9) it is clear that a f.p. integral can be evaluated by means of these formulae only if the corresponding derivatives of f are known. But even then, the computation can become cumbersome. It would therefore be desirable to have a quadrature formula for the numerical evaluation of such f.p. integrals. We shall present and discuss two kinds of such quadrature formulae in chapters III and IV.

CHAPTER IIPROPERTIES OF FINITE-PART INTEGRALS

In the first section of chapter I we mentioned that both HADAMARD and L. SCHWARTZ noticed some very strange properties of f.p. integrals. One we have observed is that if the integrand of a f.p. integral is positive throughout the open integration interval, the value of the integral can nevertheless be negative. We also noticed (see page 21) that a change of the integration variable yields a different result if λ is an integer. Therefore we may suppose that the standard classical rules for integration do not, in general, apply to f.p. integrals.

In this chapter we shall study the behaviour of f.p. integrals when subjected to the most common integration rules, and also their linearity and continuity properties and properties concerning inequalities. Throughout, we shall require the integrand function to be of $C^n[s, r]$ so that the definition formulae may be applied.

2.1 The basic rules of classic integration applied to finite-part integrals

From our definition formulae (1.4.6) and (1.4.9) it follows that a f.p. integral is a linear functional.

Thus it is clear that

$$(a) \int_s^r \sum_{i=1}^k (x-s)^{\lambda-n} \alpha_i f_i(x) dx = \sum_{i=1}^k \alpha_i \int_s^r (x-s)^{\lambda-n} f_i(x) dx, \quad -1 < \lambda \leq 0,$$

α_i real
 $s < r$

holds for every (finite) linear combination of functions $f_i(x)$.

- (b) We remember that up to now we always assumed the singular point s to have a value smaller than that of the other interval end point r . But this is only an apparent restriction since the case $r < s$ can easily be transformed to our standard case in the following way.

Given

$$\int_r^s \frac{f(x)}{(s-x)^{n-\lambda}} dx, \quad r < s, \quad -1 < \lambda \leq 0,$$

then by setting $x = -y$ we can transform this f.p. integral to

$$\int_{-s}^{-r} \frac{f(-y)}{[y - (-s)]^{n-\lambda}} dy.$$

The latter f.p. integral now has the standard form since $-s < -r$ and its value is given by our formulae.

- (c) From the definition of a f.p. integral it follows that any proper integral may also be considered as a f.p. integral. We can therefore split up $[s, r]$ into $[s, a]$ and $[a, r]$ and can write (omitting the integrand)

$$\int_s^r = \int_s^a + \int_a^r, \quad \text{with } a \text{ between } s \text{ and } r,$$

where the latter integral is now proper.

(d) For ordinary integrals there is the well-known rule that if the integrand $f(x) \geq 0$ in the integration interval $[a, b]$, then

$$\int_a^b f(x) dx \geq 0. \quad \text{But in the case of a f.p. integral, this rule}$$

is not applicable as the following counterexample shows.

Assume $f(x) \equiv 1$ in $[0, 1]$. Then, for instance,

$$\int_0^1 \frac{dx}{x^{n-\lambda}} = \frac{1}{\lambda-n+1} < 0 \quad \text{if } -1 < \lambda \leq 0 \quad \text{and } n=2, 3, \dots$$

It is also not true here that the equality holds if and only if the integrand vanishes almost everywhere in the integration interval. In order to show this, we again take $f(x) \equiv 1$ in $[0, 1]$ and calculate

$$\int_0^1 \frac{dx}{x} = 0,$$

i.e. the value of this f.p. integral is zero although the integrand function is positive within the whole open-integration interval.

(e) Furthermore, the classical rule that if $f(x) \geq g(x)$ in $[a, b]$

then $\int_a^b f(x) dx \geq \int_a^b g(x) dx$ is also not applicable to f.p. in-

tegrals. As a counterexample we consider $f(x) = x+1$ and $g(x) \equiv 1$ and calculate

$$\int_0^1 \frac{x+1}{x^3} dx = -\frac{3}{2}, \quad \int_0^1 \frac{dx}{x^3} = -\frac{1}{2}.$$

(f) In general, we may also not apply the classic inequality

$$\left| \int_a^b f(x) dx \right| \leq \int_a^b |f(x)| dx \quad \text{to f.p. integrals as is seen from}$$

the following example. Assume $f(x) \equiv -1$ in $[0,1]$. Then

$$\left| \int_0^1 \frac{-dx}{x^2} \right| = 1,$$

but
$$\int_0^1 \left| \frac{-1}{x^2} \right| dx = -1.$$

Summarizing, we can say that as far as equalities are concerned the common rules for ordinary integrals are also valid for f.p. integrals but rules concerning inequalities are, in general, not applicable to them.

2.2 Basic transformations of a finite integration interval

Given any f.p. integral of the form

$$I(s,r) = \int_s^r (x-s)^{\lambda-n} f(x) dx, \quad -1 < \lambda \leq 0, \quad s < r \quad (2.2.1)$$

with $f(x) \in C^n[s,r]$.

We first consider the simplest transformation of a finite integration interval, i.e. pure translation. Assume that the interval $[s,r]$ is shifted by the distance a . Equivalently we can say that this translation corresponds to a change of the variable of the form $y = x \pm a$. With the new variable y , (2.2.1) becomes

$$I(s \pm a, r \pm a) = \int_{s \pm a}^{r \pm a} [y - (s \pm a)]^{\lambda - n} f(y \mp a) dy = \int_{s'}^{r'} (y - s')^{\lambda - n} f(y \mp a) dy. \quad (2.2.2)$$

According to

$$r' - s' = r - s,$$

$$f^{(k)}(y \mp a) / y = s' = f^{(k)}(s),$$

$$f^{(k)}(y \mp a) / y = r' = f^{(k)}(r)$$

$$\text{and } f^{(n)}(y \mp a) / y = (r' - s')t + s' = f^{(n)}[(r - s)t + s]$$

we see immediately that the application of the definition formula (1.4.6) or (1.4.9) to (2.2.2) yields the value of $I(s, r)$, i.e.

$$\boxed{I(s \pm a, r \pm a) \equiv I(s, r)} \quad (2.2.3)$$

The f.p. integral (2.2.1) is therefore invariant with respect to any pure translation of its integration interval.

We now consider a transformation of $[s, r]$ consisting of a translation and a scaling. Assume that the interval $[s, r]$ is transformed to $[s', r']$, $s' < r'$. This can be achieved by setting

$$y = \frac{(x - s)(r' - s')}{r - s} + s'. \quad (2.2.4)$$

With the new variable y , the f.p. integral (2.2.1) becomes

$$I(s', r') = \left(\frac{r-s}{r'-s'} \right)^{1+\lambda-n} \int_{s'}^{r'} (y-s')^{\lambda-n} f(y) dy, \quad (2.2.5)$$

where

$$F(y) = f \left[\frac{(y-s')(r-s)}{r'-s'} + s \right].$$

Forming the corresponding derivatives which occur in the definition formulae we find that

$$F^{(k)}(y)/y=s' = \left(\frac{r-s}{r'-s'} \right)^k f^{(k)}(s)$$

$$F^{(k)}(y)/y=r' = \left(\frac{r-s}{r'-s'} \right)^k f^{(k)}(r)$$

$$F^{(n)}(y)/y=(r'-s')t+s' = \left(\frac{r-s}{r'-s'} \right)^n f^{(n)}[(r-s)t+s].$$

Applying the formula (1.4.9) to (2.2.5) and using the above expressions for the derivatives, we obtain the identity

$$\boxed{I(s', r')} \equiv I(s, r) \quad -1 < \lambda < 0, \quad (2.2.6)$$

i.e. the value of the f.p. integral $\int_s^r (x-s)^{\lambda-n} f(x) dx$, with

$-1 < \lambda < 0$, does not change if its integration interval $[s, r]$ is transformed to any finite interval $[s', r']$. This property agrees with that for ordinary integrals.

We now apply the definition formula (1.4.6) to (2.2.5), i.e. we assume λ to be zero, and again use the above expressions for the derivatives. This yields the relation

$$I(s', r') \equiv I(s, r) - \frac{f^{(n-1)}(s)}{(n-1)!} \ln \frac{r-s}{r'-s'} \quad (2.2.7)$$

which means that the f.p. integral $\int_s^r (x-s)^{-n} f(x) dx$ is not invariant with respect to a transformation of its integration interval which involves a scaling¹.

We thus have the important fact that our kind of f.p. integral is invariant with respect to the general linear transformation (2.2.4) only if the exponent is a non-integer. If the exponent is an integer, the original f.p. integral and the transformed one differ by the term $f^{(n-1)}(s) \ln [(r-s)/(r'-s')] / (n-1)!$, which stems from the basic difference between the corresponding definition formulae.

This behaviour has consequences for the evaluation of such f.p. integrals by a quadrature formula which has been derived for a certain fixed integration interval. In the following two chapters, we shall give quadrature formulae which refer to the integration interval $[0, 1]$. In order to compute the value $I(s, r)$ of $\int_s^r (x-s)^{-n} f(x) dx$ by these formulae, we must therefore set

$$I(s, r) = I(0, 1) + \frac{f^{(n-1)}(s)}{(n-1)!} \ln (r-s),$$

where $I(0, 1)$ is the value of $\int_0^1 x^{-n} f[(r-s)x + s] dx$.

¹ It should be noted that the behaviour of "associated functions" under a similarity transformation is similar to (2.2.7). See e.g. [7, page 82].

2.3 Transformation of an infinite integration interval

Up to now we have considered f.p. integrals with a finite integration interval $[s,r]$, s denoting the point where the integrand becomes infinite in $[s,r]$. The situation is completely different if we consider integrals with an unbounded integration interval $[r,\infty]$ and which do not exist as classical improper integrals. Thereby we assume that, as $x \rightarrow \infty$, the integrand $F(x)$ does not tend to zero faster than $1/x$. Since by setting $x=r/y$ such an integral can be transformed to a f.p. integral of the form

$$r \int_1^0 F(r/y) \frac{dy}{y^2} = r \int_0^1 \frac{f(y)}{y^2} dy, \quad r \neq 0,$$

we say that the original integral also represents a f.p. integral where the singularity is located at infinity.

Of course $x=r/y$ is not the only transformation which changes $[r,\infty]$ to a finite interval, but it is the simplest and certainly admissible. F.p. integrals involving a singularity at ∞ have in fact the strange property that they are not invariant under any arbitrary transformation which yields a finite integration interval. We demonstrate this by the following example.

Consider the integral

$$I = \int_0^{\infty} \frac{x^2}{1+x^2} dx, \quad r=0 \tag{2.3.1}$$

which does not exist classically, but can be given a meaning if we take the f.p. of the integral in question.

In order to calculate (2.3.1) we use the transformation $x = 1/y$ and thus obtain

$$I = \int_0^{\infty} \frac{dy}{y^2(1+y^2)}. \quad (2.3.2)$$

This integrand is now singular at the origin and has a finite limit as $y \rightarrow \infty$. Splitting up the integrand, we can write

$$I = \int_0^{\infty} \frac{dy}{y^2} - \int_0^{\infty} \frac{dy}{1+y^2}, \quad (2.3.3)$$

where the latter integral is regular and equal to $\pi/2$. Since the f.p. integral in (2.3.3) vanishes, we have

$$\int_0^{\infty} \frac{x^2}{1+x^2} dx = -\pi/2.$$

Instead of the above transformation, we now change the integration variable x in three different ways, viz

$$(i) \quad x = \frac{1}{y} - 1,$$

$$(ii) \quad x = \frac{\sqrt{1-z^2}}{z},$$

$$(iii) \quad x = \sqrt{\frac{2-t}{t}}.$$

By means of these transformations, (2.3.1) changes to

$$I_1 = \int_0^1 \frac{(1-y)^2}{y^2 + (1-y)^2} \frac{dy}{y}, \quad (2.3.4)$$

$$I_2 = \int_0^1 \frac{\sqrt{1-z^2}}{z^2} dz, \quad (2.3.5)$$

and

$$I_3 = \frac{1}{2} \int_0^2 \frac{\sqrt{2-t}}{t^{3/2}} dt \text{ respectively.} \quad (2.3.6)$$

To calculate (2.3.4) we can write

$$\begin{aligned} I_1 &= \int_0^1 \frac{y^2 + (1-y)^2 - y^2}{y^2 + (1-y)^2} \frac{dy}{y^2} = \int_0^1 \frac{dy}{y^2} - \int_0^1 \frac{dy}{2y^2 - 2y + 1} \\ &= -1 - \arctan(2y-1) \Big|_0^1 = -1 - \pi/2. \end{aligned}$$

Applying the formula (1.4.6) to (2.3.5), we obtain

$$I_2 = - \int_0^1 \frac{d^2}{dz^2} (\sqrt{1-z^2}) \ln z dz$$

and integration by parts yields

$$I_2 = \frac{z \ln z}{\sqrt{1-z^2}} \Big|_0^1 + \int_0^1 \frac{-dz}{\sqrt{1-z^2}} = -\pi/2.$$

(2.3.6) can be calculated by the formula (1.4.9) which yields

$$I_3 = -\frac{1}{2} \int_0^1 \frac{dt}{\sqrt{t(1-t)}} = -\pi/2.$$

We see that the transformations (ii) and (iii) yield the correct value of (2.3.1) but the transformation (i) does not, although all three transformations are very similar.

This example shows that the transformation of a f.p. integral with an infinite integration interval has to be chosen with great caution.

To be on the safe side, it is recommended that the pure reflection $x = r/y$ be applied to the integration variable x .

4. The continuity of the finite-part integral as a functional

We remember that according to our first definition (1.3.1), a f.p. integral was considered as a regularization of a certain distribution. From the definition of the regularization it thus follows that a f.p. integral represents a continuous functional.

In order to free us from the restriction to test functions, we said at the end of the previous chapter that the assumption $f(x) \in C^n [s,r]$ is sufficient for the existence of the f.p. integral under discussion. But then the question arises as to whether this f.p. integral is still a continuous functional.

In the following we shall show that under certain assumptions this question may be answered in the affirmative.

For ordinary integrals we know that if a sequence of integrable functions converges uniformly, the integral of this sequence is equal to the integral of the limit function. But for f.p. integrals, the uniform convergence of a sequence of f.p. integrable functions is not sufficient. We here need another definition of convergence, the so-called strong convergence in $C^n [s,r]$:

Definition

Given a sequence $\{f_\nu(x)\}$, where all $f_\nu(x) \in C^n[s,r]$. Then we say that $\{f_\nu(x)\}$ converges to $f(x)$ in $C^n[s,r]$ and write $\lim_{\nu \rightarrow \infty} \{f_\nu(x)\} = f(x)$, if the sequences $\{f_\nu^{(k)}(x)\}$ uniformly converge to $f^{(k)}(x)$ for $k=0,1,2,\dots,n$.

Alternatively we may say that we can, for every given $\epsilon > 0$, find an integer N which depends only on ϵ but not on $x \in [s,r]$ so that

$$|f_\nu^{(k)}(x) - f^{(k)}(x)| < \epsilon, \quad k=0,1,2,\dots,n,$$

for all $\nu > N(\epsilon)$.

Since $f(x) \in C^n[s,r]$, it is f.p. integrable and we can say that

Theorem

For any sequence $\{f_\nu(x)\}$ which converges to $f(x)$ in $C^n[s,r]$,

$$\lim_{\nu \rightarrow \infty} \int_s^r (x-s)^{\lambda-n} f_\nu(x) dx = \int_s^r (x-s)^{\lambda-n} \lim_{\nu \rightarrow \infty} f_\nu(x) dx, \quad -1 < \lambda \leq 0, \quad (2.4.1)$$

i.e. the f.p. integral is a continuous functional on $C^n[s,r]$ and thus we may interchange the limit and the integral symbol.

Proof

We consider only the case $\lambda = 0$, since the proof is the same for $\lambda \neq 0$, and denote the integrals on the left-hand and right-hand sides of (2.4.1) by I_ν and I respectively.

Then by means of the definition formula (1.4.6) we can write

$$\begin{aligned}
 |I_\nu - I| &= |[f_\nu^{(n-1)}(s) - f^{(n-1)}(s)] \dots + \sum_{k=0}^{n-2} \{ [f_\nu^{(k)}(s) - f^{(k)}(s)] \dots - \\
 &\quad - [f_\nu^{(n-k-2)}(r) - f^{(n-k-2)}(r)] \dots + \\
 &\quad + \frac{k!}{(n-1)!} \sum_{m=0}^{k+1} [f_\nu^{(n-1-m)}(s) - f^{(n-1-m)}(s)] \dots \} + \\
 &\quad + \frac{r-s}{(n-1)!} \int_0^1 \{ f_\nu^{(n)}[(r-s)t+s] - f^{(n)}[(r-s)t+s] \ln(1/t) dt \} \leq \\
 &\leq |f_\nu^{(n-1)}(s) - f^{(n-1)}(s)| \dots + \sum_{k=0}^{n-2} \{ |f_\nu^{(k)}(s) - f^{(k)}(s)| \dots + \\
 &\quad + |f_\nu^{(n-k-2)}(r) - f^{(n-k-2)}(r)| \dots + \\
 &\quad + \frac{k!}{(n-1)!} \sum_{m=0}^{k+1} |f_\nu^{(n-1-m)}(s) - f^{(n-1-m)}(s)| \dots \} + \\
 &\quad + \frac{r-s}{(n-1)!} \int_0^1 |f_\nu^{(n)}[(r-s)t+s] - f^{(n)}[(r-s)t+s]| \ln(1/t) dt,
 \end{aligned}$$

where the dots indicate the terms of (1.4.6) independent of f_ν and f .

According to the convergence of $\{f_\nu(x)\}$, all absolute values of the differences in the latter expression are smaller than some ε .

Therefore, $|I_\nu - I|$ can be made arbitrarily small, i.e. $\lim_{\nu \rightarrow \infty} I_\nu = I$.

This proves our statement.

To ensure that the f.p. integrals of a sequence of functions converge to the f.p. integral of the limit function, we had to require the strong convergence.

We now consider a f.p. integral such that the integrand function, besides depending on the integration variable, also depends on a second independent variable, i.e. we have a function

$$g(x) = \int_s^r \frac{f(x,y)}{(y-s)^{n-\lambda}} dy, \quad -1 < \lambda \leq 0, \quad s < r. \quad (2.4.2)$$

Here y is the integration variable and x a second independent variable or a parameter.

We ask under what assumptions on f is $g(x)$ continuous and when is the relation

$$g'(x) = \frac{d}{dx} \int_s^r \frac{f(x,y)}{(y-s)^{n-\lambda}} dy = \int_s^r \frac{\partial f(x,y)}{\partial x} \frac{dy}{(y-s)^{n-\lambda}} \quad (2.4.3)$$

valid, i.e. when may the differentiation be performed under the integral symbol?

In the case of an ordinary integral, it is well known that if $f(x,y)$ is one-valued and continuous in the closed region

$R : \alpha \leq x \leq \beta, \quad s \leq y \leq r$ then $g(x)$ is continuous in $[\alpha, \beta]$.

If furthermore besides $f(x,y)$, $f_x(x,y)$ also exists in R and is

continuous there, then $g(x)$ is differentiable in (α, β) and (2.4.3) is satisfied.

These assumptions are not sufficient for f.p. integrals but the following theorem holds.

Theorem

If $f(x, y)$ and its partial derivatives $\frac{\partial^k}{\partial y^k} f(x, y)$ for $k=1, 2, \dots, n$ are one-valued and continuous in the closed region $R : \alpha \leq x \leq \beta, s \leq y \leq r$, then $g(x)$ given by (2.4.2) is continuous in $[\alpha, \beta]$.

If furthermore besides $f(x, y)$ and the $\frac{\partial^k}{\partial y^k} f(x, y)$ also the function $f_x(x, y)$ and its partial derivatives $\frac{\partial^k}{\partial y^k} f_x(x, y)$ for $k=1, 2, \dots, n$ exist in R and are continuous there, then $g(x)$ is differentiable in (α, β) and (2.4.3) is valid.

Proof

First we prove that under the above assumptions the function $g(x)$ is continuous. We have

$$|g(x+h) - g(x)| = \left| \int_s^r \frac{f(x+h, y) - f(x, y)}{(x-s)^{n-\lambda}} dy \right| .$$

Applying either of the definition formulae (1.4.6) and (1.4.9)

to the latter f.p. integral, we obtain an inequality for

$|g(x+h) - g(x)|$ similar to that for $|I_\nu - I|$ in the proof of the previous theorem. The right-hand side of this inequality is a sum which contains terms of the form

$$\left| \frac{\partial^k}{\partial y^k} f(x+h, y) - \frac{\partial^k}{\partial y^k} f(x, y) \right|, \quad k=0, 1, 2, \dots, n.$$

According to the theorem of uniform continuity, there exists for any given number $\varepsilon > 0$ a number $\delta(\varepsilon) > 0$ which depends only on ε but not on x and y such that

$$\left| \frac{\partial^k}{\partial y^k} f(x+h, y) - \frac{\partial^k}{\partial y^k} f(x, y) \right| < \varepsilon$$

for all $|h| < \delta$. Thus, for a suitable choice of ε , the aforesaid sum becomes arbitrarily small, i.e. $\lim_{h \rightarrow 0} |g(x+h) - g(x)| = 0$.

The function $g(x)$ is therefore continuous in $[\alpha, \beta]$.

In order to prove the second statement of the theorem, we form

$$g(x+h) - g(x) = \int_s^r \frac{f(x+h, y) - f(x, y)}{(x-s)^{n-\lambda}} dy.$$

Due to the mean value theorem of the differential calculus we have

$$f(x+h, y) - f(x, y) = h f_x(x+\theta h, y), \quad 0 < \theta < 1.$$

Thus

$$\left| \frac{g(x+h) - g(x)}{h} - \int_s^r \frac{f_x(x, y)}{(x-s)^{n-\lambda}} dy \right| = \left| \int_s^r \frac{f_x(x+\theta h, y) - f_x(x, y)}{(x-s)^{n-\lambda}} dy \right|. \quad (2.4.4)$$

The application of formula (1.4.6) or (1.4.9) to this latter f.p. integral again yields an inequality as in the first part of the proof; the right-hand side is a sum containing terms of the form

$$\left| \frac{\partial^k}{\partial y^k} f_x(x+\vartheta h, y) - \frac{\partial^k}{\partial y^k} f_x(x, y) \right|, \quad k=0, 1, 2, \dots, n.$$

Since $\frac{\partial^k}{\partial y^k} f_x(x, y)$ ($k=0, 1, 2, \dots, n$) is also uniformly continuous in R , there exists for all $\varepsilon > 0$ a number $\delta(\varepsilon) > 0$ which is independent of x and y such that

$$\left| \frac{\partial^k}{\partial y^k} f_x(x+\vartheta h, y) - \frac{\partial^k}{\partial y^k} f_x(x, y) \right| < \varepsilon, \quad k=0, 1, 2, \dots, n \quad (2.4.5)$$

for all $|h| < \delta$.

In view of (2.4.5) the right-hand side of (2.4.4) can be made arbitrarily small, and therefore

$$\lim_{h \rightarrow 0} \frac{g(x+h) - g(x)}{h} = g'(x) = \int_s^r \frac{f_x(x, y)}{(x-s)^{n-\lambda}} dy.$$

q.e.d.

At the end we still consider the two functions

$$g(s) = \int_s^r \frac{f(x)}{(x-s)^{\lambda+n}} dx, \quad s < r, \quad 0 \leq \lambda < 1, \quad (2.4.6)$$

and

$$h(s) = \int_r^s \frac{f(x)}{(s-x)^{\lambda+n}} dx, \quad s > r, \quad 0 \leq \lambda < 1, \quad (2.4.7)$$

with the singularity s as argument. If $0 < \lambda < 1$, we know (see page 33) that the f.p. integrals in (2.4.6) and (2.4.7) commute with differentiation, i.e.

$$\frac{dg}{ds} = \int_s^r \frac{d}{ds} \left(\frac{f(x)}{(x-s)^{\lambda+n}} dx \right) = (\lambda+n) \int_s^r \frac{f(x)}{(x-s)^{\lambda+n+1}} dx.$$

and

$$\frac{dh}{ds} = \int_r^s \frac{d}{ds} \left(\frac{f(x)}{(s-x)^{\lambda+n}} dx \right) = -(\lambda+n) \int_r^s \frac{f(x)}{(s-x)^{\lambda+n+1}} dx.$$

In this case we may differentiate under the integral symbol. It was previously mentioned that this commutation does not hold for our definition of a f.p. integral with $\lambda = 0$. Therefore we ask ourselves what happens if we differentiate g and h with respect to s in that particular case.

We start with the differentiation of $g(s)$. By means of the definition formula (1.4.6) we can write

$$\frac{dg}{ds} = \frac{d}{ds} \int_s^r \frac{f(x)}{(x-s)^n} dx = \frac{f^{(n)}(s)}{(n-1)!} \ln(r-s) - \frac{f^{(n-1)}(s)}{(n-1)!(r-s)} +$$

$$\begin{aligned}
& + \sum_{k=0}^{n-2} \left\{ \frac{(r-s)^{-n+k+1}}{k!(-n+k+1)} f^{(k+1)}(s) - \frac{(r-s)^{-n+k}}{k!} f^{(k)}(s) - \right. \\
& - \frac{(k+1)!}{(r-s)^{k+2}} f^{(n-k-2)}(r) + \\
& + \frac{k!}{(n-1)!} \sum_{m=0}^{k+1} \left[\frac{m}{(k+1-m)!(r-s)^{m+1}} f^{(n-1-m)}(s) + \right. \\
& \left. + \frac{1}{(k+1-m)!(r-s)^m} f^{(n-m)}(s) \right] \left. \right\} + \\
& + \frac{1}{(n-1)!} \int_0^1 f^{(n)}[(r-s)t+s] \ln t \, dt + \\
& + \frac{r-s}{(n-1)!} \int_0^1 (1-t) f^{(n+1)}[(r-s)t+s] \ln(1/t) \, dt.
\end{aligned}$$

Integrating the latter integral by parts and recasting the sums over k and m in a suitable way (we omit the procedure here since it is lengthy and merely contains elementary steps) it follows that

$$\begin{aligned}
\frac{d}{ds} \int_s^r \frac{f(x)}{(x-s)^n} dx &= \int_s^r \frac{d}{ds} \left(\frac{f(x)}{(x-s)^n} dx \right) - \frac{f^{(n)}(s)}{n!} \\
&= n \int_s^r \frac{f(x)}{(x-s)^{n+1}} dx - \frac{f^{(n)}(s)}{n!} \tag{2.4.8}
\end{aligned}$$

if $s < r$.

From (2.4.8) we see that the derivative (with respect to s) of the f.p. integral and the f.p. integral with the differentiated integrand differ by the term $f^{(n)}(s)/n!$

We come now to the differentiation of $h(s)$. We remember that in order to apply our definition formula to the right-hand side of (2.4.7) where $s > r$, we have to transform the f.p. integral in the following way (see also page 46), viz

$$h(s) = \int_r^s \frac{f(x)}{(s-x)^n} dx = \int_{-s}^{-r} \frac{f(-x)}{[x - (-s)]^n} dx.$$

We have thus for the derivative of h ,

$$\frac{dh}{ds} = \frac{d}{ds} \int_{-s}^{-r} \frac{f(-x)}{[x - (-s)]^n} dx.$$

If we apply the formula (1.4.6) to the latter integral, differentiate it with respect to s and recast that expression similarly as in the former case, we obtain the relation

$$\begin{aligned} \frac{d}{ds} \int_r^s \frac{f(x)}{(s-x)^n} dx &= \int_r^s \frac{d}{ds} \left(\frac{f(x)}{(s-x)^n} \right) dx + \frac{(-1)^n f^{(n)}(s)}{n!} \\ &= -n \int_r^s \frac{f(x)}{(s-x)^{n+1}} dx + \frac{(-1)^n f^{(n)}(s)}{n!} \end{aligned} \quad (2.4.9)$$

if $s > r$.

We consider now a special case of the above formulae.

For $n=1$, (2.4.8) and (2.4.9) become

$$\frac{d}{ds} \int_s^{r'} \frac{f(x)}{x-s} dx = \int_s^{r'} \frac{f(x)}{(x-s)^2} dx - f'(s) \quad (2.4.10)$$

and

$$\frac{d}{ds} \int_r^s \frac{-f(x)}{x-s} dx = - \int_r^s \frac{f(x)}{(x-s)^2} dx - f'(s) \quad (2.4.11)$$

respectively, where we take as upper boundary in (2.4.10) a point $r' > r$.

Subtraction of (2.4.11) from (2.4.10) yields (since the additional terms cancel)

$$\boxed{\frac{d}{ds} \text{P.V.} \int_r^{r'} \frac{f(x)}{x-s} dx = \int_r^{r'} \frac{f(x)}{(x-s)^2} dx} \quad r < s < r', \quad (2.4.12)$$

where the integral on the left-hand side represents a Cauchy principal value integral. The statement of (2.4.12) is remarkable. It means that if we differentiate a Cauchy principal value integral with respect to its singularity, we obtain a f.p. integral. This connects the theory of f.p. integral equations (with exponent two) to the Hilbert transform theory; for further developments see [27, chapter V].

CHAPTER IIIAN INTERPOLATORY QUADRATURE FORMULA

The (numerical) evaluation of a f.p. integral by means of the definition can be cumbersome, even if analytic functions are involved. Furthermore, in many problems the integrand function, $f(x)$, is not given in closed form but it may be possible to compute its values at arbitrary points. Thus we seek appropriate numerical procedures for approximating the value of the f.p. integral I .

In the following, we derive an interpolatory quadrature formula based on equispaced stations, while the problem of finding a Gaussian-type quadrature formula is treated in the next chapter.

3.1 Derivation of the formula

For simplicity, we consider the f.p. integral

$$\int_0^1 \frac{g(x)}{x^\lambda} dx; \quad \lambda \text{ real and } \geq 1 \quad (3.1.1)$$

$$g(x) \in C^{[\lambda]} [0,1]$$

instead of the general form I . We assume that N distinct points $x_i \in [0,1)$ are given by $x_i = (i-1)/N$, $i=1,2,\dots,N$. Thus the points are equally spaced in $[0,1)$ and the first coincides with the origin.

With these points as interpolation points, we form (for the continuous function $g(x)$) the interpolation polynomial $P_{N-1}(x)$ of

degree $N-1$ such that $g(x_i) = P_{N-1}(x_i)$, $i=1,2,\dots,N$.

Then as an approximation to the f.p. integral (3.1.1), we set

$$I_N\{g\} = \int_0^1 P_{N-1}(x) x^{-\lambda} dx.$$

This integral is easily evaluated. In fact, by using the Lagrange form for the interpolation polynomial

$$P_{N-1}(x) = \sum_{i=1}^N \Phi_{N-1,i}(x) g(x_i),$$

where

$$\Phi_{N-1,i}(x) = \prod_{\substack{k=1 \\ k \neq i}}^N \frac{(x-x_k)}{(x_i-x_k)}; \quad i=1,2,\dots,N$$

we obtain the quadrature formula

$$I_N\{g\} = \sum_{i=1}^N w_i g(x_i), \quad (3.1.2a)$$

with the coefficients given by

$$w_i = \int_0^1 x^{-\lambda} \Phi_{N-1,i}(x) dx. \quad (3.1.2b)$$

The N distinct points x_i are called the quadrature points, or nodes, or "stations", and the quantities w_i are called the quadrature coefficients or "weights".

It is clear that the weights w_i are completely determined by the end points of the interval of integration and by the interpolation points x_i ; the weights are independent of the integrand function $g(x)$. A quadrature formula of the form (3.1.2a and b) is called an interpolatory formula.

We proved in section 2.2 that if λ is an integer I is not scale-invariant, but satisfies the relationship

$$\int_s^r \frac{f(x)}{(x-s)^\lambda} dx = (r-s)^{1-\lambda} \int_0^1 \frac{f[(r-s)t+s]}{t^\lambda} dt + \frac{f^{(\lambda-1)}(s)}{(\lambda-1)!} \ln|r-s|. \quad (3.1.3)$$

This strange property of f.p. integrals does not permit a direct approximation of I by the formula (3.1.2a). In principle, I may always (omitting the integrand) be split up into

$$\int_s^{s+1} + \int_{s+1}^r \quad (3.1.4)$$

where the last integral is regular and may be evaluated by a standard method. Shifting the interval of the f.p. integral in (3.1.4) to $[0,1]$, the last term in (3.1.3) vanishes and we obtain

$$\int_s^{s+1} \frac{f(x)}{(x-s)^\lambda} dx = \int_0^1 \frac{f(t+s)}{t^\lambda} dt. \quad (3.1.5)$$

Applying (3.1.2a) to the right-hand side of (3.1.5), it therefore follows that

$$I \approx \sum_{i=1}^N w_i f(s+x_i) + \int_{s+1}^r \frac{f(x)}{(x-s)^\lambda} dx. \quad (3.1.6)$$

This method is inconvenient, however, for the following reasons: firstly, two different quadrature formulae are applied and thus further function values have to be computed; secondly, if r is close to the singularity s , the numerical value of the regular integral can become very inaccurate.

If $f(x)$ is known analytically, another method that can be used is to differentiate $f(x)$ formally and then use (3.1.3). But to determine the $(\lambda-1)$ th derivative could still be a laborious and difficult task. If $f(x)$ is merely given by a set of data this method cannot be used. We shall therefore try to approximate $f^{(\lambda-1)}(s)$ numerically by a formula involving the same (equally spaced) stations as were used in (3.1.2a).

Setting $g(t) = f[(r-s)t+s]$ and differentiating both sides $(\lambda-1)$ times, we obtain for $t=0$

$$f^{(\lambda-1)}(s) = (r-s)^{1-\lambda} g^{(\lambda-1)}(0). \quad (3.1.7)$$

Approximating $g^{(\lambda-1)}(0)$ by

$$D_N\{g\} = P_{N-1}^{(\lambda-1)}(0)$$

we obtain the formula

$$D_N\{g\} = \sum_{i=1}^N c_i g(x_i) \quad (3.1.8a)$$

with the coefficients given by

$$c_i = \Phi_{N-1,i}^{(\lambda-1)}(0). \quad (3.1.8b)$$

Applying the formulae (3.1.2a) and (3.1.8a) for the approximation of the right-hand side in (3.1.3) we obtain the quadrature formula

for λ an *integer*

$$\int_s^r \frac{f(x)}{(x-s)^\lambda} dx \approx (r-s)^{1-\lambda} \sum_{i=1}^N [w_i + c_i \ln|r-s| / (\lambda-1)!] f[(r-s)(i-1)/N+s]$$

(3.1.9)

Since a f.p. integral with a non-integer power λ is scale-invariant, (3.1.2a) may be used to approximate the integral directly, i.e.

for λ a *non-integer*

$$\int_s^r \frac{f(x)}{(x-s)^\lambda} dx \approx (r-s)^{1-\lambda} \sum_{i=1}^N w_i f[(r-s)(i-1)/N+s] \quad (3.1.10)$$

We remark that in the formulae (3.1.9) and (3.1.10) the station x_i was replaced by $(i-1)/N$.

3.2 Computation of the coefficients w_i and c_i

Since the interpolation points are of the form $x_i = (i-1)/N$, $i=1,2,\dots,N$, the coefficients w_i and c_i of the formulae (3.1.2b) and (3.1.8b) can be written as

$$\begin{aligned}
 w_i &= \int_0^1 x^{-\lambda} \Phi_{N-1,i}(x) dx \\
 &= \int_0^1 x^{-\lambda} \prod_{\substack{k=1 \\ k \neq i}}^N \frac{Nx-k+1}{i-k} dx \\
 &= \frac{(-1)^{N-i}}{(N-1)!} \binom{N-1}{i-1} \int_0^1 x^{-\lambda} \prod_{\substack{k=1 \\ k \neq i}}^N (Nx-k+1) dx, \quad i=1,2,\dots,N \quad (3.2.1)
 \end{aligned}$$

and

$$\begin{aligned}
 c_i &= \Phi_{N-1,i}^{(\lambda-1)}(0) \\
 &= \left[\prod_{\substack{k=1 \\ k \neq i}}^N \frac{Nx-k+1}{i-k} \right]_{/x=0}^{(\lambda-1)} \\
 &= \frac{(-1)^{N-i}}{(N-1)!} \binom{N-1}{i-1} \left[\prod_{\substack{k=1 \\ k \neq i}}^N (Nx-k+1) \right]_{/x=0}^{(\lambda-1)}, \quad i=1,2,\dots,N. \quad (3.2.2)
 \end{aligned}$$

Since the integrand function in (3.2.1) is a polynomial of degree $N-1$ which is integrated over $[0,1]$, the weights w_i will all be rational numbers.

From (3.2.2) it is clear that the coefficients c_i are also rational numbers. Though (3.2.1) and (3.2.2) are simple formulae, it would be too laborious to use them for computing the w_i and c_i . We therefore chose an alternative indirect procedure, called the method of undetermined coefficients, to determine the coefficients for the formulae (3.1.2a) and (3.1.8a). This method is quite practical for unequally spaced stations as well as fairly large values of N .

In order uniquely to determine the N unknowns w_i (or c_i) associated with N fixed stations x_i , we set up a linear system. This can easily be obtained by requiring (3.1.2a), or (3.1.8a), to be exact for all polynomials of degree $\leq N-1$, i.e. the formulae are to yield the exact value whenever $g(x) = 1, x, x^2, \dots, x^{N-1}$.

Writing out each of these conditions and using the abbreviation $\int_0^1 x^{j-\lambda} dx = \lambda^{m_j}$ [or $(x^{j-\lambda})_{/x=0}^{(\lambda-1)} = \lambda^{m_j}$], we have

$$w_1 x_1^j + w_2 x_2^j + \dots + w_N x_N^j = \lambda^{m_j} \quad (j=0, 1, 2, \dots, N-1), \quad (3.2.3)$$

$$\text{or } c_1 x_1^j + c_2 x_2^j + \dots + c_N x_N^j = \lambda^{m_j}.$$

The coefficients λ^{m_j} are called moments and are given by

$$\lambda^{m_j} = \begin{cases} 1/(j+1-\lambda) & \text{for } j+1 \neq \lambda \\ 0 & \text{otherwise} \end{cases} \quad \text{for the } w_i$$

and by

$$\lambda^{m_j} = \begin{cases} (\lambda-1)! & \text{for } j+1 = \lambda \\ 0 & \text{otherwise} \end{cases} \quad \text{for the } c_i.$$

The determinant of the linear system (3.2.3) is the Van der Monde determinant V , generated by the N equispaced stations x_i . Since the stations are distinct, it follows that $V \neq 0$. Therefore (3.2.3) may be solved uniquely for the N unknowns w_i (or c_i) which may then be used in the formulae (3.1.2a) or (3.1.8a).

The rationality of the w_i and c_i in this case follows immediately from the fact that the matrix and the right-hand side of (3.2.3) consist of rational numbers.

Before a linear system is solved numerically, it is advantageous to know something about the condition of the matrix involved. The usual criteria defining the condition number of a matrix by means of certain eigenvalues can hardly be applied in our case as it is too difficult to obtain reasonable estimates of those eigenvalues. But it is possible to estimate the ratio of the absolute value of the determinant and the product of the Euclidean norms of all its row or column vectors. If this ratio is much smaller than 1, the matrix is said to be ill-conditioned, i.e. the solution is very sensitive to small errors occurring in the coefficients. The determinant of (3.2.3) has the value (see [34] for example)

$$\begin{aligned}
 |V| &= \left(\frac{1}{N}\right) \left(\frac{2}{N}\right) \left(\frac{3}{N}\right) \dots \left(\frac{N-1}{N}\right) \\
 &\quad \left(\frac{1}{N}\right) \left(\frac{2}{N}\right) \dots \left(\frac{N-2}{N}\right) \\
 &\quad \left(\frac{1}{N}\right) \dots \left(\frac{N-3}{N}\right) \\
 &\quad \cdot \\
 &\quad \cdot \\
 &\quad \left(\frac{1}{N}\right)
 \end{aligned}
 = N^{(N-N^2)/2} \prod_{i=1}^{N-1} (N-i)! \quad (3.2.4)$$

The product of the Euclidean norms of, for instance, the column vectors of the matrix is

$$E = \sqrt{\prod_{i=1}^N \left[\sum_{j=0}^{N-1} x_i^{2j} \right]}$$

and thus greater than 1.

The ratio of $|V|$ to E can be estimated, for instance, by

$$\frac{|V|}{E} < |V| < \left(\frac{N-1}{N}\right)^{(N^2-N)/2}$$

which is bad, even for a small N . The linear system (3.2.3) is therefore rather ill-conditioned.

To solve (3.2.3) numerically, we first used some of the known iterative methods as well as the direct method (triangular decomposition) with iterative improvement of FORSYTHE and MOLER [5]. But we found the solution obtained by one of these methods not accurate enough; for instance not even ten significant digits were correct with $N > 10$. The task we set ourselves was to find the coefficients w_i and c_i to thirty significant digits, since the double word length of some modern computers comes close to this number of significant digits.

The safest way of ensuring that we shall obtain such a highly accurate solution is to determine the rational (exact) solution first and afterwards to divide the numerators by their corresponding denominators. The exact solution of (3.2.3) was computed by the Gaussian elimination process, performed in rational arithmetic [17].

The weights w_i were calculated for the powers $\lambda=1, 4/3, 3/2, 5/3, 2, 3, 4, 5$ and in each case with $N = 3(1)20$ equally spaced stations $x_i = (i-1)/N$. The coefficients for $f^{(\lambda-1)}(s)$, c_i , were also computed for the same values of λ and N , except of course the cases $\lambda < 2$. Both coefficients, the w_i and the c_i , have been tabulated in [18] with a mantissa length of thirty digits (the last one correctly rounded off).

3.3 General properties of the w_i and c_i

Apart from the rationality of the coefficients w_i and c_i , we cannot unfortunately derive any further property from their explicit representations (3.2.1) and (3.2.2) respectively.

To do so we should have to know explicitly the coefficients of

the polynomial $\prod_{\substack{k=1 \\ k \neq i}}^N (Nx-k+1)$.

Owing to the factor $(-1)^{N-i}$ in (3.2.1) and (3.2.2) we may conjecture an alternating sign for the w_i and c_i . This conjecture was verified numerically in nearly all the computed cases.

From the formulae for w_i and c_i we observe that their absolute numerical values increase with the number of stations, N , and the value of the power λ . The largest absolute value of the weights in the cases we have computed is of the order 10^{11} and that of the coefficients c_i is of order 10^{12} . Comparing the absolute values of the corresponding w_i and c_i , we can say that for $\lambda \leq 3$ the coefficients c_i are smaller, by at most one order of magnitude, than the weights w_i . Exactly the reverse is the

case when $\lambda = 4$ or 5 . Furthermore, we notice that corresponding w_i and c_i have opposite signs.

The varying sign and the increasing (absolute) value of the coefficients w_i and c_i have consequences for the evaluation of the scalar products (3.1.2a) and (3.1.8a). In order to keep the rounding-off error as small as possible during the computation of these scalar products, the positive and negative terms should be added up separately so that at the end the subtraction need be performed only once. Nevertheless, since in most cases the magnitude of the result will be much smaller than that of the w_i and c_i used, significant digits are lost. We note that this loss is not caused by a rounding-off error. Thus in general the highest-order quadrature formula is not numerically the most accurate.

CHAPTER IVTHE OPTIMAL QUADRATURE FORMULA

In the previous chapter we showed that for N arbitrarily fixed stations x_i we can find a quadrature formula of interpolatory type which is exact for all polynomials of degree $\leq N-1$. This requirement and the interval of integration completely define the weights w_i .

In order to increase the precision of (3.1.2) the choice of the stations x_i ($i=1,2,\dots,N$) is still at our disposal. We might hope that for a suitable choice of these stations the degree of precision can be increased by N and cause the quadrature formula to become exact for all polynomials of degree $\leq 2N-1$; this is the highest degree of precision which can be obtained using N stations. Such formulae are usually called Gaussian quadrature formulae because they were first studied by Gauss [6].

Under what circumstances a Gaussian-type formula for the f.p. integral

$$\int_0^1 \frac{g(x)}{x^\lambda} dx; \quad \lambda \text{ real and } \geq 1, \quad g(x) \in C^{[\lambda]}[0,1]$$

can be derived will be shown in the following.

4.1 The orthogonal polynomials associated with the optimal quadrature formula

We write the above integral in the form

$$\int_0^1 w(x)g(x)dx \quad (4.1.0,1)$$

and formally consider $w(x) = \langle x^{-\lambda}$ as a weight function¹. The possibility of constructing formulae with degree of precision $\leq 2N-1$ (N is the number of stations) is closely related to the existence of polynomials of degree up to N which are orthogonal with respect to the weight function involved in the integrand, and the most widely studied classes of orthogonal polynomials (such as for instance the Legendre, Tschebyscheff, Jacobi, Laguerre and Hermite polynomials) are for weight functions which are positive on the integration interval (see, for example, [14,30,31]). The assumption that $w(x)$ be positive is, however, not necessary to develop certain fundamental properties of the quadrature formulae. For example the fact that one cannot obtain a formula exact for all polynomials of degree higher than $2N-1$ is a consequence of a certain determinant condition and does not follow from the assumption $w(x) > 0$. On the other hand, most of the very important properties of Gaussian-type formulae, such as the fact that all stations x_i are real and located within the integration interval, are a consequence of this assumption.

In our case, the symbolic weight function $\langle x^{-\lambda}$ is only apparently positive on $[0,1]$. This follows immediately from

$$\int_0^1 x^{-\lambda} dx \begin{cases} = 0 & \text{for } \lambda = 1 \\ < 0 & \text{for } \lambda > 1. \end{cases}$$

¹ Since $x^{-\lambda}$ actually represents a distribution and not an ordinary function we choose Dirac's "bra" notation for distributions (the symbol \langle is read "bra").

Definition

Given a sequence of polynomials

$$P_n(x) = x^n + a_{n-1}x^{n-1} + \dots + a_1x + a_0, \quad n=0,1,2,\dots \quad (4.1.0.2)$$

which - for any weight function $w(x)$ integrable over $[a,b]$ and not identically zero there - satisfy

$$\int_a^b w(x)P_1(x)P_n(x)dx = 0 \quad (1 \neq n; 1, n=0,1,2,\dots), \quad (4.1.0.3)$$

$a < b$

then the $P_n(x)$ are said to form an *orthogonal sequence* on $[a,b]$ with respect to the weight function $w(x)$.

If $w(x) > 0$ in $[a,b]$ we know that such a sequence exists, and it is always possible, by multiplying each $P_n(x)$ by a suitable constant, to obtain

$$\int_a^b w(x)P_1^*(x)P_n^*(x)dx = \delta_{1n} \quad (\text{the Kronecker symbol}). \quad (4.1.0.4)$$

A sequence of polynomials for which (4.1.0.4) holds is called *orthonormal*.

We shall now investigate whether it is possible to construct a unique sequence of polynomials which are orthonormal with respect to $\langle x^{-\lambda} \rangle$ on $[0,1]$. To do so, we shall first analyse the Gram determinants closely connected with the existence of such polynomials. Also, we shall consider the use of the Gram-Schmidt process of orthonormalization to enable us to construct those polynomials.

4.1.1 In order to obtain a sequence of orthogonal polynomials associated with a given weight function $w(x)$ we consider the real linear space \mathcal{H} consisting of the non-negative powers of

$x : 1, x, x^2, \dots, x^n, \dots$ in which an inner product is given. This

inner product of any two elements x^i and x^j of \mathcal{H} is defined by

$$(x^i, x^j) = \int_a^b w(x) x^i x^j dx; \quad i, j = 0, 1, 2, \dots$$

It is well-known from the theory of orthogonal polynomials (see, for example [3,12,14,31]) that a unique and complete² sequence of orthogonal polynomials exists and $\int_a^b w(x) [P_n(x)]^2 dx \neq 0$ if and only if the Gram determinants

$$G_1 = \begin{vmatrix} (1,1) & (1,x) & \dots & (1,x^1) \\ (x,1) & (x,x) & \dots & (x,x^1) \\ \dots & \dots & \dots & \dots \\ (x^1,1) & (x^1,x) & \dots & (x^1,x^1) \end{vmatrix} \quad l = 0, 1, 2, \dots \quad (4.1.1.5)$$

are all different from zero. It is also known that then the orthonormal polynomials are given by

$$P_0^*(x) = (G_0)^{-\frac{1}{2}},$$

$$P_n^*(x) = (G_{n-1} G_n)^{-\frac{1}{2}} \begin{vmatrix} (1,1) & (1,x) & \dots & (1,x^n) \\ (x,1) & (x,x) & \dots & (x,x^n) \\ \dots & \dots & \dots & \dots \\ (x^{n-1},1) & (x^{n-1},x) & \dots & (x^{n-1},x^n) \\ 1 & x & \dots & x^n \end{vmatrix} \quad n > 0. \quad (4.1.1.6)$$

² We call here a sequence of orthogonal polynomials $\{P_n(x)\}$, $n=0,1,2,\dots,N$, complete if n (the degree of the polynomial $P_n(x)$) takes all values from 0 up to N .

The Gram matrix $G_1 = (g_{ik})$ with $g_{ik} = (x^i, x^k)$ ($i, k=0, 1, \dots, 1$) is the fundamental tensor of \mathcal{H} with respect to the basis $1, x, x^2, \dots$. All "major subsets" of basis vectors (i.e. all sets $\{x^i | i=0, 1, \dots, 1\}$ with arbitrary 1) must be linearly independent. From this it follows that $G_1 > 0$ if $w(x)$ is assumed to be positive. In this case it is always possible to find a unique and complete sequence of orthogonal polynomials. In our case, the metric generated in \mathcal{H} by $\langle x^{-\lambda}$ is no longer positive definite but indefinite, i.e. (x^i, x^j) can be positive, negative or zero depending on the vectors x^i, x^j and the power λ . Our inner product space \mathcal{H} is therefore a pseudo-Euclidean space [8, chapter XIII].

It should be noted that the usual norm of a vector $x \in \mathcal{H}$ exists if and only if $(x, x) > 0$. Therefore, we shall call (x, x) in the following the inner product of the vector x with itself. As in the positive definite case two vectors $x, y \in \mathcal{H}$ are called *orthogonal* if $(x, y) = 0$.

Definition

A basis e_i ($i=1, 2, \dots, n$) in \mathcal{H} is called *orthonormal* if

$$(e_i, e_j) = \epsilon_i \delta_{ij}$$

where

$$\epsilon_i = \begin{cases} +1 & (i=1, \dots, s) \\ -1 & (i=s+1, \dots, n). \end{cases}$$

Definition

A vector $x \in \mathcal{H}$ is called *normalized* if $(x,x) = \pm 1$.

We remark that a vector which can be normalized need not have a norm in the classical sense.

No theorem on the existence (or non-existence) of orthogonal polynomials in the case of an indefinite metric could be found in the standard literature. The only way to be assured of the existence of the orthogonal polynomials here seems to be to examine the Gram determinants G_1 ($l=0,1,2,\dots$) themselves. Before doing so, we shall still show the connection of G_1 with the coefficients of the orthogonal polynomials. Taking $[0,1]$ as $[a,b]$, (4.1.0.3) is obviously equivalent to

$$\int_0^1 x^{-\lambda} P_n(x) dx = 0 \quad (0 \leq l < n; n=1,2,\dots)$$

and therefore - using

the abbreviation $m_i = \int_0^1 x^{i-\lambda} dx$ - we can construct $P_n(x)$ by

solving the system of simultaneous linear equations

$$\begin{aligned} m_0 a_0 + m_1 a_1 + \dots + m_{n-1} a_{n-1} &= -m_n \\ m_1 a_0 + m_2 a_1 + \dots + m_n a_{n-1} &= -m_{n+1} \\ \dots & \\ m_{n-1} a_0 + m_n a_1 + \dots + m_{2n-2} a_{n-1} &= -m_{2n-1} \end{aligned} \tag{4.1.1.7}$$

for the unknown coefficients of $P_n(x)$. The quantities m_i (identical to the above inner products) are generally called moments or monomials.

Examining (4.1.1.7) we see immediately that the system determinant is in fact the Gram determinant G_{n-1} . Thus it is clear why it is necessary and sufficient for the major Gram determinants not to vanish in order that a unique and complete sequence of orthogonal polynomials should exist.

We now investigate the behaviour of the Gram determinants, separating the cases when

- (a) the power λ is an integer and
 - (b) λ is not an integer.
- (a) λ is an integer ≥ 1

We write the inner products (moments)

$$(x^i, x^j) = \int_0^1 x^{i+j-\lambda} dx = \begin{cases} 0 & \text{for } i+j+1 = \lambda \\ 1/(i+j+1-\lambda) & \text{otherwise} \end{cases}$$

$i, j = 0, 1, 2, \dots$

using the following scheme:

	$\lambda=5$	$\lambda=4$	$\lambda=3$	$\lambda=2$	$\lambda=1$				
...	$-\frac{1}{4}$	$-\frac{1}{3}$	$-\frac{1}{2}$	-1	0	1	$\frac{1}{2}$	$\frac{1}{3}$...
...	$-\frac{1}{3}$	$-\frac{1}{2}$	-1	0	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$...
...	$-\frac{1}{2}$	-1	0	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$...
...	-1	0	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$...
...	0	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	$\frac{1}{7}$...
...	1	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	$\frac{1}{7}$	$\frac{1}{8}$...
...	$\frac{1}{2}$	$\frac{1}{3}$	$\frac{1}{4}$	$\frac{1}{5}$	$\frac{1}{6}$	$\frac{1}{7}$	$\frac{1}{8}$	$\frac{1}{9}$...
...	:	:	:	:

(4.1.1.8)

(4.1.1.8) represents the Gram determinants G_1 ($l=0,1,2,\dots$) bounded at the left-hand side by the dashed vertical lines for different λ 's. Owing to their structure, all determinants are of the Hankel type³ (see, for example, [13]). We immediately deduce from (4.1.1.8) that $G_0 = 0$ if $\lambda=1$. In this case, the corresponding equation of (4.1.1.7) is $0 \cdot a_0 = -1$, which yields no finite solution (see page 93) for the unknown coefficient a_0 of $P_1(x)$, i.e. the linear polynomial cannot exist. Furthermore, it follows that $P_0^*(x)$ and therefore also $P_0(x)$ cannot exist either. But this is not the only case where a determinant vanishes. Consider for instance, a $G_{\lambda-1}$ where λ is odd:

$$G_2 = \begin{vmatrix} -\frac{1}{2} & -1 & 0 \\ -1 & 0 & 1 \\ 0 & 1 & \frac{1}{2} \end{vmatrix} \quad \text{when } \lambda = 3.$$

In such a case we can always, achieve by interchanging the columns (in the above example the first and the last column have to be interchanged) that $G_{\lambda-1}$ becomes a skew-symmetric determinant. As we know from the theory of determinants (see, for example, [13]), a skew-symmetric determinant of odd order is equal to zero. In these cases, the corresponding linear systems (4.1.1.7) have vanishing determinants; the rows (columns) are linearly dependent

³It is easily seen from (4.1.1.8) that if $\lambda = 0$ the major Gram matrices are segments of the (infinite) Hilbert matrix, which is a special type of Hankel matrix.

and thus the rank of the system matrix is less than λ .

But since the rank of the extended matrix is equal to λ no solution exists⁴. Thus we may conclude that the sequence of orthogonal polynomials is certainly not complete for odd values of λ .

No attempt will here be made to prove whether for an arbitrary integer λ the Gram determinants G_1 vanish or not.

We constructed the orthogonal polynomials ${}_{\lambda}P_n(x)$ for $\lambda = 1, 2, 3, 4, 5$ and $n = 1(1)20$ (except the cases $n = \lambda$ if λ is odd) numerically, i.e. we solved the corresponding linear equations (4.1.1.7) exactly by Gauss elimination performed in a rational arithmetic [17]. We remark that all coefficients of (4.1.1.7) are rational numbers and therefore the solution - if it exists - must also be rational. We thus obtained for each of $\lambda = 1, 2, 3, 4, 5$ a set of orthogonal polynomials ${}_{\lambda}P_{20}$ consisting of

⁴ Denoting the column vectors of the system matrix by c_j , there exists a linear combination $\sum_{j=1}^n a_j c_j = 0$ such that at least one coefficient, say a_i , is non-zero. We now consider the linear combination $\sum_{\substack{j=1 \\ j \neq i}}^n a_j c_j + b\tau = 0$, where the coefficient $b \neq 0$ and τ denotes the right-hand side vector. With the aid of the first linear combination, this last equation can be written as $-a_i c_i + b\tau = 0$. Since each column vector c_j contains one zero component, but all components of τ are non-zero, this equation is only satisfied if $a_i = b = 0$. This is a contradiction and thus the vectors $c_1, \dots, c_{i-1}, c_{i+1}, \dots, c_n, \tau$ are linearly independent and the extended matrix has the rank λ .

$$\begin{aligned}
 &P_0(x), P_1(x), P_2(x), \dots, P_{20}(x) && \text{for even } \lambda, \\
 &P_0(x), P_1(x), \dots, P_{\lambda-1}(x), P_{\lambda+1}(x), \dots, P_{20}(x) && \text{for odd } \lambda > 1 \\
 \text{and } &P_2(x), P_3(x), P_4(x), \dots, P_{20}(x) && \text{for } \lambda = 1.
 \end{aligned}$$

We now want to normalize these polynomials, i.e. we construct $P_n^*(x)$ from $P_n(x)$ so that $(P_n^*, P_n^*) = \pm 1$. In order to find the normalization factors λ_n^k for the above set of orthogonal polynomials, we computed $\int_0^1 x^{-\lambda} [P_n(x)]^2 dx = \pm 1/\lambda k_n^2$ again by rational arithmetic. The coefficients of the orthogonal polynomials

$$\begin{aligned}
 &{}_{\lambda}P_2(x), {}_{\lambda}P_3(x), \dots, {}_{\lambda}P_{20}(x) && \text{for } \lambda = 2, 4 \\
 \text{and } &{}_{\lambda}P_{\lambda+1}(x), {}_{\lambda}P_{\lambda+2}(x), \dots, {}_{\lambda}P_{20}(x) && \text{for } \lambda = 1, 3, 5
 \end{aligned}$$

including their normalization factors are given in [18].

(b) $\lambda > 1$ and not an integer

In this case the inner products are given by

$$(x^i, x^j) = \int_0^1 x^{i+j-\lambda} dx = 1/(i+j+1-\lambda) \quad i, j = 0, 1, 2, \dots$$

and the Gram determinants G_{n-1} thus have the form

$$\begin{vmatrix} \frac{1}{1-\lambda} & \frac{1}{2-\lambda} & \cdots & \frac{1}{n-\lambda} \\ \frac{1}{2-\lambda} & \frac{1}{3-\lambda} & & \frac{1}{n+1-\lambda} \\ \dots & \dots & \dots & \dots \\ \frac{1}{n-\lambda} & \frac{1}{n+1-\lambda} & \cdots & \frac{1}{2n-1-\lambda} \end{vmatrix} \quad n = 1, 2, 3, \dots \quad (4.1.1.9)$$

By interchanging the first column in (4.1.1.9) and its immediate neighbour on the right (n-1) times, then interchanging the second column and its immediate neighbour on the right (n-2) times, and so on, till we interchange the penultimate column and the last, we finally obtain

$$G_{n-1} = (-1)^{n(n-1)/2} \begin{vmatrix} \frac{1}{n-\lambda} & \frac{1}{n-1-\lambda} & \cdots & \frac{1}{1-\lambda} \\ \frac{1}{n+1-\lambda} & \frac{1}{n-\lambda} & \cdots & \frac{1}{2-\lambda} \\ \dots & \dots & \dots & \dots \\ \frac{1}{2n-1-\lambda} & \frac{1}{2n-2-\lambda} & \cdots & \frac{1}{n-\lambda} \end{vmatrix} \quad (4.1.1.10)$$

Setting $k = n-\lambda$, the matrix corresponding to the determinant in (4.1.1.10) can be written as

$$(u_{rs}) = \begin{pmatrix} \frac{1}{k} & \frac{1}{k-1} & \cdots & \frac{1}{k-n+1} \\ \frac{1}{k+1} & \frac{1}{k} & \cdots & \frac{1}{k-n+2} \\ \dots & \dots & \dots & \dots \\ \frac{1}{k+n-1} & \frac{1}{k+n-2} & \cdots & \frac{1}{k} \end{pmatrix} \quad (4.1.1.11)$$

(4.1.1.11) may be regarded as a segment of a generalized Hilbert matrix; for if the columns are written in reversed order and k is restricted to positive integer values greater than $n-1$, the resultant matrix is a segment of the Hilbert matrix $[1/(i+j-1)]$. COLLAR has represented [2] the elements of the inverse of (4.1.1.11) explicitly, where k is no integer within the range $\pm(n-1)$ inclusive but is otherwise arbitrary. Applying his formula with k defined as above, we obtain for the inverse of (4.1.1.11)

$$(u_{rs})^{-1} = (-1)^{n+r-s-1} \frac{\prod_{k=n+1}^{2n} (k-\lambda-r) \prod_{k=0}^{n-1} (k+s-\lambda)}{(n-\lambda-r+s)(r-1)!(n-r)!(s-1)!(n-s)!},$$

$$r, s = 1, 2, \dots, n. \quad (4.1.1.12)$$

From (4.1.1.7) it follows that the coefficients of the orthogonal polynomials $P_n(x)$ are given by

$$a_{n-r} = - \sum_{s=1}^n (u_{rs})^{-1} m_{n+s-1}, \quad \begin{matrix} r = 1, 2, \dots, n \\ n = 1, 2, \dots \end{matrix}$$

or, if we insert (4.1.1.12)

$$a_{n-r} = \frac{(2n-\lambda-r)(2n-1-\lambda-r)\dots(n+1-\lambda-r)}{(r-1)!(n-r)!}$$

$$\sum_{s=1}^n (-1)^{n+r-s} \frac{(n-1+s-\lambda)(n-2+s-\lambda)\dots(s-\lambda)}{(n-r+s-\lambda)(n+s-\lambda)(n-s)!(s-1)!}. \quad (4.1.1.13)$$

This proves that for any non-integer $\lambda > 1$ a uniquely determined complete sequence of orthogonal polynomials exists.

The coefficients of these polynomials are given by (4.1.1.13) and can thus be easily calculated.

This concludes our examination of the Gram determinants.

Before we turn our attention towards the Gram-Schmidt process a very important property of orthogonal polynomials will be briefly discussed.

Theorem 1

Let $\{P_n(x)\}$ ($n=0,1,2,\dots$) be a unique sequence of polynomials which are orthogonal with respect to $w(x)$ on $[a,b]$. Then any three consecutive $P_n(x)$ of $\{P_n(x)\}$ are related by a recursion formula of the form

$$P_n(x) = (x-\beta_n)P_{n-1}(x) - \gamma_n P_{n-2}(x), \quad n=2,3,4,\dots \quad (4.1.1.14)$$

$$P_1(x) = x-\beta_1 \quad \text{and} \quad P_0(x) = 1.$$

The coefficients β_n and γ_n are given by

$$\beta_n = \frac{I_{n,n-1}}{I_{n-1,n-1}} + a_{n-1,n-2} \quad (4.1.1.15)$$

$$\gamma_n = \frac{I_{n-1,n-1}}{I_{n-2,n-2}}, \quad (4.1.1.16)$$

where we have written $I_{n,m} = \int_a^b w(x)x^n P_m(x) dx$ and $a_{n-1,n-2}$ denotes the coefficient of the power x^{n-2} in $P_{n-1}(x)$.

A proof of this theorem is given in [30], for instance.

A recursion formula similar to (4.1.1.14) also exists for the corresponding sequence of orthonormal polynomials.

For any non-integer $\lambda > 1$, $\{P_n(x)\}$ ($n=0,1,2,\dots$) is unique and therefore (4.1.1.14) is valid. Inserting (4.1.1.13) in

$$P_m(x) = x^m + \sum_{i=1}^m a_{m-i} x^{m-i}, \text{ we obtain}$$

$$I_{n,n-1} = \frac{1}{2n-\lambda} + \sum_{i=1}^{n-1} \left\{ \frac{(2n-2-\lambda-i)(2n-3-\lambda-i)\dots(n-\lambda-i)}{(n-1-i)!(i-1)!(2n-\lambda-i)} \right. \\ \left. \sum_{s=1}^{n-1} (-1)^{n-1+i-s} \frac{(n-2+s-\lambda)(n-3+s-\lambda)\dots(s-\lambda)}{(n-1-i+s-\lambda)(n-1+s-\lambda)(n-1-s)!(s-1)!} \right\}$$

$$I_{n-1,n-1} = \frac{1}{2n-1-\lambda} + \sum_{i=1}^{n-1} \left\{ \frac{(2n-2-\lambda-i)(2n-3-\lambda-i)\dots(n-\lambda-i)}{(n-1-i)!(i-1)!(2n-1-\lambda-i)} \right. \\ \left. \sum_{s=1}^{n-1} (-1)^{n-1+i-s} \frac{(n-2+s-\lambda)(n-3+s-\lambda)\dots(s-\lambda)}{(n-1-i+s-\lambda)(n-1+s-\lambda)(n-1-s)!(s-1)!} \right\}$$

$$I_{n-2,n-2} = \frac{1}{2n-3-\lambda} + \sum_{i=1}^{n-2} \left\{ \frac{(2n-4-\lambda-i)(2n-5-\lambda-i)\dots(n-1-\lambda-i)}{(n-2-i)!(i-1)!(2n-3-\lambda-i)} \right. \\ \left. \sum_{s=1}^{n-2} (-1)^{n-2+i-s} \frac{(n-3+s-\lambda)(n-4+s-\lambda)\dots(s-\lambda)}{(n-2-i+s-\lambda)(n-2+s-\lambda)(n-2-s)!(s-1)!} \right\}.$$

Since (4.1.1.15) and (4.1.1.16) become extremely cumbersome in our case, the orthogonal polynomials were directly computed, again using the rational arithmetic mentioned previously, by (4.1.1.13) instead of applying (4.1.1.14).

What can be said about the orthonormal polynomials

${}_{\lambda}P_n^*(x)$ in this case?

Since $G_0 = 1/(1-\lambda)$ it is clear that $(P_0^*, P_0^*) = -1$.

For $n > 0$ we consider (4.1.1.6). If all G_1 ($1 \geq 0$) had the same sign, then $(P_n^*, P_n^*) = 1$ for $n \geq 1$.

From [2], we do not only know the inverse of (4.1.1.11) but also the value of the determinant $|u_{rs}|$, which is equal to⁵

$$\frac{(-1)^{n(n-1)/2} \{0!1! \dots (n-1)!\}^2}{(k-n+1)(k-n+2)^2 \dots (k-1)^{n-1} k^n (k+1)^{n-1} \dots (k+n-2)^2 (k+n-1)}$$

Thus

$$G_{n-1} = \frac{\{0!1! \dots (n-1)!\}^2}{(1-\lambda)(2-\lambda)^2 \dots (n-1-\lambda)^{n-1} (n-\lambda)^n (n+1-\lambda)^{n-1} \dots (2n-2-\lambda)^2 (2n-1-\lambda)}$$

$(n = 1, 2, \dots).$ (4.1.1.17)

Assume $i < \lambda < i+1$ ($i = 1, 2, \dots$) then it is not difficult to see from (4.1.1.17) that all G_{n-1} where $n-1 \geq [(i-1)/2] + 1$ have the same sign as $(-1)^{i(i+1)/2}$. If $1 < \lambda < 2$ or $2 < \lambda < 3$, the

G_0, G_1, G_2, \dots are negative and therefore $(P_n^*, P_n^*) = 1$ for $n \geq 1$.

The coefficients of the orthogonal polynomials

$$\lambda P_2(x), \lambda P_3(x), \dots, \lambda P_{20}(x) \quad \text{for } \lambda = \frac{4}{3}, \frac{3}{2}, \frac{5}{3}$$

and their normalization factors are given in [18].

We remember that the existence of a complete sequence of orthogonal polynomials for $\lambda = 2, 4$ was secured by solving the linear systems (4.1.1.7). Thus we may apply the recursion

⁵ The formula in [2] contains a misprint: $(-1)^n$ should be replaced by $(-1)^{n(n-1)/2}$.

formula (4.1.1.14) in these cases. We have shown that if λ is an integer and odd, the sequence of orthogonal polynomials is not complete. The question as to whether in this case a recursion formula exists at all will be treated later in section 4.2 of this chapter.

4.1.2 The method by which a set of orthonormal polynomials $\{p_n^*(x)\}$ can be determined is a special case of a general procedure in which an orthonormal set of functions is constructed from an arbitrary linearly independent set. This process is known as the Gram-Schmidt orthonormalization method and can be described in our case as follows.

Given the inner product space \mathcal{H} (see section 4.1.1), then the elements $1, x, x^2, \dots$ can be orthonormalized by setting

$$\begin{aligned} p_0 &= 1 & p_0^* &= p_0 / \sqrt{|(p_0, p_0)|} \\ p_1 &= x - (x, p_0^*) p_0^* & \text{and } p_1^* &= p_1 / \sqrt{|(p_1, p_1)|} \\ &\vdots & & \\ p_n &= x^n - \sum_{k=0}^{n-1} (x^n, p_k^*) p_k^* & \text{and } p_n^* &= p_n / \sqrt{|(p_n, p_n)|} \end{aligned} \quad (4.1.2.1)$$

such that

$$|(p_i^*, p_j^*)| = \delta_{ij} \quad i, j = 0, 1, 2, \dots \quad (4.1.2.2)$$

If the metric in (4.1.2.2) is positive or negative definite, i.e. $(p_i, p_i) \neq 0$ ($i = 0, 1, 2, \dots$), then a unique and complete sequence of orthonormal polynomials (4.1.2.1) is obtained by the Gram-Schmidt process. But our metric is indefinite and therefore this procedure may or may not work.

In the following, we shall not consider the cases $\lambda = 2, 4$ - the sequences $\{p_n^*(x)\}$ were already constructed for $n = 1(1)20$ - but analyse the Gram-Schmidt process if λ is odd; we showed that then $\{p_n^*(x)\}$ is not complete.

Let us first consider the case $\lambda = 1$.

We set, according to (4.1.2.1),

$$p_0(x) = \ell_0 = 1$$

and

$$p_0^*(x) = 1/\sqrt{|(1,1)|}.$$

But now we have $(\ell_0, \ell_0) = \int_0^1 x^{-1} dx = 0$, i.e. ℓ_0 is orthogonal to itself (in a pseudo-Euclidean space, such a vector is called a light-vector). Thus $p_0^*(x)$ cannot be constructed and the Gram-Schmidt procedure comes to an end. At this point, we modify the procedure in the following way.

We introduce a linear polynomial $p_1(x) = x + a_0$ instead of $p_0(x) = 1$, while still allowing for another linear polynomial $\tilde{p}_1(x) = x + b_0$. Then we require

$$(p_1, p_1) \neq 0, \quad (\tilde{p}_1, \tilde{p}_1) \neq 0 \quad (4.1.2.3)$$

and

$$(p_1, \tilde{p}_1) = 0, \quad (4.1.2.4)$$

i.e. $p_1(x)$ and $\tilde{p}_1(x)$ are to be orthogonal to each other, but neither is any longer a light-vector. Therefore we are now able to continue the Gram-Schmidt process. For the time being we shall assume that a_0 and b_0 exist; we shall return to this point later.

The two linear polynomials can be normalized by setting

$$p_1^*(x) = p_1(x) / \sqrt{|(p_1, p_1)|} \quad (4.1.2.5)$$

$$\tilde{p}_1^*(x) = \tilde{p}_1(x) / \sqrt{|(\tilde{p}_1, \tilde{p}_1)|} \quad (4.1.2.6)$$

The next steps in the orthonormalization procedure formally agree with the Gram-Schmidt process if $p_0^*(x)$ and $p_1^*(x)$ are replaced by $p_1^*(x)$ and $\tilde{p}_1^*(x)$. The quadratic polynomial $p_2^*(x)$ is obtained by setting

$$p_2(x) = x^2 - (x^2, p_1^*)p_1^* - (x^2, \tilde{p}_1^*)\tilde{p}_1^* \quad (4.1.2.7)$$

and

$$p_2^*(x) = p_2(x) / \sqrt{|(p_2, p_2)|}.$$

A simple computation verifies that $p_2^*(x)$ is orthogonal to $p_1^*(x)$ and $\tilde{p}_1^*(x)$. For $n > 2$, the n -th orthonormal polynomial $p_n^*(x)$ is obtained by

$$p_n(x) = x^n - (x^n, p_1^*)p_1^* - (x^n, \tilde{p}_1^*)\tilde{p}_1^* - \sum_{k=2}^{n-1} (x^n, p_k^*)p_k^*, \quad (4.1.2.8)$$

$$p_n^*(x) = p_n(x) / \sqrt{|(p_n, p_n)|}.$$

In order to prove that $p_n(x)$ given by (4.1.2.8) is orthogonal to $p_1^*(x), \tilde{p}_1^*(x), p_2^*(x), \dots, p_{n-1}^*(x)$, we proceed by induction. We assume that for $2 \leq i \leq n-1$ we have proved $(p_i, p_1^*) = 0$, $(p_i, \tilde{p}_1^*) = 0$, $(p_i, p_j^*) = 0$ (the last equality holds only if $n > 3$; then $2 \leq j < i$). Then for $2 \leq j \leq n-1$

$$\begin{aligned}
(p_n, p_j^*) &= (x^n - (x^n, p_1^*)p_1^* - (x^n, \tilde{p}_1^*)\tilde{p}_1^* - \sum_{k=2}^{n-1} (x^n, p_k^*)p_k^*, p_j^*) \\
&= (x^n, p_j^*) - (x^n, p_1^*)(p_1^*, p_j^*) - (x^n, \tilde{p}_1^*)(\tilde{p}_1^*, p_j^*) - \sum_{k=2}^{n-1} (x^n, p_k^*)(p_k^*, p_j^*) \\
&= (x^n, p_j^*) - (x^n, p_j^*) = 0.
\end{aligned}$$

Replacing p_j^* by p_1^* or \tilde{p}_1^* in the above proof yields $(p_n, p_1^*) = 0$ and $(p_n, \tilde{p}_1^*) = 0$ respectively and therefore $p_n^*(x)$ is indeed orthogonal to $p_1^*(x), \tilde{p}_1^*(x), p_2^*(x), \dots, p_{n-1}^*(x)$.

We have said nothing so far about the parameters a_0 and b_0 occurring in $p_1(x)$ and $\tilde{p}_1(x)$; actually we assumed their existence so that (4.1.2.3) and (4.1.2.4) are satisfied. We want to determine them now. From (4.1.2.4) it follows that

$$a_0 + b_0 + \frac{1}{2} = 0. \quad (4.1.2.9)$$

If we assume, for instance, a_0 fixed, we can write

$$p_1(x) = x + a_0 \quad (4.1.2.10)$$

and
$$\tilde{p}_1(x) = x - a_0 - \frac{1}{2}. \quad (4.1.2.11)$$

We have a one-parameter family of pairs of polynomials; if one member of a pair satisfies (4.1.2.10) and the other satisfies (4.1.2.11) the two members are orthogonal.

Forming the inner product of $p_1(x)$ given by (4.1.2.10) with itself yields

$$(p_1, p_1) = \int_0^1 x^{-1} (x + a_0)^2 dx = 2(a_0 + \frac{1}{4}) = \pm N^2 \quad (N \geq 0). \quad (4.1.2.12)$$

The normalized polynomial $p_1^*(x)$ is therefore (we always take the positive square root)

$$p_1^*(x) = \frac{1}{N} (x + a_0) \quad \text{if } N \neq 0.$$

From (4.1.2.12) it now follows that (p_1, p_1) vanishes if $a_0 = -\frac{1}{4}$. Thus the inner product of $p_1(x)$ with itself is certainly positive for $a_0 > -\frac{1}{4}$ and negative for any $a_0 < -\frac{1}{4}$.

From this fact and (4.1.2.11) it follows immediately that either (p_1, p_1) is positive and $(\tilde{p}_1, \tilde{p}_1)$ is negative, or vice versa. Therefore, setting $a_0 = -\frac{1}{4}$, both linear polynomials must be identical and represent a light vector ℓ_1 . This is easily verified.

We now write $p_1(x)$ and $\tilde{p}_1(x)$ in a form such that the value of their inner products with themselves acts as parameter. First we introduce a new parameter a instead of a_0 , such that

$$a = a_0 + \frac{1}{4}. \quad (4.1.2.13)$$

Then

$$p_1(x) = x + a - \frac{1}{4} \quad (4.1.2.14)$$

$$\tilde{p}_1(x) = x - a - \frac{1}{4}, \quad (4.1.2.15)$$

i.e. $\tilde{p}_1(x)$ is obtained from $p_1(x)$ by merely writing $-a$ instead of a . (4.1.2.12) with (4.1.2.13) becomes $2a = \pm N^2$, or

$$a = \pm \frac{1}{2} N^2. \quad (4.1.2.16)$$

Inserting (4.1.2.16) in (4.1.2.14) and (4.1.2.15) we finally obtain

$$\left. \begin{aligned} p_1(x) &= x + \frac{1}{2}(\pm N^2 - \frac{1}{2}) \\ \tilde{p}_1(x) &= x + \frac{1}{2}(\mp N^2 - \frac{1}{2}) \end{aligned} \right\} \quad (4.1.2.17)$$

This representation of $p_1(x)$ and $\tilde{p}_1(x)$ clearly shows that if $(p_1, p_1) = +N^2$ then $(\tilde{p}_1, \tilde{p}_1) = -N^2$ and vice versa. Assuming from now on that $(p_1, p_1) = +N^2$ the normalized linear polynomials needed in the modified Gram-Schmidt process, are thus

$$\left. \begin{aligned} p_1^*(x) &= x + \frac{1}{4} \\ \tilde{p}_1^*(x) &= x - \frac{3}{4} \end{aligned} \right\} \quad (4.1.2.18)$$

Inserting these normalized linear polynomials in (4.1.2.7), we have

$$p_2(x) = x^2 - \frac{1}{2}x - \frac{1}{12}.$$

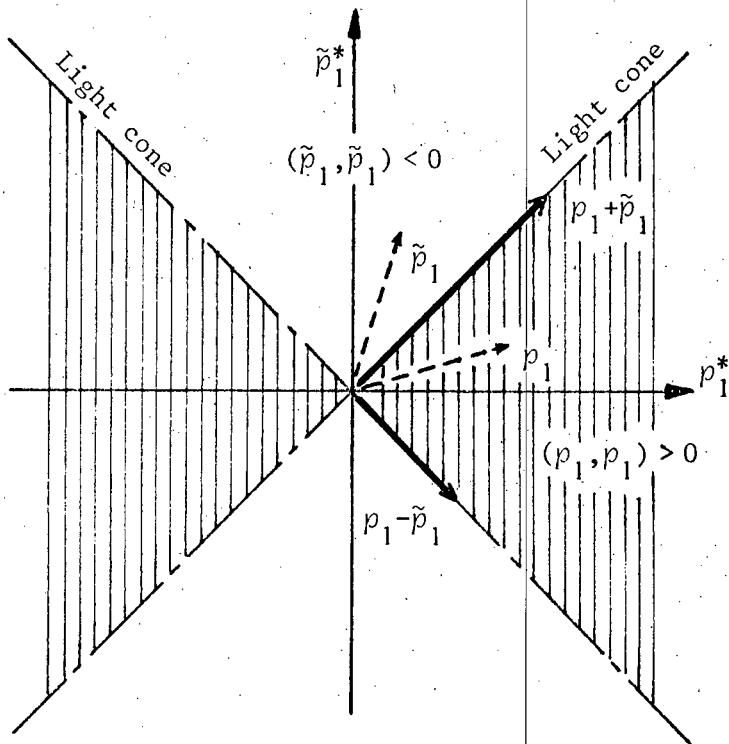
The same quadratic polynomial could also have been obtained by solving the corresponding linear system (4.1.1.7), i.e.

$$c_1 = -\frac{1}{2}$$

$$c_0 + \frac{1}{2}c_1 = -\frac{1}{3}$$

for the coefficients c_0 and c_1 of $p_2(x) = x^2 + c_1x + c_0$.

The pseudo-Euclidean subspace spanned by the linear polynomials p_1^* and \tilde{p}_1^* can be represented by the following graph



Since the vectors p_1 and \tilde{p}_1 are symmetric with respect to the light-cone (this is the set of all light-vectors) their sum and difference respectively must yield two light-vectors. It is easily verified that these light-vectors are - apart from a constant factor - identical with ℓ_1 and ℓ_0 .

We shall now briefly discuss the case $\lambda = 3$.

By the Gram-Schmidt process we set

$$p_0(x) = 1$$

and obtain

$$p_0^*(x) = 1/\sqrt{|(1,1)|} = \sqrt{2}.$$

The next two steps yield

$$p_1(x) = x - 2$$

$$p_1^*(x) = 1/\sqrt{2} (x-2)$$

and

$$p_2(x) = l_2 = x^2 - \frac{1}{2}x + 1.$$

Since now $(l_2, l_2) = 0$, we have the same situation as in the previous case, i.e. l_2 is a light-vector and the Gram-Schmidt process comes to an end. It must again be modified to enable us to continue. We introduce $p_3(x) = x^3 + a_2x^2 + a_1x + a_0$ instead of $p_2(x)$ and still allow for another cubic polynomial $\tilde{p}_3(x) = x^3 + b_2x^2 + b_1x + b_0$. Then we require the orthogonality conditions

$$(p_3, 1) = 0, \quad (p_3, x) = 0, \quad (\tilde{p}_3, 1) = 0, \quad (\tilde{p}_3, x) = 0, \quad (4.1.2.19a)$$

$$(p_3, \tilde{p}_3) = 0 \quad (4.1.2.19b)$$

to be satisfied. Furthermore, none of the cubic polynomials shall be orthogonal to itself, i.e.

$$(p_3, p_3) \neq 0 \quad \text{and} \quad (\tilde{p}_3, \tilde{p}_3) \neq 0. \quad (4.1.2.20)$$

From (4.1.2.19a) follow the equations

$$\frac{1}{2} a_0 + a_1 = 1$$

$$a_0 - a_2 = \frac{1}{2}$$

$$\frac{1}{2} b_0 + b_1 = 1$$

$$b_0 - b_2 = \frac{1}{2}.$$

In order to satisfy (4.1.2.19b) now, we merely need to require that $(p_3, x^3 + b_2 x^2) = 0$, yielding

$$\frac{1}{4} + \frac{1}{3}(a_2 + b_2) + \frac{1}{2}(a_1 + a_2 b_2) + a_0 + a_1 b_2 = 0.$$

If as before we assume a_0 to be fixed, we obtain

$$p_3(x) = x^3 + (a_0 - \frac{1}{2})x^2 + (-\frac{1}{2}a_0 + 1)x + a_0, \quad (4.1.2.21)$$

$$\tilde{p}_3(x) = x^3 + (-a_0 - \frac{7}{13})x^2 + (\frac{1}{2}a_0 + \frac{53}{52})x + (-a_0 - \frac{1}{26}); \quad (4.1.2.22)$$

i.e. a one-parameter family of pairs of cubic polynomials; each two members of a pair satisfying (4.1.2.21) and (4.1.2.22) are orthogonal.

If we form the inner product (p_3, p_3) with the aid of (4.1.2.21) and set it equal to $\pm N^2$ ($N \geq 0$) we obtain

$$\frac{13}{6}(a_0 + \frac{1}{52}) = \pm N^2,$$

i.e. if $a_0 > -\frac{1}{52}$, then (p_3, p_3) is positive, and it is negative for $a_0 < -\frac{1}{52}$. Since the constant in $\tilde{p}_3(x)$ is $-a_0 - \frac{1}{26}$, we here have the same behaviour for the inner products of $p_3(x)$ and $\tilde{p}_3(x)$ as previously with $p_1(x)$ and $\tilde{p}_1(x)$. Both cubic polynomials become identical and represent a light-vector ℓ_3 if

$$a_0 = -\frac{1}{52}.$$

Introducing a new parameter as before,

$$a = a_0 + \frac{1}{52}$$

the equations corresponding to (4.1.2.16), (4.1.2.17) and (4.1.2.18) are here

$$a = \pm \frac{6}{13} N^2$$

$$p_3(x) = x^3 + \frac{6}{13}(\pm N^2 - \frac{9}{8})x^2 - \frac{3}{13}(\pm N^2 - \frac{35}{8})x + \frac{6}{13}(\pm N^2 - \frac{1}{24})$$

$$\tilde{p}_3(x) = x^3 + \frac{6}{13}(\mp N^2 - \frac{9}{8})x^2 - \frac{3}{13}(\mp N^2 - \frac{35}{8})x + \frac{6}{13}(\mp N^2 - \frac{1}{24}).$$

Assuming from now on that $(p_3, p_3) = +N^2$, we obtain the normalized cubic polynomials

$$p_3^*(x) = x^3 - \frac{3}{52} x^2 + \frac{81}{104} x + \frac{23}{52}$$

$$\tilde{p}_3^*(x) = x^3 - \frac{51}{52} x^2 + \frac{129}{104} x - \frac{25}{52}$$

by means of which the Gram-Schmidt process may be continued.

The polynomial $p_4^*(x)$ can now be obtained by setting

$$p_4(x) = x^4 - (x^4, p_0^*)p_0^* - (x^4, p_1^*)p_1^* - (x^4, p_3^*)p_3^* - (x^4, \tilde{p}_3^*)\tilde{p}_3^*$$

$$p_4^*(x) = p_4 / \sqrt{|(p_4, p_4)|}.$$

The same pseudo-Euclidean space is spanned here by p_3^* and \tilde{p}_3^* as previously by p_1^* and \tilde{p}_1^* . The sum or the difference of any pair of vectors p_3, \tilde{p}_3 yields again a light-vector which is - apart from a constant factor - identical with ℓ_3 or ℓ_2 .

Having analysed the Gram-Schmidt process for the examples $\lambda = 1$ and $\lambda = 3$ it may be evident how this orthonormalization process has to be modified for an arbitrary odd λ .

Let $\lambda = 2m+1$ ($m=0,1,\dots$), then we assume the existence of a pseudo-Euclidean subspace as in the example with $\lambda=1$, but now spanned by the orthonormal polynomials $p_\lambda^*(x)$ and $\tilde{p}_\lambda^*(x)$. The construction of these polynomials will be given later. We start with the Gram-Schmidt process and continue until

$(p_{\lambda-1}, p_{\lambda-1}) = 0$. This point will be reached since the Gram determinant $G_{\lambda-1}$ vanishes. Up to this point, the orthonormal polynomials $p_0^*, p_1^*, \dots, p_{\lambda-2}^*$ were constructed. Now we modify

the process by introducing $p_\lambda = x^\lambda + \sum_{i=1}^{\lambda} a_{\lambda-i} x^{\lambda-i}$ instead of

$p_{\lambda-1}(x)$ while still allowing for another polynomial of degree

λ : $\tilde{p}_\lambda(x) = x^\lambda + \sum_{i=1}^{\lambda} b_{\lambda-i} x^{\lambda-i}$. Then we require p_λ and \tilde{p}_λ to

satisfy the orthogonality conditions

$$\left. \begin{aligned} (p_\lambda, x^j) &= 0 \\ (\tilde{p}_\lambda, x^j) &= 0 \end{aligned} \right\} \quad (j=0,1,\dots,\lambda-2) \quad (4.1.2.23a)$$

$$(p_\lambda, \tilde{p}_\lambda) = 0 \quad (4.1.2.23b)$$

but not to be orthogonal to themselves, i.e.

$$(p_\lambda, p_\lambda) \neq 0 \quad \text{and} \quad (\tilde{p}_\lambda, \tilde{p}_\lambda) \neq 0.$$

From (4.1.2.23a) follow the systems of linear equations

$$\left. \begin{aligned} \sum_{i=1}^{\lambda} a_{\lambda-i} \frac{1}{(i-j-1)} &= \frac{1}{j+1} \\ \sum_{i=1}^{\lambda} b_{\lambda-i} \frac{1}{(i-j-1)} &= \frac{1}{j+1} \end{aligned} \right\} \quad (j=0,1,\dots,\lambda-2) \quad (4.1.2.24)$$

In order to satisfy (4.1.2.23b) now, we merely need to require that $(p_{\lambda}, x^{\lambda} + b_{\lambda-1} x^{\lambda-1}) = 0$, yielding

$$b_{\lambda-1} \left[\frac{1}{\lambda} + \sum_{i=1}^{\lambda} a_{\lambda-i} \left(\frac{1}{\lambda-i} \right) \right] + \frac{1}{\lambda+1} + \sum_{i=1}^{\lambda} a_{\lambda-i} \left(\frac{1}{\lambda-i+1} \right) = 0.$$

Since the coefficients $a_{\lambda-i}$ and $b_{\lambda-i}$ are not uniquely determined by (4.1.2.24) we assume, for instance, that a_0 is fixed. Then we can express the remaining coefficients $a_1, a_2, \dots, a_{\lambda-1}$ and $b_0, b_1, \dots, b_{\lambda-1}$ by the parameter a_0 (we assumed the existence of the normalized polynomials p_{λ}^* and \tilde{p}_{λ}^*). By means of these parameter-dependent expressions for the coefficients $a_{\lambda-i}, b_{\lambda-i}$ we obtain a one-parameter family of pairs of polynomials $\{p_{\lambda}, \tilde{p}_{\lambda}\}$; each two of a pair are orthogonal. Applying the same normalization procedure as in the previous two examples, we finally obtain $p_{\lambda}^*(x)$ and $\tilde{p}_{\lambda}^*(x)$.

Now the Gram-Schmidt process may be continued by setting

$$p_{\lambda+1}(x) = x^{\lambda+1} - \sum_{k=0}^{\lambda-2} (x^{\lambda+1}, p_k^*) p_k^* - (x^{\lambda+1}, p_{\lambda}^*) p_{\lambda}^* - (x^{\lambda+1}, \tilde{p}_{\lambda}^*) \tilde{p}_{\lambda}^*$$

$$p_{\lambda+1}^*(x) = p_{\lambda+1} / \sqrt{|(p_{\lambda+1}, p_{\lambda+1})|}$$

for the next element.

4.1.3 Before we derive the optimal quadrature formula, we want to consider the modified Gram-Schmidt process in the corresponding matrix notation. We note that owing to our indefinite metric the eigenvalues of the Gram matrices are positive up to exactly one negative eigenvalue.

With $\chi^T = \{1, x, x^2, \dots, x^n\}$ and $p^T = \{p_0^*, p_1^*, \dots, p_n^*\}$ the modified Gram-Schmidt process can be written as

$$\chi^T = P^T U \quad (4.1.3.1)$$

where U is an almost upper triangular matrix, i.e. the lower main diagonal contains just one non-zero element (it must be remembered that there are two orthonormal polynomials of degree λ but none of degree $\lambda-1$). Since the p_i^* are normalized, we have

$$PP^T = I \quad (4.1.3.2)$$

Denoting by C the matrix containing the coefficients of the p_i^* , i.e. the "decomposition components" of the vectors p_i^* in the basis $\{1, x, x^2, \dots, x^n\}$, P can be represented by

$$P = C^T \chi \quad (4.1.3.3)$$

Inserting this expression for P in (4.1.3.1), it follows that

$$U = C^{-1}.$$

If we insert $C = U^{-1}$ in (4.1.3.3) another representation of U is obtained, viz

-105-

$$U = PX^T,$$

i.e. U is the matrix of the "projection components" of the vectors p_i^* in the basis $\{1, x, x^2, \dots, x^n\}$.

It is clear that $G = XX^T$. From this equation it follows by the aid of (4.1.3.1) and (4.1.3.2) that

$$G = XX^T = U^T P P^T U = U^T U.$$

This means that if λ is odd, the corresponding Gram matrix can be decomposed in the following way:

$$G = \begin{array}{|c|c|} \hline & U \\ \hline U^T & \\ \hline \end{array}$$

This decomposition is remarkably similar to that by Cholesky of a symmetric and positive definite matrix.

4.2 Theory of the optimal quadrature

In this section we follow the development of the theory given by V.I. Krylov [14]. The quadrature formula

$$\int_0^1 x^{-\lambda} f(x) dx \approx \sum_{i=1}^N w_i f(x_i), \quad (4.2.1)$$

for a fixed N , contains the $2N$ parameters w_i and x_i ($i=1, 2, \dots, N$). The problem is to select these parameters so that formula (4.2.1)

will be exact for all polynomials up to the highest possible degree (i.e. for all polynomials of degree $\leq k$, where k is as large as possible).

In the following, we shall only give the most important theorems of the theory. These theorems concern the degree of precision of the quadrature formula as well as the Christoffel-Darboux relationship by means of which the weights w_i can be very conveniently computed.

Let us consider the polynomial $p(x) = (x-x_1)(x-x_2)\dots(x-x_n)$ with the stations x_i of (4.2.1) as zeros, instead of considering the stations themselves. If we know the x_i , then we can easily find the coefficients of $p(x)$. Conversely, if we know the polynomial $p(x) = x^n + a_{n-1}x^{n-1} + \dots + a_0$, then the roots of $p(x)$ will give us the stations x_i .

The connection of this polynomial with the optimal quadrature formula is explained by

Theorem 1

If formula (4.2.1) is to be exact for all polynomials of degree $\leq 2N-1$, then it is necessary and sufficient that (4.2.1) be interpolatory and that the polynomial $p(x)$ be orthogonal with respect to $\langle x^{-\lambda}$ to all polynomials of degree $< N$.

The proof of this theorem is the same as that for the case of a positive weight function and is therefore omitted here.

We only remark that no formula (4.2.1) exact for all polynomials of degree $\leq 2\lambda-1$ exists for an odd λ . We remember that

in such a case the orthogonal polynomial of degree $\lambda-1$ was replaced by a one-parameter family of polynomials of degree λ . Each polynomial of this family is orthogonal to $1, x, \dots, x^{\lambda-2}$ (for $\lambda > 1$) and to a certain polynomial of the family, but it is not orthogonal to $x^{\lambda-1}$ and this violates a postulate of the theorem. The above observation then follows from taking that fact into consideration in the proof of theorem 1.

The question of the circumstances under which $2N-1$ is the highest degree of precision for formula (4.2.1) is answered by

Theorem 2

If $p(x)$ is orthogonal with respect to $x^{-\lambda}$ to all polynomials of degree $< N$ and if it can be normalized (i.e. $(p, p) \neq 0$), then, no matter how we choose the x_i and w_i , (4.2.1) cannot be exact for all polynomials of degree $2N$.

Proof

For the polynomial $\hat{p}(x) = [p(x)]^2$, which has degree $2N$, the integral $\int_0^1 x^{-\lambda} \hat{p}(x) dx \neq 0$ because we assumed $p(x)$ to be normalizable.

The quadrature sum $\sum w_i f(x_i)$ is zero because $p(x_i) = 0$. Hence (4.2.1) cannot be exact for $\hat{p}(x)$.

In order to calculate explicitly the weights in (4.2.1) the Christoffel-Darboux relationship will be useful. The proof of this relationship is based on the existence of recursion formulae for a given sequence of orthonormal polynomials $\{p^*(x)\}$. From theorem 1 of section 4.1 we know that if λ is integer and even or not integer a recursion formula for the corresponding (complete)

sequence of orthogonal polynomials exists. The recursion formula for the sequence of orthonormal polynomials is in these cases given by (see e.g. [31])

$$p_{n+1}^*(x) = (A_n x + B_n) p_n^*(x) - C_n p_{n-1}^*(x), \quad n \geq 1. \quad (4.2.2)$$

If a_k and b_k represent the coefficients of the terms of degree k and $k-1$ in $p_k^*(x)$ it can be shown that

$$A_n = \frac{a_{n+1}}{a_n}, \quad B_n = \frac{a_{n+1}}{a_n} \left(\frac{b_{n+1}}{a_{n+1}} - \frac{b_n}{a_n} \right), \quad C_n = \frac{a_{n+1} a_{n-1}}{a_n^2} \quad (4.2.3)$$

We remark that (4.2.2) and (4.2.3) remain valid for $n=0$ if we define $a_{-1} = p_{-1}^* = 0$.

It was shown in the previous section that for an odd power λ the corresponding sequence of orthonormal polynomials contains no polynomial of degree $\lambda-1$, but two polynomials of degree λ . Thus the recursion formula (4.2.2) cannot hold for all polynomials of the sequence. But we shall show

Lemma

If λ is odd and ≥ 3 and the corresponding sequence of orthonormal polynomials is denoted by $p_0^*, p_1^*, \dots, p_{\lambda-2}^*, p_\lambda^*, \tilde{p}_\lambda^*, p_{\lambda+1}^*, \dots, p_n^*, \dots$ where both p_λ^* and \tilde{p}_λ^* are of degree λ (assuming $(p_\lambda^*, p_\lambda^*) = +1$), then the following recursion formulae are valid:

(a) formula (4.2.2) with the coefficients given by (4.2.3) for $n \geq \lambda+2$ and for $0 \leq n \leq \lambda-3$.

(b) $p_{\lambda+2}^*(x) = (A_{\lambda+1} x + B_{\lambda+1}) p_{\lambda+1}^*(x) - C_{\lambda+1} \tilde{p}_\lambda^*(x) - D_{\lambda+1} p_\lambda^*(x)$
with the coefficients

$$\left. \begin{aligned}
 A_{\lambda+1} &= 1 / \int_0^1 x^{-\lambda} x p_{\lambda+2}^*(x) p_{\lambda+1}^*(x) dx \\
 B_{\lambda+1} &= - A_{\lambda+1} \int_0^1 x^{-\lambda} x [p_{\lambda+1}^*(x)]^2 dx \\
 C_{\lambda+1} &= - A_{\lambda+1} \int_0^1 x^{-\lambda} x p_{\lambda+1}^*(x) \tilde{p}_{\lambda}^*(x) dx \\
 D_{\lambda+1} &= A_{\lambda+1} \int_0^1 x^{-\lambda} x p_{\lambda+1}^*(x) p_{\lambda}^*(x) dx.
 \end{aligned} \right\} (4.2.4)$$

- (c) $p_{\lambda+1}^*(x) = (A_{\lambda}x + B_{\lambda})\tilde{p}_{\lambda}^*(x) - C_{\lambda}p_{\lambda}^*(x) - D_{\lambda}p_{\lambda-2}^*(x)$ with the coefficients

$$\left. \begin{aligned}
 A_{\lambda} &= 1 / \int_0^1 x^{-\lambda} x p_{\lambda+1}^*(x) \tilde{p}_{\lambda}^*(x) dx \\
 B_{\lambda} &= A_{\lambda} \int_0^1 x^{-\lambda} x [\tilde{p}_{\lambda}^*(x)]^2 dx \\
 C_{\lambda} &= A_{\lambda} \int_0^1 x^{-\lambda} x \tilde{p}_{\lambda}^*(x) p_{\lambda}^*(x) dx \\
 D_{\lambda} &= A_{\lambda} \int_0^1 x^{-\lambda} x \tilde{p}_{\lambda}^*(x) p_{\lambda-2}^*(x) dx.
 \end{aligned} \right\} (4.2.5)$$

- (d) $p_{\lambda+1}^*(x) = (A_{\lambda-1}x + B_{\lambda-1})p_{\lambda}^*(x) - C_{\lambda-1}\tilde{p}_{\lambda}^*(x) - D_{\lambda-1}p_{\lambda-2}^*(x)$ with the coefficients

$$\left. \begin{aligned}
 A_{\lambda-1} &= 1 / \int_0^1 x^{-\lambda} x p_{\lambda+1}^*(x) p_{\lambda}^*(x) dx \\
 B_{\lambda-1} &= - A_{\lambda-1} \int_0^1 x^{-\lambda} x [p_{\lambda}^*(x)]^2 dx \\
 C_{\lambda-1} &= - A_{\lambda-1} C_{\lambda} / A_{\lambda} \\
 D_{\lambda-1} &= A_{\lambda-1} \int_0^1 x^{-\lambda} x p_{\lambda}^*(x) p_{\lambda-2}^*(x) dx.
 \end{aligned} \right\} (4.2.6)$$

(e) $p_{\lambda}^*(x) - \tilde{p}_{\lambda}^*(x) = (A_{\lambda-2}x + B_{\lambda-2}) p_{\lambda-2}^*(x) - C_{\lambda-2} p_{\lambda-3}^*(x)$

with the coefficients

$$\left. \begin{aligned}
 A_{\lambda-2} &= 1 / \int_0^1 x^{-\lambda} x \tilde{p}_{\lambda}^*(x) p_{\lambda-2}^*(x) dx \\
 &= 1 / \int_0^1 x^{-\lambda} x p_{\lambda}^*(x) p_{\lambda-2}^*(x) dx \\
 B_{\lambda-2} &= - A_{\lambda-2} \int_0^1 x^{-\lambda} x [p_{\lambda-2}^*(x)]^2 dx \\
 C_{\lambda-2} &= A_{\lambda-2} \int_0^1 x^{-\lambda} x p_{\lambda-2}^*(x) p_{\lambda-3}^*(x) dx.
 \end{aligned} \right\} (4.2.7)$$

If $\lambda = 1$ then (d) with $p_{-1}^* \equiv 0$ is the last formula.

Proof

Assume $n \geq \lambda$ or $0 \leq n \leq \lambda-3$; then with A_n given by (4.2.3) it follows that

$$p_{n+1}^*(x) - A_n x p_n^*(x) \equiv Q_n(x)$$

is a polynomial of degree at most n . Hence, $Q_n(x)$ can be expanded as

$$\begin{aligned} Q_n(x) &= \alpha_n p_n^*(x) + \alpha_{n-1} p_{n-1}^*(x) + \dots \\ &+ \alpha_\lambda \tilde{p}_\lambda^*(x) + \alpha_{\lambda-1} p_{\lambda-1}^*(x) + \alpha_{\lambda-2} p_{\lambda-2}^*(x) + \dots + \alpha_0 p_0^*(x). \end{aligned} \quad (4.2.8)$$

By the orthogonality, however, we find that

$$\begin{aligned} \alpha_k &= \int_0^1 x^{-\lambda} Q_n(x) p_k^*(x) dx \\ &= \int_0^1 x^{-\lambda} p_{n+1}^*(x) p_k^*(x) dx - A_n \int_0^1 x^{-\lambda} x p_n^*(x) p_k^*(x) dx \quad (4.2.9) \\ &= \begin{cases} 0 & \text{for } k=0,1,\dots,n-2 \text{ if } n \geq \lambda+2 \text{ or } 2 \leq n \leq \lambda-3 \\ 0 & \text{for } k=0,1,\dots,n-3 \text{ if } \lambda \leq n \leq \lambda+1. \end{cases} \end{aligned}$$

Thus, setting $\alpha_n = B_n$, $\alpha_{n-1} = -C_n$ and $\alpha_{n-2} = -D_n$ we obtain the recursion formulae (a), (b) and (c). In principle, each coefficient of (4.2.4) and (4.2.5) is obtained in the same manner. In order to determine $B_{\lambda+1}$ (for instance) we multiply both sides of the recursion formula (b) by $p_{\lambda+1}^*(x)$. Then using the orthonormality, the explicit representation for $B_{\lambda+1}$ follows.

Since both p_λ^* and \tilde{p}_λ^* are of degree λ they may be interchanged in (c), yielding the recursion formula (d). The integral representations of the coefficients (4.2.6) of (d) are obtained in the

same manner as that described above.

So far we have constructed recursion formulae such that on the right-hand side the p_i^* ($i=\lambda, \lambda+1, \dots$) is multiplied by a linear term. Our aim is to find further recursion formulae involving the product of a linear term and p_i^* ($i=0, 1, \dots, \lambda-2$).

We know that both orthonormal polynomials which have the degree λ are of the form $x^\lambda + \dots$. Therefore, the difference $p_\lambda^* - \tilde{p}_\lambda^*$ represents a polynomial of degree at most $\lambda-1$.

If we choose $A_{\lambda-2}$ as in (4.2.3), it follows that

$$p_\lambda^*(x) - \tilde{p}_\lambda^*(x) - A_{\lambda-2} x p_{\lambda-2}^*(x) \equiv Q_{\lambda-2}(x)$$

is a polynomial of degree at most $\lambda-2$. Therefore $Q_{\lambda-2}(x)$ can be expanded as

$$Q_{\lambda-2}(x) = \beta_{\lambda-2} p_{\lambda-2}^*(x) + \beta_{\lambda-3} p_{\lambda-3}^*(x) + \dots + \beta_0 p_0^*(x). \quad (4.2.10)$$

By the orthogonality we find in the same manner as that used above that

$$\begin{aligned} \beta_{\lambda-2} &\neq 0, & \beta_{\lambda-3} &\neq 0 \\ \beta_0 &= \beta_1 = \dots = \beta_{\lambda-4} = 0. \end{aligned}$$

Thus, setting $\beta_{\lambda-2} = B_{\lambda-2}$ and $\beta_{\lambda-3} = -C_{\lambda-2}$ we obtain the recursion formula (e) with the coefficients given by (4.2.7).

We have thus demonstrated the existence and validity of the recursion formulae (a) - (e) in the case of an odd $\lambda \geq 3$. If $\lambda=1$, it is easily seen that formula (d) is the final one (remembering our convention $p_{-1}^* \equiv 0$).

This completes the proof for all odd λ .

q.e.d.

Theorem 3 (Christoffel-Darboux)

The orthonormal polynomials $p_0^*, p_1^*, \dots, p_{n+1}^*$ satisfy

$$(x-\xi) \sum_{i,k=0}^n p_i^*(x) g_{ik} p_k^*(\xi) = \frac{a_n}{a_{n+1}} [p_{n+1}^*(x)p_n^*(\xi) - p_n^*(x)p_{n+1}^*(\xi)], \quad (4.2.11)$$

$$n \geq \lambda + 1 \quad \text{if } \lambda \text{ odd}$$

$$n \geq 0 \quad \text{otherwise,}$$

where a_n denotes the coefficient of x^n in the orthonormal polynomial $p_n^*(x)$ and g_{ik} denotes the metric of the involved real linear space⁶.

Proof

We consider the recursion formula (4.2.2) and multiply both sides by $p_n^*(\xi)$ (with arbitrary ξ) to get:

$$p_{n+1}^*(x)p_n^*(\xi) = (A_n x + B_n)p_n^*(x)p_n^*(\xi) - C_n p_{n-1}^*(x)p_n^*(\xi).$$

Since this is an identity, it holds if we interchange the arguments x and ξ . Subtracting this interchanged form from the original form and multiplying by A_n^{-1} yields, with the aid of (4.2.3)

$$(x-\xi)p_n^*(x)p_n^*(\xi) = A_n^{-1} [p_{n+1}^*(x)p_n^*(\xi) - p_n^*(x)p_{n+1}^*(\xi)] - A_n^{-1} [p_n^*(x)p_{n-1}^*(\xi) - p_{n-1}^*(x)p_n^*(\xi)]. \quad (4.2.12)$$

⁶ $g_{ik} = \delta_{ik}$ in the case of the usual Euclidean space, whereas $g_{ik} = \varepsilon_i \delta_{ik}$ (see page 81) for a pseudo-Euclidean space.

We know that (4.2.2) is valid for all $n \geq 0$ if λ is not odd. Thus if we sum the identities (4.2.12) over $0, 1, 2, \dots, n$ all terms, except the last cancel (for $n=0$, we use the convention $a_{-1} = 0$). This yields the Christoffel-Darboux relationship (4.2.11).

If λ is odd, we first assume $n \geq \lambda+2$. Then, by the Lemma, the recursion formula (4.2.2) is valid and therefore also the identity (4.2.12). By applying the procedure described above to all feasible lower-order recursion formulae (b) - (e) similar identities are obtained.

From (4.2.4) - (4.2.7) it is easily verified that

$$\left. \begin{aligned} A_{\lambda} &= -A_{\lambda+1}/C_{\lambda+1} \\ A_{\lambda-1} &= A_{\lambda+1}/D_{\lambda+1} \\ A_{\lambda-2} &= A_{\lambda-1}/D_{\lambda-1} = A_{\lambda}/D_{\lambda} \end{aligned} \right\} \quad (4.2.13)$$

If we now sum the identities over $0, 1, 2, \dots, n$ all terms except the last cancel, because of (4.2.3) and (4.2.13). This last term represents the right-hand side of (4.2.11) and thus the Christoffel-Darboux relationship has also been proved for an odd λ . We remark that the above arguments remain valid for $n \geq \lambda+1$.

q.e.d.

Summarizing the statements of the theorems 1-3 we can say that an optimal quadrature formula for f.p. integrals exists. Its degree of precision is $2N-1$ (N is the number of stations) and the Christoffel-Darboux relationship is also satisfied.

We now finally discuss our main problem, the actual construction of the optimal quadrature formula. Let us consider the system of polynomials $p_N^*(x)$ ($N=0,1,2,\dots$; but if λ is odd we restrict N to the values $\geq \lambda+1$) orthonormal with respect to $\langle x^{-\lambda}$ on $[0,1]$. The roots of $p_N^*(x)$ will thus be the stations x_j ($j=1,2,\dots,N$) which are to be used in the optimal quadrature formula.

In the theory of orthogonal polynomials it is shown that if the weight function is positive in the integration interval, the roots of the corresponding orthogonal polynomials are real, distinct and located within that interval.

No conditions governing the weight function were found in the standard literature (for instance [3,12,14,30,31]) necessary for such a behaviour of the roots.

In our case, the stations may therefore be located outside the integration interval and even be complex.

Because (4.2.1) is of interpolatory type, the weights w_j are given by equation (3.1.2b) which here corresponds to

$$w_j = \int_0^1 x^{-\lambda} \frac{p_N^*(x)}{(x-x_j)p_N^*(x_j)} dx \quad (j=1,2,\dots,N). \quad (4.2.14)$$

In order to calculate w_j by (4.2.14) we make use of the Christoffel-Darboux relationship (4.2.11) by substituting x_j for ξ in the equation. After dividing by $x-x_j$ we obtain

$$\sum_{i,k=0}^N p_i^*(x) g_{ik} p_k^*(x_i) = -\frac{a_N}{a_{N+1}} \frac{p_N^*(x)p_{N+1}^*(x_j)}{x-x_j}$$

where a_N is the coefficient of x^N in $p_N^*(x)$. Let us multiply this last equation by $x^{-\lambda}$ and integrate in the sense of f.p. over $[0, 1]$. If $\lambda > 1$, the integral

$$\int_0^1 x^{-\lambda} p_k^*(x) p_k^*(x_j) dx \quad (4.2.15)$$

is zero for $k \geq 1$ by the orthogonality of $p_k^*(x)$, and is 1 for $k=0$ by the normality of $p_0^*(x)$. After carrying out the integration we have

$$1 = -\frac{a_N}{a_{N+1}} p_{N+1}^*(x_i) \int_0^1 x^{-\lambda} \frac{p_N^*(x)}{x-x_j} dx.$$

Hence we obtain

$$w_j = -\frac{a_{N+1}}{a_N} \frac{1}{p_N^*(x_j) p_{N+1}^*(x_j)} \quad j=1, 2, \dots, N \quad (4.2.16)$$

with $N \geq \lambda+1$ if λ is odd, otherwise $N \geq 1$.

We remember that in the case $\lambda=1$ there exists no polynomial of degree zero which can be normalized. Thus by the orthogonality of $p_k^*(x)$ (4.2.15) vanishes only for $k \geq 2$ and differs from zero for $k=0, 1$. It is easily shown that (4.2.16), however, remains valid in this case.

Let x_j be any root of $p_N^*(x)$ ($N \geq 2$ since λ is odd).

With $p_1^*(x)$ and $\tilde{p}_1^*(x)$ given by (4.1.2.18) we obtain

$$\begin{aligned} \sum_{i,k=0}^1 \int_0^1 x^{-1} p_i^*(x) g_{ik} p_k^*(x_j) dx &= \int_0^1 x^{-1} (x + \frac{1}{4})(x_j + \frac{1}{4}) dx - \\ &\quad - \int_0^1 x^{-1} (x - \frac{3}{4})(x_j - \frac{3}{4}) dx \\ &= \int_0^1 x^{-1} (x + x_j - \frac{1}{2}) dx \\ &= 1 \end{aligned}$$

and thus (4.2.16) also holds for $\lambda = 1$.

The above expression for w_j can be changed slightly by making use of the recursion relation (4.2.2) for orthonormal polynomials.

Let us substitute the root x_j of $p_N^*(x)$ for x in (4.2.2). This gives

$$a_N^2 p_{N+1}^*(x_j) + a_{N+1} a_{N-1} p_{N-1}^*(x_j) = 0.$$

With this relationship we can write (4.2.16) in the form

$$w_j = \frac{a_N}{a_{N-1}} \frac{1}{p_N^*(x_j) p_{N-1}^*(x_j)} \quad j=1,2,\dots,N. \quad (4.2.17)$$

We remark that (4.2.17) is valid only for $N \geq \lambda+2$, if λ is odd.

Because the formulae (4.2.16) and (4.2.17) were derived for any root of $p_N^*(x)$, they are valid even for a complex station x_j , in this case yielding a complex weight.

With this explicit representation of the weights, we consider the theory of the optimal quadrature for f.p. integrals as closed. The next section contains a brief discussion of quadrature formulae with preassigned stations.

4.3 Quadrature formulae containing preassigned stations

In applied problems it may be convenient to use quadrature formulae in which some of the stations are given in advance, while the others are free and may be chosen by any criterion we wish.

Consider the quadrature formula

$$\int_0^1 x^{-\lambda} f(x) dx \approx \sum_{i=1}^n w_i f(x_i) + \sum_{j=1}^m a_j f(y_j) \quad (4.3.1)$$

in which the m stations y_1, \dots, y_m are prescribed in advance and where the $m+2n$ constants a_j , w_i and x_i are to be determined so that (4.3.1) may be exact for polynomials of as high a degree as possible.

We shall not develop a special theory of such quadrature formulae here but give the following theorem showing the connection between this type of quadrature formula and the optimal ones.

Let us introduce the two polynomials

$$\Omega(x) = (x - y_1) \dots (x - y_m)$$

$$\omega(x) = (x - x_1) \dots (x - x_n).$$

By counting the number of ways in which the coefficients a_j and w_i can be chosen, we see that formula (4.3.1) can be made exact for polynomials of degree $\leq n+m-1$. This can be accomplished by requiring that the formula be interpolatory. In order to achieve a higher degree of precision we have at our disposal only the choice of the nodes x_i .

Theorem

In order that formula (4.3.1) may be exact for all polynomials of degree $\leq 2n+m-1$ it is necessary and sufficient that it should be interpolatory, and that the polynomial $\omega(x)$ should be orthogonal on $[0,1]$ with respect to the weight function $x^{-\lambda}\Omega(x)$ to every polynomial of degree $< n$.

A proof of this theorem, but involving a positive weight function, can be found for instance in [14]. That proof may be applied to our case and is thus omitted.

Since formula (4.3.1) is interpolatory the coefficients w_i and a_j have the following values:

$$w_i = \int_0^1 x^{-\lambda} \frac{\omega(x)\Omega(x)}{(x-x_i)\omega'(x_i)\Omega(x_i)} dx \quad i=1,2,\dots,n \quad (4.3.2)$$

$$a_j = \int_0^1 x^{-\lambda} \frac{\omega(x)\Omega(x)}{(x-y_j)\omega(y_j)\Omega'(y_j)} dx \quad j=1,2,\dots,m. \quad (4.3.3)$$

Another representation for the coefficients w_i which is easier to use for computation than (4.3.2) can be obtained if we assume

that there exists a unique system of polynomials $\pi_k(x)$ ($k=0,1,\dots$) forming an orthonormal system with respect to the weight function $\langle x^{-\lambda} \Omega(x)$ on $[0,1]$ where $\pi_k(x)$ has degree k . Clearly, the polynomial $\pi_n(x)$ differs from $\omega(x)$ by only a constant factor, so that

$$w_i = \frac{1}{\pi_n'(x_i)\Omega(x_i)} \int_0^1 \rho(x) \frac{\pi_n(x)}{x-x_i} dx$$

where

$$\rho(x) = \langle x^{-\lambda} \Omega(x).$$

The integral in this expression was calculated in the previous section using a different notation. We obtained the following two expressions for this integral:

$$\int_0^1 \rho(x) \frac{\pi_n(x)}{x-x_i} dx = \frac{a_{n+1}}{a_n \pi_{n+1}'(x_i)} = \frac{a_n}{a_{n-1} \pi_{n-1}'(x_i)},$$

where a_n is the coefficient of x^n in the polynomial $\pi_n(x)$.

Thus

$$w_i = - \frac{a_{n+1}}{a_n \pi_n'(x_i) \pi_{n+1}'(x_i) \Omega(x_i)} = \frac{a_n}{a_{n-1} \pi_n'(x_i) \pi_{n-1}'(x_i) \Omega(x_i)}. \quad (4.3.4)$$

If we compare (4.3.4) with the expressions (4.2.16) and (4.2.17) for the weights of the optimal formula then it is clear that the w_i in (4.3.1) differ only by the factor $1/\Omega(x_i)$ from the corres=

ponding weights in the quadrature formula with weight function

$$\rho(x) = \langle x^{-\lambda} \Omega(x) \rangle$$

$$\int_0^1 \rho(x) f(x) dx \approx \sum_{i=1}^n \hat{w}_i f(x_i) \quad (4.3.5)$$

which is exact for polynomials of degree $\leq 2n-1$.

We shall now discuss the quadrature formula with $y_1 = 0$ as the one preassigned station. In the classical theory of Gauss integration the case with a single fixed station is mostly called Radau integration⁷ [26]. If in what follows we speak of a Radau-type formula we mean the quadrature formula (4.3.1) with $m=1$ and $y_1 = 0$.

In the case of a Radau-type formula we have $\Omega(x) = x$ and as the previous theorem shows, we must determine the polynomial $\omega(x)$ orthogonal on $[0,1]$ with respect to the weight function $\rho(x) = \langle x^{1-\lambda}$ to every polynomial of degree $< n$ (n is the number of stations x_i). Then the roots of $\omega(x)$ are the stations x_i ($i=1,2,\dots,n$). It can immediately be recognized that the stations of the Radau-type formula are identical with those of the optimal quadrature formula with the weight function $\rho(x) = \langle x^{1-\lambda}$. The weights of the Radau-type formula are simply related to those of (4.3.5) by $w_i = \hat{w}_i/x_i$ ($i=1,2,\dots,n$).

⁷ Some Russian authors, for instance V.I. Krylov, attribute the study of the cases with

- (a) one single fixed station $y_1=0$ and
 - (b) two fixed stations $y_1=0, y_2=1$
- to A. Markoff [22].

In particular, we consider the Radau-type formula for $\lambda = 1$. Here, $\rho(x) \equiv 1$ and thus the stations are identical with the zeros of the so-called shifted Legendre polynomials, or

$$x_i = \frac{x_i^* + 1}{2} \quad (i=1,2,\dots,n) \quad (4.3.6)$$

where x_i^* denotes a zero of the classical Legendre polynomial of order n .

Denoting by w_i^* the weights of the classical Gauss-Legendre quadrature formula, we obtain for the corresponding weights

$$w_i = \frac{w_i^*}{x_i^* + 1}. \quad (4.3.7)$$

Since (4.3.1) is exact for $f(x) \equiv 1$ we can write

$$a_1 = - \sum_{i=1}^n w_i$$

and together with (4.3.6) and (4.3.7) the Radau-type formula

$$\int_0^1 \frac{f(x)}{x} dx \approx \sum_{i=1}^n \frac{w_i^*}{x_i^* + 1} \left[f\left(\frac{x_i^* + 1}{2}\right) - f(0) \right]$$

follows, involving the stations and weights of the classical Gauss-Legendre quadrature formula. We observe that the weights given by (4.3.7) are positive because the w_i^* are positive and $|x_i^*| < 1$.

This Radau-type formula is the only one among all possible quadrature formulae with one preassigned station which is related to a classical quadrature formula. If $\lambda = 2, 3, 4, 5$ then the corresponding Radau-type formula involves the stations and weights of the optimal quadrature formula with the weight function $\rho(x) = \langle x^{-1}, \langle x^{-2}, \langle x^{-3}, \langle x^{-4}$; i.e. the singularity of the weight function decreases by one power when a Radau-type formula is applied.

We next briefly investigate the second important case with preassigned stations, viz. the case when $y_1 = 0$ and $y_2 = 1$ are fixed stations. In agreement, once more, with the theory of Gauss integration we in this case call the quadrature formula (4.3.1) the Lobatto-type formula [20].

There is a remarkable correspondence between the Lobatto-type formula and the classical theory of integral approximation if $\lambda = 1$. We therefore here restrict our attention to

$$\int_0^1 \frac{f(x)}{x} dx \approx a_1 f(0) + a_2 f(1) + \sum_{i=1}^n w_i f(x_i). \quad (4.3.7)$$

The corresponding $\Omega(x)$ is equal to $x(x-1)$. In order to find the stations x_i in (4.3.7) we have to determine that polynomial which is orthogonal on $[0, 1]$ with respect to the weight function $\rho(x) = x^{-1}$ to every polynomial of degree $< n$. Since by the linear transformation $x = (t+1)/2$

$$\int_0^1 (x-1) f(x) dx = - \int_0^1 (1-x) f(x) dx = - \frac{1}{2} \int_{-1}^1 (1-t) F(t) dt, \quad (4.3.8)$$

it follows that

$$x_i = \frac{x_i^* + 1}{2} \quad (i=1,2,\dots,n). \quad (4.3.9)$$

Let $P_n^{(\alpha,\beta)}(x)$ ($n=0,1,\dots$) be the general system of Jacobi polynomials orthogonal on $[-1,+1]$ with respect to the weight function $(1-x)^\alpha(1+x)^\beta$, then x_i^* in (4.3.9) denotes the i -th root of the special Jacobi polynomial $P_n^{(1,0)}(x)$. According to (4.3.5) and (4.3.8) the weights in (4.3.7) are given by

$$w_i = \frac{w_i^*}{1 - x_i^{*2}}, \quad (4.3.10)$$

where w_i^* is the weight corresponding to x_i^* .

Because (4.3.7) is exact at least for $f(x) \equiv 1$ and $f(x) = x$, we have

$$a_1 = \sum_{i=1}^n w_i (x_i - 1) = -1,$$

$$a_2 = 1 - \sum_{i=1}^n w_i x_i.$$

Inserting these expressions together with (4.3.9) and (4.3.10) in (4.3.7) we obtain the Lobatto-type formula

$$\int_0^1 \frac{f(x)}{x} dx \approx \sum_{i=1}^n \frac{w_i^*}{1-x_i^{*2}} \left[\frac{x_i^*-1}{2} f(0) - \frac{x_i^*+1}{2} f(1) + f\left(\frac{x_i^*+1}{2}\right) \right] -f(0) + f(1)$$

involving the stations and weights derived from the special Jacobi polynomials $P^{(1,0)}(x)$. These coefficients are given, for instance, in [15].

4.4 Computation of the stations and weights for the optimal quadrature formula

In principle, there are three possible methods of computing the coefficients of the orthogonal polynomials: in the first place, the recursion formula (4.1.1.14) could be used; secondly, the Gram-Schmidt process could be applied (modified if λ is an odd integer); and thirdly the systems of linear equations (4.1.1.7) could be solved. Since the first two methods involve the process of integration they are inconvenient for practical purposes, and thus we chose the third possibility.

It is well-known that such linear systems arising in Gaussian-type quadrature are mostly rather ill-conditioned. Indeed, using some direct and iterative numerical methods for linear system solving we observed a behaviour of the solution similar to that obtained when computing the weights for an interpolatory quadrature formula: i.e. at most ten significant digits of the solution were correct with $N \geq 12$, and this accuracy we did not regard as sufficient. Therefore, to be on the safe side, the linear systems for the coefficients of the orthogonal polynomials were again solved exactly by the Gaussian elimination

process performed in a rational arithmetic [17] for the cases $\lambda = 1, 2, 3, 4, 5$ with $N = 2(1)20$ (for $\lambda = 3, 5$ of course $N \neq \lambda$). It was shown in section 4.1 that the coefficients of the orthogonal polynomials can be calculated explicitly by (4.1.1.13) if λ is not integer. With the aid of that formula and using a rational arithmetic [17] in the cases $\lambda = \frac{4}{3}, \frac{3}{2}, \frac{5}{3}$ and $N = 2(1)20$, we computed the coefficients precisely.

The next step was to determine the roots of the orthogonal polynomials. First, we found the approximate zeros of these polynomials by one of the standard methods, the coefficients being expressed merely to double precision accuracy and the calculations being also carried out in double precision. Then, using the exact (rational) representation of the polynomial coefficients and applying a special multi-precision floating point arithmetic⁸, the approximate zeros were refined to high accuracy by Newton's method. It should be noted that the rate of quadratic convergence of Newton's method is effective only if the number of significant digits used is sufficient. We used 56 significant digits in order to be sure that the refined zeros would be correct to at least 31 significant digits.

Finally, by means of (4.2.16) and (4.2.17), and again using multi-precision floating point arithmetic, we computed the corresponding weights.

The exact values of the coefficients of the polynomials, as well as the stations and weights in floating point representation

⁸ The four basic operations involving real or complex numbers may be performed by this multi-precision floating point arithmetic with an arbitrary number of digits. The method is based on an integer arithmetic [17].

to thirty significant digits (the last one correctly rounded off) are given in [18] for $\lambda = 1, \frac{4}{3}, \frac{3}{2}, \frac{5}{3}, 2, 4$ with $N = 2(1)20$ and for $\lambda = 3, 5$ with $N = \lambda+1(1)20$.

4.5 Properties of the stations and weights

According to a well-known theorem from the theory of orthogonal polynomials, the stations of a Gaussian-type quadrature formula are located within the integration interval if the weight function involved is non-negative there. To our knowledge, there is no theorem giving a necessary condition for the stations to lie within the integration interval. Such a condition might be very difficult to find. In most of the literature on Gaussian quadrature (for instance [3,12,14,30]) it is said that if the weight function $w(x)$ does not satisfy the assumption $w(x) \geq 0$ on the integration interval, the zeros of the corresponding orthogonal polynomials (provided they exist) can also lie outside the interval of integration or even be complex. In fact, for the cases we have computed the stations have the following behaviour:

$$\lambda = 1, \frac{4}{3}, \frac{3}{2}, \frac{5}{3} \quad \text{and} \quad N = 2(1)20:$$

one station is negative but relatively close to the origin ($\geq -0.1601 \dots$) and all the others are located within $[0,1]$.

$$\lambda = 2, 4 \quad \text{and} \quad N = 2(1)20:$$

there are $\lambda/2$ pairs of complex conjugate stations and the real ones lie within $[0,1]$.

$\lambda = 3,5$ and $N = \lambda+1(1)20$:

there are $[\lambda/2]$ pairs of complex conjugate stations, one negative station but not as close to the origin as previously ($\geq -0.4113 \dots$) and the remaining stations again lie within $[0,1]$.

In the theory of Gauss quadrature it is shown that if the weight function is non-negative in the integration interval then all weights are positive. But this property of the weight function is again merely sufficient. In our case, we can expect some weights to be negative or complex. Owing to the computed values we observe that to a negative, positive or complex station corresponds a negative, positive or complex weight. Of course, the complex weights occur in complex conjugate pairs. The absolute values of the real weights decrease as the absolute values of the real stations increase and their orders vary from 10^{-1} up to 10^8 . The real and imaginary parts of complex weights are of the same order of magnitude which increases with λ and N and lies between 10 and 10^8 in the computed cases.

Obviously, the application of the optimal quadrature formula is limited to f.p. integrals where the integrand function $f(x)$ is also defined outside the integration interval and where it can be evaluated for complex arguments. This means that $f(x)$ is either given analytically or its value for points not located within the interval and for complex arguments is computable by a certain procedure.

The value of the quadrature sum, in general, will be complex (unless the function satisfies $f(\bar{z}) = \overline{f(z)}$). The real part of this complex number can be considered a (real) approximation to the f.p. integral while the imaginary part gives an indication of the error of the approximation.

CHAPTER VA DERIVATIVE-FREE ERROR BOUND5.1 Error estimates for f.p. integrals in general

The analysis of errors committed when regular integrals in one dimension are evaluated by numerical integration rules has received considerable attention. Most of the quadrature error bounds which appear in the literature can be classified as either derivative-dependent or derivative-free. Derivative-dependent error bounds express a bound of the error committed when approximate formulae of integration are used, in terms of the higher derivatives of the function operated upon. Such expressions for the error bound are valid for the class of real functions which are sufficiently differentiable, and the expressions are thus widely applicable. On the other hand, they have several drawbacks. In the first place, since the error terms applicable to different rules may contain different orders of derivatives, there is no common basis enabling the rules to be compared with one another. Secondly, data on higher derivatives may be unavailable or may be difficult to obtain. This may be the case when operating with functions given in closed form but which are highly composite.

OSSICINI in [25] gave a derivative-dependent error bound for an interpolatory quadrature formula for f.p. integrals. In that paper the integrand function f is assumed to be $\in C^n[-1,1]$ where $[-1,1]$ represents the integration interval and $n \geq 1$ denotes

the number of stations. The given error bound contains an integral involving $f^{(n)} [1 + \xi(x-1)]$ ($-1 < \xi < 1$) as integrand. An error bound of this form appears to have drawbacks where practical application is concerned.

Our aim is therefore to find a derivative-free error bound for f.p. integrals, by means of which the remainder can be bounded more easily.

The integrand function f will be assumed to be analytic merely in $|z - \frac{1}{2}| < \frac{1}{2} + \epsilon$ ($\epsilon > 0$), containing the basic integration interval $[0, 1]$. For this reason, we here restrict ourselves to an error bound for the equispaced station quadrature formula. The application of the optimal quadrature formula, however, would require f to be analytically given in a larger region since some stations are negative or complex in this case.

The basic work on derivative-free error bounds for errors committed by the approximations of regular integrals, of derivatives or of real functions was done by DAVIS [4]. His derivative-free error bound is of the form $|E(f)| \leq \sigma \|f\|$. Here $f(z)$ ($z = x+iy$) is required to be analytic in a disc containing the considered interval of the real axis, and to be continuous on the boundary of the disc. The quantity σ depends solely upon the approximation rule employed while the quantity $\|f\|$ is the norm of f in the Hilbert space of analytic functions. For certain classes of analytic functions such derivative-free error bounds have been studied by several authors: [1, 11, 19, 23, 29, 33]. Most of this work is restricted to Gaussian quadrature rules.

Since almost all assumptions made by the above authors are violated by the behaviour of f.p. integrals, it is not possible to apply any of their derivative-free error bounds. For this reason we developed such an error bound with the aid of the general method given in [4].

Denoting by $E_n(f)$ the error committed in the use of our interpolatory quadrature formula with n equally spaced stations, we shall show in the following that $E_n(f)$ can be bounded in the form

$$|E_n(f)| \leq \sigma_{n,p} T_{f,q}. \quad (5.1.1)$$

p and q are parameters $\in [1, \infty]$ and must satisfy the relationship $\frac{1}{p} + \frac{1}{q} = 1$, which is deduced from the Hölder inequality involved in the derivation of (5.1.1). For p fixed, the quantity $\sigma_{n,p}$ depends merely on the n -point formula used, while $T_{f,q}$ depends only on the integrand function f . It should be noted that due to the freedom of choice of p (or q) there are - for a fixed n and f - different possible values of $\sigma_{n,p}$ and $T_{f,q}$. Ideally, the best p (or q) is that which minimizes these error quantities. But this problem is not pursued here.

We shall derive $\sigma_{n,p}$ and $T_{f,q}$ by two different methods: the first is based on an analytical continuation of the integrand function f in the sense of Borel and thus simplifies the proof of certain convergence properties. The other method dispenses with any analytical continuation of f but involves some cumbersome estimates for certain inequalities. In either case, we prove the existence of the error quantities for two practically important

values of p , viz. $p = \frac{1}{2}$ and $p = \infty$. We then bring $\sigma_{n,p}$ into a form suitable for computational purposes and give some values of it for different powers λ and $n = 3(1)20$. After a few comments on the computation of $T_{f,q}$, we conclude both cases with an example; eventually we compare the results.

Finally in this chapter we compare this analytic error bound with a graphical method for finding the number of correct significant digits. The reasons why we mention such a feasible graphical method at all are that it is simple to apply and yields fairly good results.

Before we turn our attention to the first method of obtaining the error quantities we give the condition which must be satisfied a priori by the integrand function $f(x)$ for both methods. We want to obtain a derivative-free error bound for the remainder

$$E_n(f) = \int_0^1 \frac{f(x)}{x^\lambda} dx - \sum_{i=1}^n w_i f(x_i) \quad (5.1.2)$$

in the case when the interpolatory quadrature formula of chapter III is used for approximation.

The function $f(z)$ is assumed to be an analytic function of z , regular in the disc $|z - \frac{1}{2}| < \frac{1}{2} + \epsilon$ ($\epsilon > 0$) which contains the integration interval $[0, 1]$; i.e.

$$f(z) = \sum_{k=0}^{\infty} a_k (z - \frac{1}{2})^k, \quad |z - \frac{1}{2}| < \frac{1}{2} + \epsilon \quad (5.1.3)$$

with

$$a_k = \frac{f^{(k)}(\frac{1}{2})}{k!}.$$

5.2 The first method of obtaining the error quantities

In the following, we prefer to use a simpler representation of $f(z)$ than that given in (5.1.3), namely

$$f(z) = \sum_{k=0}^{\infty} b_k z^k \quad (5.2.1)$$

with

$$b_k = \frac{f^{(k)}(0)}{k!} = \sum_{\nu=k}^{\infty} \binom{\nu}{k} \left(-\frac{1}{2}\right)^{\nu-k} a_{\nu}.$$

This representation of $f(z)$ is the essential feature of this method. But it is clear that by this change of representation the convergence radius of $f(z)$ is also changed, i.e. the series in (5.2.1) now converges absolutely and uniformly only for $|z| < \epsilon$. Therefore (5.2.1) may not be integrated termwise over $[0,1]$ as will be necessary. In order to overcome this disadvantage we apply the following

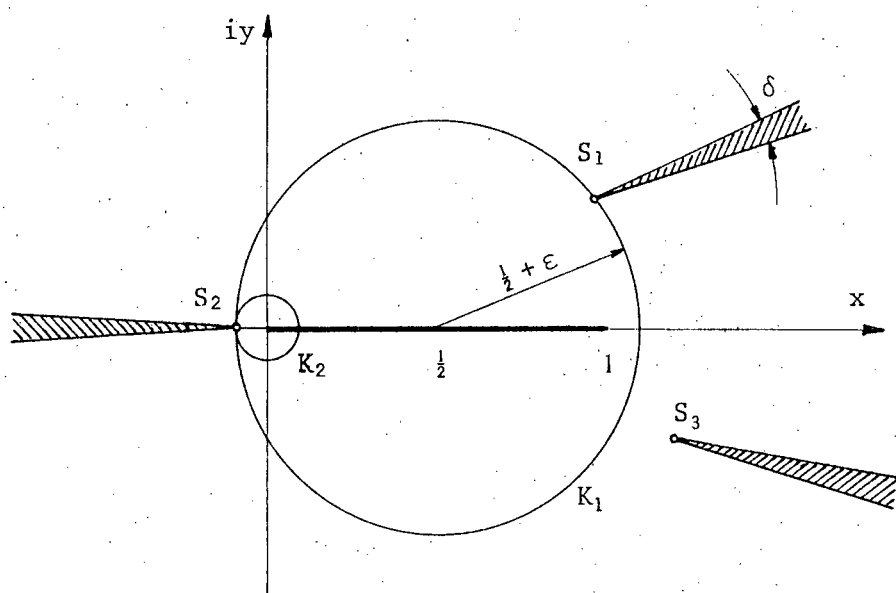
Theorem (method of analytic continuation in the sense of Borel)

Let $f(z) = \sum_{k=0}^{\infty} a_k z^k$ be convergent for $|z| < r$. Then the integral

$$\int_0^{\infty} e^{-t} F(zt) dt, \quad (5.2.2)$$

where $F(z) = \sum_{k=0}^{\infty} a_k \frac{z^k}{\Gamma(1+k)}$, represents a radial analytic continuation of $f(z)$ on a certain region of summability $B(f,1)$.

A proof of this theorem is given for instance in [10, page 83]. We illustrate the construction of such a region $B(f,1)$ in our case by the following graph.



K_1 represents the convergence circle of the series in (5.1.3). We know that at least one singular point must lie on K_1 . If S_1 is such a point, $f(z)$ can be analytically continued in a radial direction by taking out a small sector with angle δ around S_1 . In the worst possible case, the convergence circle of the series in (5.2.1) is K_2 with the radius ϵ . In such a case, there can be only one singularity S_2 on K_2 and this must lie on the negative real axis at $-\epsilon$. Again, taking out a small sector around S_2 , the radial analytic continuation of $f(z)$ is rendered possible. This process may

be continued for all singular points of $f(z)$; the remaining part of the complex plane is then the region of summability $B(f,1)$ where

(5.2.2) represents $f(z)$. It is clear that the integration interval $[0,1]$ belongs to $B(f,1)$ in any case. Thus, the radial analytic continuation of (5.2.1) which has the form

$$f(z) = \int_0^{\infty} e^{-t} \left[\sum_{k=0}^{\infty} b_k \frac{(tz)^k}{k!} \right] dt \quad (5.2.3)$$

may now be integrated termwise over $[0,1]$.

The error $E_n(f)$ can be bounded as follows.

$$\begin{aligned} |E_n(f)| &= \left| \int_0^1 \frac{f(x)}{x^\lambda} dx - \sum_{i=1}^n w_i f(x_i) \right| \\ &= \left| \int_0^1 x^{-\lambda} \int_0^{\infty} e^{-t} \sum_{k=0}^{\infty} b_k \frac{(tx)^k}{k!} dt dx - \sum_{i=1}^n w_i \int_0^{\infty} e^{-t} \sum_{k=0}^{\infty} b_k \frac{(tx_i)^k}{k!} dt \right| \\ &= \left| \int_0^{\infty} e^{-t} \sum_{k=0}^{\infty} \frac{t^k b_k}{k!} \left[\int_0^1 x^{k-\lambda} dx - \sum_{i=1}^n w_i x_i^k \right] dt \right|. \end{aligned} \quad (5.2.4)$$

We remark that the last interchange of the order of summation

yielding (5.2.4) is admissible since $\sum_k b_k \frac{(tz)^k}{k!}$ is uniformly convergent in $[0,1]$.

Since the interpolatory quadrature formula has the degree of precision $n-1$, where we require $n \geq \lambda \geq 1$ (i.e. the number of stations is not smaller than λ), the differences in (5.2.4) vanish for

$k=0,1,\dots,n-1$. Thus we can write

$$|E_n(f)| = \left| \int_0^{\infty} e^{-t} \sum_{k=0}^{\infty} \frac{t^{n+k} b_{n+k}}{(n+k)!} e_{n,k} dt \right| \quad (5.2.5)$$

where

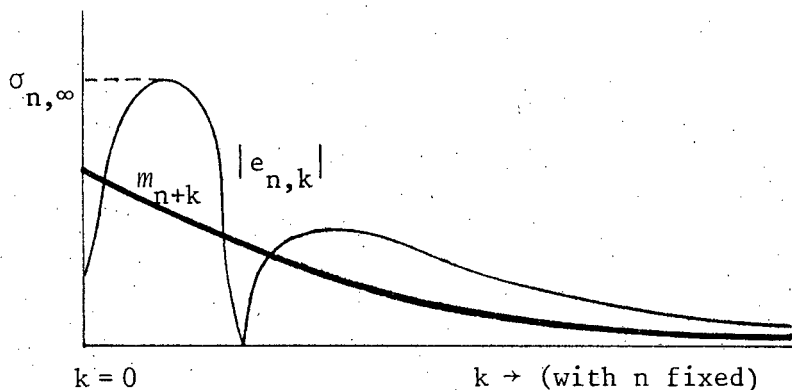
$$e_{n,k} = \int_0^1 x^{n+k-\lambda} dx - \sum_{i=1}^n w_i x_i^{n+k}. \quad (5.2.6)$$

It should be noted that owing to the above restriction on n the integral in (5.2.6) is now regular for any λ . For n fixed, the quantities $e_{n,k}$ ($k=0,1,\dots$) represent the errors of the quadrature formula when integrating the powers x^{n+k} ($k=0,1,\dots$). We can thus write $e_{n,k} = E_n(x^{n+k})$.

As we shall later see, the numerical behaviour of the quantities $e_{n,k}$ has a far-reaching effect in that it determines the existence of $\sigma_{n,p}$ and therefore also that of the derivative-free error bound.

STENGER [29] showed for instance that in the case of a symmetric Gauss-type quadrature formula, $e_{n,k} > 0$. In our case, it is easily verified numerically that the $e_{n,k}$ do not have a constant sign. Also, the sequence $\{|e_{n,k}|\}_{k=0}^{\infty}$ does not decrease monotonically as one would perhaps be inclined to assume. But this non-monotonic behaviour of $|e_{n,k}|$ is not due to the f.p. quadrature; the previously mentioned symmetric Gauss-type formula was found to exhibit similar behaviour.

A typical graph illustrating the relationship between $|e_{n,k}|$ and the higher-order moments $m_{n+k} = \int_0^1 x^{n+k-\lambda} dx$ is given below.



It follows from (5.2.5) that

$$|E_n(f)| \leq \int_0^\infty e^{-t} \sum_{k=0}^\infty \left| \frac{t^{n+k} b^{n+k}}{(n+k)!} e_{n,k} \right| dt. \quad (5.2.7)$$

Assuming that the sequence $\{e_{n,k}\}_{k=0}^\infty$ is in ℓ^p ($1 \leq p \leq \infty$) we apply Hölder's inequality to (5.2.7) and obtain

$$|E_n(f)| \leq \int_0^\infty e^{-t} \left[\sum_{k=0}^\infty \left| \frac{t^{n+k} b^{n+k}}{(n+k)!} \right|^q \right]^{1/q} \left[\sum_{k=0}^\infty |e_{n,k}|^p \right]^{1/p} dt \quad (5.2.8)$$

with $\frac{1}{p} + \frac{1}{q} = 1$.

The last factor of the integrand in (5.2.8) is independent of t and we can thus write the error bound in the form

$$|E_n(f)| \leq \sigma_{n,p} T_{f,q}$$

with the error quantities given by

$$\sigma_{n,p} = \left[\sum_{k=0}^{\infty} |e_{n,k}|^p \right]^{1/p} \quad (5.2.9)$$

and

$$T_{f,q} = \int_0^{\infty} e^{-t} \left[\sum_{k=0}^{\infty} \left| \frac{t^{n+k} b_{n+k}}{(n+k)!} \right|^q \right]^{1/q} dt. \quad (5.2.10)$$

In accordance with the Hölder inequality for each pair of parameters p and q the error quantities are expressed in a different norm which we may still choose.

We shall now consider the important error quantity $\sigma_{n,p}$.

It is easily seen from (5.2.9) that apart from the parameter p , $\sigma_{n,p}$ depends solely upon the n -point quadrature formula used and therefore can be computed once and for all.

With a view to practical application we choose the following two cases in particular:

(a) $p = q = 2$ which corresponds to the Euclidean norm of σ , i.e.

$$\sigma_{n,2}^2 = \sum_{k=0}^{\infty} e_{n,k}^2 \quad (5.2.11)$$

(b) $p = \infty$, $q = 1$ by which we obtain the supremum norm, i.e.

$$\sigma_{n,\infty} = \sup_{k=0,1,\dots} |e_{n,k}| \quad (5.2.12)$$

The question whether $\sigma_{n,2}$ and $\sigma_{n,\infty}$ exist at all is answered in the following.

Since the integral as well as the sum in (5.2.6) tend to zero when $k \rightarrow \infty$, the existence of $\sigma_{n,\infty}$ is assured for all powers λ .

In order to examine the existence of $\sigma_{n,2}$, we investigate the series $\sum_k e_{n,k}^2$. Replacing $\int_0^1 x^{n+k-\lambda} dx$ by the moment notation m_{n+k} , we can rewrite (5.2.11) in the form

$$\sigma_{n,2}^2 = \sum_{k=0}^{\infty} m_{n+k}^2 - 2 \sum_{k=0}^{\infty} m_{n+k} B_k + \sum_{k=0}^{\infty} B_k^2 \quad (5.2.13)$$

where $B_k = \sum_{i=1}^n w_i x_i^{n+k}$.

The value of m_{n+k} is $1/(n+k+1-\lambda)$ which is certainly less than one if $n > \lambda \geq 1$. Thus the first series on the right-hand side in (5.2.13) represents a general harmonic series which converges absolutely. Since

$$|B_k| < \sum_{i=1}^n |w_i| x_i^{n+k} < W y^{n+k},$$

with $W = \sum_{i=1}^n |w_i|$ and $y = \max_i x_i < 1$,

the geometric series $\sum_k W y^{n+k}$ is a convergent majorant series for $\sum_k B_k$.

Therefore the second and third series in (5.2.14) are also absolutely convergent and $\sigma_{n,2}$ exists.

Having demonstrated the existence of $\sigma_{n,p}$ for $p=2$ and $p=\infty$ we shall discuss the numerical evaluation of $\sigma_{n,2}$.

An expression such as (5.2.13) is obviously unsuitable for computing the numerical value of $\sigma_{n,2}$. We therefore recast each series in (5.2.13) as follows.

If we add the terms $1, \frac{1}{2^2}, \dots, \frac{1}{(n-\lambda)^2}$ to the first series $\sum_k m_{n+k}^2$, the new series represents Riemann's ζ function $\zeta(s) = \sum_{i=1}^{\infty} i^{-s}$ for $s=2$. But $\zeta(2) = \pi^2/6$ and we thus have

$$\sum_{k=0}^{\infty} m_{n+k}^2 = \frac{\pi^2}{6} - \sum_{j=1}^{n-\lambda} \frac{1}{j^2}. \quad (5.2.14)$$

Using the integral representation for the moments m_{n+k} , the second series can be written in the form

$$\begin{aligned} \sum_{k=0}^{\infty} m_{n+k} B_k &= \sum_{k=0}^{\infty} \int_0^1 y^{n+k-\lambda} dy \sum_{i=1}^n w_i x_i^{n+k} \\ &= \int_0^1 y^{n-\lambda} \sum_{k=0}^{\infty} y^k \sum_{i=1}^n w_i x_i^{n+k} dy \\ &= \int_0^1 y^{n-\lambda} \sum_{i=1}^n w_i x_i^n \sum_{k=0}^{\infty} (x_i y)^k dy \\ &= \int_0^1 y^{n-\lambda} \sum_{i=1}^n \frac{w_i x_i^n}{1-x_i y} dy. \end{aligned} \quad (5.2.15)$$

Recasting the third series in (5.2.13) in a similar way, we finally obtain

$$\sigma_{n,2}^2 = \frac{\pi^2}{6} - \sum_{j=1}^{n-\lambda} \frac{1}{j^2} - 2 \int_0^1 y^{n-\lambda} \sum_{i=1}^n \frac{w_i x_i^n}{1-x_i y} dy + \sum_{i=1}^n \sum_{j=1}^n \frac{w_i w_j (x_i x_j)^n}{1-x_i x_j} . \quad (5.2.16)$$

This now is an expression containing easily computable finite sums.

We computed the quantities $\sigma_{n,2}$ and $\sigma_{n,\infty}$ for $\lambda = 1, 2$ and $n = 3(1)20$.

Their values are given in the tables below (we remember that the weights w_i are given in [18]).

n	$\sigma_{n,2}$	$\sigma_{n,\infty}$
3	0,393	0,988 E-1
4	0,289	0,559 E-1
5	0,266	0,465 E-1
6	0,223	0,336 E-1
7	0,210	0,296 E-1
8	0,186	0,236 E-1
9	0,178	0,214 E-1
10	0,162	0,180 E-1
11	0,156	0,166 E-1
12	0,145	0,145 E-1
13	0,140	0,135 E-1
14	0,132	0,120 E-1
15	0,128	0,114 E-1
16	0,121	0,103 E-1
17	0,118	0,976 E-2
18	0,113	0,893 E-2
19	0,110	0,854 E-2
20	0,106	0,789 E-2

$$\lambda = 1$$

n	$\sigma_{n,2}$	$\sigma_{n,\infty}$
3	0,817	0,500
4	0,103 E1	0,430
5	0,743	0,306
6	0,910	0,297
7	0,698	0,252
8	0,835	0,230
9	0,662	0,187
10	0,781	0,190
11	0,633	0,159
12	0,738	0,162
13	0,608	0,138
14	0,704	0,142
15	0,587	0,123
16	0,675	0,127
17	0,568	0,111
18	0,650	0,115
19	0,552	0,101
20	0,628	0,105

$$\lambda = 2$$

According to these computed values one might guess that the error quantities $\sigma_{n,p}$ increase with λ^1 . Since the values of $\sigma_{n,\infty}$ are smaller than those of $\sigma_{n,2}$ they might yield a lower error bound (see the following example). Comparing our error quantities with those given in [29] for the classic Gauss-Legendre quadrature formula, we observe that they are of the same order of magnitude.

We now discuss the second error quantity $T_{f,q}$ which for a fixed q (i.e. any choice of p) depends merely on the given analytic

¹ In order to prove it, one would have to know the order of magnitude of the corresponding weights for arbitrary λ . At present this seems not to be feasible.

function f . It is relatively easy to compute $\sigma_{n,p}$, especially if $p=2$ or $p=\infty$, but it does not appear to be as easy to evaluate $T_{f,q}$.

It might be difficult to obtain an estimate of $T_{f,q}$ by developing a simpler expression not involving the Taylor coefficients b_k . But we point out here that most of the derivative-free error bounds contain a factor similar to the series in $T_{f,q}$. However, in the case of an arbitrary analytic function it does not seem to be easier to compute or estimate the value of those factors than it is to calculate $T_{f,q}$. We shall return to this point in the next section.

How can the quantity $T_{f,q}$ be computed in practice? First we need the derivatives of the given function f at the origin. For some analytic functions $f^{(k)}(0)$ ($k=0,1,2,\dots$) is known, perhaps in closed form. In the case of many analytic functions $f^{(k)}(0)$ can be computed with the aid of some symbolic string-handling language². The series involved in $T_{f,q}$ may converge mostly very rapidly owing to the denominator $(n+k)!$ and thus only a few terms need to be summed. The exponential integral itself can be conveniently computed by the classic Gauss-Laguerre quadrature formula [30].

Example 1

We bounded the error caused by applying our 3-point, 10-point and 20-point interpolatory quadrature formula to

² e.g. FORMAC which enables symbolic algebraic manipulations to be performed.

$$\int_0^1 \frac{dx}{x^2 \sqrt{(x-2)^2 + 1}}$$

The quantities $T_{f,2}$ and $T_{f,1}$ (corresponding to $p=2$ and $p=\infty$) as well as the error bounds are given below.

n	$T_{f,2}$	$\sigma_{n,2} \cdot T_{f,2}$	$T_{f,1}$	$\sigma_{n,\infty} \cdot T_{f,1}$	Actual error
3	0,18 E-1	0,15 E-1	0,24 E-1	0,12 E-1	0,10 E-1
10	0,33 E-4	0,26 E-4	0,44 E-4	0,84 E-5	0,25 E-6
20	0,11 E-7	0,68 E-8	0,18 E-7	,18 E-8	0,47 E-13

The actual error was computed by determining the difference between the values obtained by the definition formula and those obtained by the quadrature formula. We see here that the values of $T_{f,q}$, in contrast to those of $\sigma_{n,p}$, are almost independent of the parameter q . The error bounds computed with $\sigma_{n,\infty}$ are therefore smaller than those where $\sigma_{n,2}$ is involved. Both error bounds agree very well with the true error for the low-order quadrature formula, whereas agreement becomes worse as n increases.

The second method of obtaining the error quantities

The main difference between this method and the first is that we do not consider any analytic continuation of $f(z)$, but now directly

substitute the series of (5.1.3) in the error definition (5.1.2).

Doing so we obtain

$$\begin{aligned} |E_n(f)| &= \left| \int_0^1 x^{-\lambda} \sum_{k=0}^{\infty} a_k (x - \frac{1}{2})^k dx - \sum_{i=1}^n w_i \sum_{k=0}^{\infty} a_k (x_i - \frac{1}{2})^k \right| \\ &= \left| \sum_{k=0}^{\infty} a_k \left[\int_0^1 x^{-\lambda} (x - \frac{1}{2})^k dx - \sum_{i=1}^n w_i (x_i - \frac{1}{2})^k \right] \right|. \end{aligned}$$

Since the interpolatory quadrature formula has the degree of precision $n-1$, where we again require $n \geq \lambda$, the differences in the last expression vanish for $k=0,1,\dots,n-1$. Thus we have

$$|E_n(f)| = \left| \sum_{k=0}^{\infty} a_{n+k} \hat{e}_{n,k} \right| \quad (5.3.1)$$

with

$$\hat{e}_{n,k} = \int_0^1 x^{-\lambda} (x - \frac{1}{2})^{n+k} dx - \sum_{i=1}^n w_i (x_i - \frac{1}{2})^{n+k}. \quad (5.3.2)$$

It should be noted that in contrast to the previous coefficient $e_{n,k}$ the integral in (5.3.2) is not regular. The meaning of $\hat{e}_{n,k}$ is similar to that of $e_{n,k}$. It is easily seen from (5.3.2) that for n fixed the quantity $\hat{e}_{n,k}$ represents the error of the quadrature formula employed when the polynomial $(x - \frac{1}{2})^{n+k}$ is integrated. We can thus write $\hat{e}_{n,k} = E_n[(x - \frac{1}{2})^{n+k}]$.

The numerical behaviour of $\hat{e}_{n,k}$ is seen to be like that previously observed in the case of $e_{n,k}$, i.e. it does not have a constant sign and the sequence $\{|\hat{e}_{n,k}|\}_{k=0}^{\infty}$ does not decrease monotonically.

It follows from (5.3.1) that

$$|E_n(f)| \leq \sum_{k=0}^{\infty} |a_{n+k} \hat{e}_{n,k}|. \quad (5.3.3)$$

If we assume the sequence $\{\hat{e}_{n,k}\}_{k=0}^{\infty}$ to be in ℓ^p ($1 \leq p \leq \infty$) we may apply Hölder's inequality to (5.3.3) and obtain

$$|E_n(f)| \leq \sigma_{n,p} T_{f,q}$$

where

$$\sigma_{n,p} = \left\{ \sum_{k=0}^{\infty} |\hat{e}_{n,k}|^p \right\}^{1/p} \quad (5.3.4)$$

$$T_{f,q} = \left\{ \sum_{k=0}^{\infty} |a_{n+k}|^q \right\}^{1/q}. \quad (5.3.5)$$

For practical purposes we again choose the Euclidean and supremum norms for $\sigma_{n,p}$, i.e.

$$(a) \quad p = q = 2: \quad \sigma_{n,2}^2 = \sum_{k=0}^{\infty} \hat{e}_{n,k}^2 \quad (5.3.6)$$

$$(b) \quad p = \infty, q = 1: \quad \sigma_{n,\infty} = \sup_{k=0,1,2,\dots} |\hat{e}_{n,k}|. \quad (5.3.7)$$

In the following we shall show that both the quantities $\sigma_{n,2}$ and $\sigma_{n,\infty}$ exist, but it will be more difficult to do this now than in the previous case. Setting

$$A_k = \int_0^1 x^{-\lambda} (x - \frac{1}{2})^{n+k} dx$$

and
$$B_k = \sum_{i=1}^n w_i (x_i - \frac{1}{2})^{n+k}$$

(5.3.6) can be written as

$$\sigma_{n,2}^2 = \sum_{k=0}^{\infty} A_k^2 - 2 \sum_{k=0}^{\infty} A_k B_k + \sum_{k=0}^{\infty} B_k^2. \tag{5.3.8}$$

If we can find a convergent major series for each series in (5.3.8) then the existence of $\sigma_{n,2}$ is assured.

Considering $(x - \frac{1}{2})^{n+k}$ as integrand function and applying the definition formula for f.p. integrals where λ is an integer we can estimate A_k in the following way.

$$\begin{aligned} |A_k| &= \left| \sum_{\nu=0}^{\lambda-2} \left[\frac{-\nu!}{(\lambda-1)!} \left(\frac{1}{2}\right)^{n+k-(\lambda-\nu-2)} (n+k)(n+k-1)\dots(n+k-\lambda+\nu+3) + \right. \right. \\ &\quad \left. \left. + \frac{1}{\nu!(\nu+1-\lambda)} \left(-\frac{1}{2}\right)^{n+k-\nu} (n+k)(n+k-1)\dots(n+k-\nu+1) + \right. \right. \\ &\quad \left. \left. + \frac{\nu!}{(\lambda-1)!} \sum_{\mu=0}^{\nu+1} \frac{1}{(\nu+1-\mu)!} \left(-\frac{1}{2}\right)^{n+k-(\lambda-1-\mu)} (n+k)(n+k-1)\dots(n+k-\lambda+\mu+2) \right] + \right. \\ &\quad \left. + \frac{1}{(\lambda-1)!} (n+k)(n+k-1)\dots(n+k-\lambda+1) \int_0^1 \left(t-\frac{1}{2}\right)^{n+k-\lambda} \ell_n(1/t) dt \right| < \\ &< (\lambda-1) \left[\frac{(\lambda-2)!}{(\lambda-1)!} \left(\frac{1}{2}\right)^{k+2} (n+k)^{\lambda-2} + \left(\frac{1}{2}\right)^{k+2} (n+k)^{\lambda-2} + \right. \\ &\quad \left. + \frac{(\lambda-2)!}{(\lambda-1)!} \left(\frac{1}{2}\right)^{k+1} (n+k)^{\lambda-1} \lambda \right] + \frac{(n+k)^\lambda}{(\lambda-1)!} \left(\frac{1}{2}\right)^{n+k-\lambda} < \end{aligned}$$

$$\begin{aligned}
 < (\lambda-1) \left[\frac{1}{(\lambda-1)} \left(\frac{1}{2}\right)^k (n+k)^\lambda + (n+k)^\lambda \left(\frac{1}{2}\right)^k + \frac{\lambda}{(\lambda-1)} (n+k)^\lambda \left(\frac{1}{2}\right)^k \right] + \\
 & + (n+k)^\lambda \left(\frac{1}{2}\right)^k = (2\lambda+1) (n+k)^\lambda \left(\frac{1}{2}\right)^k.
 \end{aligned}$$

Thus we finally obtain

$$|A_k| < (2\lambda+1) (n+k)^\lambda \left(\frac{1}{2}\right)^k = u_k, \text{ if } \lambda \text{ is an integer.}$$

We now apply the definition formula for a non-integer λ , setting $\lambda = [\lambda] + \rho$ ($0 < \rho < 1$), and estimate A_k by

$$\begin{aligned}
 |A_k| &= \left| \sum_{\nu=0}^{[\lambda]-1} \frac{1}{\nu! (\nu+1-[\lambda]-\rho)} (n+k)(n+k-1)\dots(n+k-\nu+1) \left(-\frac{1}{2}\right)^{n+k-\nu} + \right. \\
 &+ \sum_{\nu=0}^{[\lambda]-1} \frac{(-1)^\nu}{(\nu+1-[\lambda]-\rho)! \prod_{\tau=0}^{\nu} (\tau+1-[\lambda]-\rho)} (n+k)(n+k-1)\dots \\
 &\quad \left. \dots (n+k-[\lambda]+1) \int_0^1 \left(t-\frac{1}{2}\right)^{n+k-[\lambda]} (1-t)^{[\lambda]-\nu-1} dt + \right. \\
 &+ \frac{(-1)^{[\lambda]}}{([\lambda]-1)! \prod_{\tau=0}^{[\lambda]-1} (\tau+1-[\lambda]-\rho)} (n+k)(n+k-1)\dots \\
 &\quad \left. \dots (n+k-[\lambda]+1) \int_0^1 \left(t-\frac{1}{2}\right)^{n+k-[\lambda]} t^{-\rho} dt \right| < \\
 &< [\lambda] \frac{(n+k)^{[\lambda]}}{\rho} \left(\frac{1}{2}\right)^{k+1} + \frac{(n+k)^{[\lambda]}}{\rho} \left(\frac{1}{2}\right)^{k+1} (1+[\lambda]).
 \end{aligned}$$

From the last expression it follows that

$$|A_k| < \rho^{-[\lambda]} (1 + 2[\lambda]) (n+k)^{[\lambda]} \left(\frac{1}{2}\right)^{k+1} = v_k, \text{ if } \lambda \text{ is not an integer.}$$

It is easily seen, for instance by applying the quotient criterion, that the series Σu_k and Σv_k are convergent. Therefore the series ΣA_k and ΣA_k^2 are absolutely convergent for any λ .

We shall now demonstrate that ΣB_k and ΣB_k^2 are absolutely convergent. Since

$$|B_k| = \left| \sum_{i=1}^n w_i (x_i - \frac{1}{2})^{n+k} \right| < \sum_{i=1}^n \frac{|w_i|}{2^{n+k}},$$

the geometric series

$$W \sum_{k=0}^{\infty} \left(\frac{1}{2}\right)^{n+k}, \text{ with } W = \sum_{i=1}^n |w_i|,$$

majorizes ΣB_k and thus this series as well as ΣB_k^2 are absolutely convergent. This proves the existence of $\sigma_{n,2}$. The existence of $\sigma_{n,\infty}$ follows from $\lim_{k \rightarrow \infty} A_k = 0$ and $\lim_{k \rightarrow \infty} B_k = 0$. Having convinced ourselves of the existence of $\sigma_{n,p}$ for $p=2$ and $p=\infty$, we now treat their numerical evaluation.

It is inconvenient to use the expression (5.3.8) for computing $\sigma_{n,2}$. But we can rewrite the right-hand side of (5.3.8) in such a way that infinite series are no longer involved. The result is then similar to (5.2.16).

We recast the first term in (5.3.8) in the following way

$$\begin{aligned}
 \sum_{k=0}^{\infty} A_k^2 &= \sum_{k=0}^{\infty} A_k \int_0^1 y^{-\lambda} (y - \frac{1}{2})^{n+k} dy \\
 &= \int_0^1 y^{-\lambda} (y - \frac{1}{2})^n \int_0^1 x^{-\lambda} (x - \frac{1}{2})^n \sum_{k=0}^{\infty} [(x - \frac{1}{2})(y - \frac{1}{2})]^k dx dy \\
 &= \int_0^1 \int_0^1 \frac{[(x - \frac{1}{2})(y - \frac{1}{2})]^n}{x^\lambda y^\lambda [1 - (x - \frac{1}{2})(y - \frac{1}{2})]} dx dy.
 \end{aligned}$$

The second and third terms in (5.3.8) may be treated in the same way, yielding

$$\begin{aligned}
 \sigma_{n,2}^2 &= \int_0^1 \int_0^1 \frac{[(x - \frac{1}{2})(y - \frac{1}{2})]^n}{x^\lambda y^\lambda [1 - (x - \frac{1}{2})(y - \frac{1}{2})]} dx dy - \\
 &\quad - 2 \int_0^1 y^{-\lambda} (y - \frac{1}{2})^n \sum_{i=1}^n \frac{w_i (x_i - \frac{1}{2})^n}{1 - (y - \frac{1}{2})(x_i - \frac{1}{2})} dy + \\
 &\quad + \sum_{i=1}^n \sum_{j=1}^n \frac{w_i w_j [(x_i - \frac{1}{2})(x_j - \frac{1}{2})]^n}{1 - (x_i - \frac{1}{2})(x_j - \frac{1}{2})} \tag{5.3.9}
 \end{aligned}$$

The error quantities $\sigma_{n,2}$ and $\sigma_{n,\infty}$ were evaluated for $\lambda = 1, 2, 3, 4, 5$ and $n = 3(1)20$ and the values obtained are given in the tables below.

n	$\sigma_{n,2}$	$\sigma_{n,\infty}$
3	0,691 E-1	0,556 E-1
4	0,929 E-2	0,729 E-2
5	0,661 E-2	0,507 E-2
6	0,101 E-2	0,753 E-3
7	0,730 E-3	0,532 E-3
8	0,118 E-3	0,838 E-4
9	0,865 E-4	0,597 E-4
10	0,145 E-4	0,974 E-5
11	0,107 E-4	0,698 E-5
12	0,184 E-5	0,116 E-5
13	0,136 E-5	0,836 E-6
14	0,238 E-6	0,141 E-6
15	0,177 E-6	0,102 E-6
16	0,313 E-7	0,187 E-7
17	0,234 E-7	0,136 E-7
18	0,418 E-8	0,244 E-8
19	0,313 E-8	0,183 E-9
20	0,563 E-9	0,330 E-9

$$\lambda = 1$$

n	$\sigma_{n,2}$	$\sigma_{n,\infty}$
3	0,962	0,556
4	0,492	0,271
5	0,222	0,122
6	0,995 E-1	0,526 E-1
7	0,423 E-1	0,221 E-1
8	0,180 E-1	0,908 E-2
9	0,746 E-2	0,371 E-2
10	0,310 E-2	0,156 E-2
11	0,126 E-2	0,637 E-3
12	0,514 E-3	0,262 E-3
13	0,207 E-3	0,106 E-3
14	0,836 E-4	0,428 E-4
15	0,334 E-4	0,171 E-4
16	0,134 E-4	0,686 E-5
17	0,532 E-5	0,271 E-5
18	0,212 E-5	0,108 E-5
19	0,839 E-6	0,424 E-6
20	0,333 E-6	0,167 E-6

$$\lambda = 2$$

n	$\sigma_{n,2}$	$\sigma_{n,\infty}$
3	0,279 E 1	0,141 E 1
4	0,231 E 1	0,118 E 1
5	0,157 E 1	0,812
6	0,940	0,482
7	0,518	0,261
8	0,269	0,133
9	0,134	0,670 E-1
10	0,648 E-1	0,325 E-1
11	0,305 E-1	0,154 E-1
12	0,140 E-1	0,711 E-2
13	0,636 E-2	0,323 E-2
14	0,284 E-2	0,145 E-2
15	0,126 E-2	0,639 E-3
16	0,549 E-3	0,279 E-3
17	0,238 E-3	0,120 E-3
18	0,102 E-3	0,516 E-4
19	0,437 E-4	0,219 E-4
20	0,185 E-4	0,925 E-5

$$\lambda = 3$$

n	$\sigma_{n,2}$	$\sigma_{n,\infty}$
4	0,461 E 1	0,216 E 1
5	0,447 E 1	0,211 E 1
6	0,370 E 1	0,180 E 1
7	0,268 E 1	0,131 E 1
8	0,175 E 1	0,865
9	0,106 E 1	0,527
10	0,610	0,304
11	0,334	0,167
12	0,176	0,883 E-1
13	0,902 E-1	0,453 E-1
14	0,451 E-1	0,227 E-1
15	0,221 E-1	0,111 E-1
16	0,106 E-1	0,533 E-2
17	0,503 E-2	0,251 E-2
18	0,235 E-2	0,117 E-2
19	0,108 E-2	0,537 E-3
20	0,495 E-3	0,244 E-3

$$\lambda = 4$$

n	$\sigma_{n,2}$	$\sigma_{n,\infty}$
5	0,811 E 1	0,359 E 1
6	0,821 E 1	0,362 E 1
7	0,763 E 1	0,340 E 1
8	0,633 E 1	0,296 E 1
9	0,474 E 1	0,226 E 1
10	0,327 E 1	0,158 E 1
11	0,211 E 1	0,103 E 1
12	0,129 E 1	0,631
13	0,752	0,370
14	0,424	0,209
15	0,231	0,114
16	0,123	0,607 E-1
17	0,640 E-1	0,315 E-1
18	0,326 E-1	0,160 E-1
19	0,163 E-1	0,797 E-2
20	0,805 E-2	0,391 E-2

$$\lambda = 5$$

Comparing these error quantities for $\lambda = 1, 2$ with those given in the previous section, we notice a significant difference in the order of magnitude. Since these $\sigma_{n,2}$ and $\sigma_{n,\infty}$ are considerably smaller, they might be preferable (see also the examples). In addition, we notice that the order of magnitude of $\sigma_{n,p}$ is now almost independent of p .

At this point we consider the investigation of the quadrature-dependent error quantity $\sigma_{n,p}$ as completed.

We now come to the problem of calculating the corresponding quantities $T_{f,2}$ and $T_{f,1}$ which depend on the integrand function $f(x)$, or more precisely, on the Taylor coefficients a_k . Clearly, the sharpness of our error bound will depend on how well the magnitudes of these Taylor coefficients can be estimated.

We were confronted with this problem before, in the previous section, and it was suggested there that the a_k could be computed by some symbolic string-handling language. But apart from this numerical method, what other possibilities are there? Since $T_{f,q}$ now involves no exponential integration we are here in a slightly better position than previously. In fact, $T_{f,2}$ can be crudely estimated by

$$T_{f,2} < \left\{ \sum_{k=0}^{\infty} |a_k|^2 \right\}^{\frac{1}{2}} \leq \max_{|z-\frac{1}{2}| \leq \frac{1}{2}} |f(z)|. \quad (5.3.10)$$

Although (5.3.10) looks very simple, it may, in practice, be cumbersome to determine the maximum.

In order to obtain bounds for $T_{f,1}$ we need an estimate of $\sum |a_k|$. Most of the estimates commonly used in the literature do not involve that series but only the Taylor coefficients, as the following examples show.

$$(a) \quad |a_{n+k}| \leq 2^{n+k} \max_{|z-\frac{1}{2}|=\frac{1}{2}} |f(z)|.$$

$$(b) \quad |a_{n+k}| \leq 2^{n+k} \max_{|z-\frac{1}{2}|=\frac{1}{2}} |f(z) + f(-z)|.$$

This estimate is obtained from Cauchy's integral formula.

It is used in [29], for instance.

$$(c) \quad |a_{n+k}| \leq 2^{n+k} \inf_{q \in \mathcal{P}} \left\{ \max_{|z-\frac{1}{2}|=\frac{1}{2}} \left| \frac{f(z) + f(-z)}{2} - q(z) \right| \right\},$$

where \mathcal{P} denotes the class of all polynomials of degree $\leq n-1$.

It is mentioned in [29] that this is a better estimate than

(b). Owing to the complexity of the expression, its practical utility might be very limited.

It is clear that only for some very specific functions will bounds for $T_{f,1}$ be obtained with the aid of one of the above estimates. In the literature, one can sometimes find examples of error bounds without any indication of what function is involved, it being assumed a priori that for instance $F_m := \max_{|z|=r} |f(z) + f(-z)|$ is given. But such examples can hardly be considered meaningful.

Example 2

We consider the same f.p. integral discussed in the previous section. The quantities $T_{f,2}$ and $T_{f,1}$ (corresponding to $p=2$ and $p=\infty$) as well as the computed error bounds are given below.

n	$T_{f,2}$	$\sigma_{n,2} \cdot T_{f,2}$	$T_{f,1}$	$\sigma_{n,\infty} \cdot T_{f,1}$	Actual error
3	0,23 E-1	0,22 E- 1	0,46 E-1	0,26 E- 1	0,10 E- 1
10	0,43 E-3	0,13 E- 5	0,79 E-3	0,12 E- 5	0,25 E- 6
20	0,58 E-6	0,19 E-12	0,12 E-5	0,20 E-12	0,47 E-13

Comparing the above error bounds with those obtained previously we observe that the bounds are now considerably better for $n=10$ and 20 , but worse for $n=3$. The reason is that $T_{f,1}$ and $T_{f,2}$ are here larger than before and thus the smaller error quantities $\sigma_{n,2}$, $\sigma_{n,\infty}$ affect only higher-order quadrature formulae.

5.4 General remarks

The main disadvantage of error bounds, whether derivative-free or derivative-dependent, is that they are applicable only to functions given analytically in closed form. Nevertheless, even if we know the analytic form of the function, it may in general be very difficult to estimate the value of the function-dependent term (a high-

order derivative at a point within the integration interval, or a series of its Taylor coefficients).

For practical purposes it might therefore be of advantage to use, for instance, a graphical method to determine, the number of correct significant digits.

A feasible graphical method is given in [18]. We shall briefly describe the principle of this method here.

Let $g(x) = (x-X)^2 + Y^2$; thus $g(x) = 0$ if $x = X \pm iY$.

We ran an extensive series of tests on the functions

$$f_0(x) = \sqrt{g(x)}$$

$$f_1(x) = 1/\sqrt{g(x)}$$

$$f_2(x) = 1/g(x)$$

$$f_\infty(x) = \exp[1/g(x)].$$

These functions have increasingly worse singularities in the complex plane at $X \pm iY$: f_0 has a branching point, f_1 has a pole of first order, f_2 a pole of second order and f_∞ an essential singularity. Of course the closer this singularity is to the interval of integration, the worse are the results. We used our interpolatory quadrature formula with $n = 10, 18$ and computed

$$\int_0^1 \frac{f_i(x)}{x^\lambda} dx \quad (i=0,1,2,\infty) \quad (5.4.1)$$

for each $\lambda = 1, \frac{4}{3}, \frac{3}{2}, \frac{5}{3}, 2, 3, 4, 5$.

Then for the function $f_1(x)$ - considered to be the most instructive - we plotted curves on the complex plane $X + iY$ connecting the points where equal numbers of correct significant digits were obtained; we varied $X = -1(0,25)2$ and $Y = 0(0,1)1$ (omitting, of course, $0 \leq X \leq 1$ and $Y = 0$). The results which the quadrature formula yielded were checked against the analytic definition of a f.p. integral (the graphs given in [18] refer to the function $f_1(x)$). The method of estimating the number of correct significant digits will now be demonstrated by an example.

Example 3

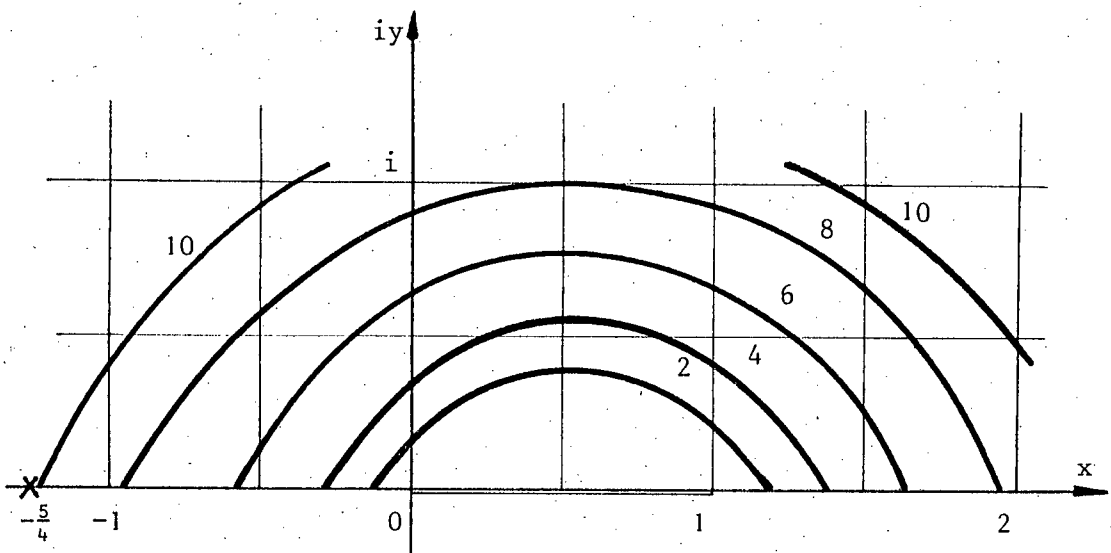
Let an f.p. integral be given where a function $f(x)$ with a simple pole is involved, for instance

$$\int_0^1 \frac{dx}{x^2 \sqrt{x + \frac{5}{4}}}$$

The corresponding $f(x)$ in (5.4.2) is $(x + \frac{5}{4})^{-\frac{1}{2}}$ and it has a pole of first order at $x = -\frac{5}{4}$. Since we are integrating from 0 to 1 and the singularity of $f(x)$ is located at $-\frac{5}{4}$ we may expect - see the graph given below - ten correct significant digits with $n = 18$.

This graph consists of the curves of equal numbers of correct significant digits for (5.4.1) with $f_1(x)$ and $n = 18$. The value of (5.4.2) yielded by our interpolatory quadrature formula with 18 stations is $-0,72938483052\dots$ and the corresponding error

bound, using $\sigma_{18,2}$ of the second method, is about $0,43 \text{ E-}10$, which means that ten significant digits of the approximation are correct. If we check the result of the approximation against the value of the definition formula for (5.4.2) we notice an actual error of about $0,23 \text{ E-}10$. In this case, both the results of the graphical method and the analytic error bound agree very well with the actual error. It is simpler and faster, however, to use the graphical method.



We shall now describe a method by which the number of correct significant digits may be estimated using only the results of the interpolatory quadrature formula.

In numerous applications of this quadrature formula it was found that the results are very stable, i.e. the accuracy attained

increased regularly with the number of stations used. This fact was made use of to devise a simple practical method of estimating the number of correct significant digits.

We consider, for instance, the application of 4-, 8- and 16-point interpolatory quadrature formulae to a given integral. It is obvious that in this case for all three quadrature formulae together only the stations of the 16-point formula are needed. Therefore three different numerical results may be obtained by merely sixteen function evaluations. But - using our tables with $N = 3(1)20$ - we can find two further ways of applying three different formulae while performing a minimum number of function evaluations.

The second possibility is to use a 5-, 10-, 20-point formula and the third involves a 6-, 9-, 18-point formula (we omit the 3-point formula since its precision is too low). In practice the last possibility seems to be the most promising since it contains neither a very low-order nor a very high-order formula.

The advantage of applying such a triplet of N -point formulae when numerically evaluating an integral is clear. Instead of computing only one scalar product by the function values and the corresponding weights, three scalar products can be computed at the expense of merely using some more weights but no additional function values. Assuming the stability of the numerical results the number of correct digits may then be estimated by comparing the three values obtained and noting the convergence.

Before concluding this chapter, we compare the values of our error bounds with the result of a derivative-free bound for regular integrals.

To do so, we apply a 4-point and 8-point Gauss-Legendre quadrature formula to

$$\int_0^1 \frac{dx}{\sqrt{(x-2)^2 + 1}}$$

and bound the errors committed by the error coefficients given in [29]. In order to be fair, the corresponding function-dependent quantities $T_{f,1} = \sum_k |a_{2n+2k}|$ and $T_{f,2} = \sqrt{\sum_k (a_{2n+2k})^2}$ were computed to the same precision as those of example 2. The results obtained are given below.

n	$\sigma_{n,2}$	$T_{f,2}$	$\sigma_{n,2} \cdot T_{f,2}$	$\sigma_{n,\infty}$	$T_{f,1}$	$\sigma_{n,\infty} \cdot T_{f,1}$	Actual error
4	0,30	0,29 E-3	0,87 E-4	0,61 E-1	0,32 E-3	0,20 E-4	0,16 E- 7
8	0,16	0,28 E-6	0,45 E-7	0,17 E-1	0,27 E-6	0,48 E-7	0,50 E-14

Comparing the error bounds with the corresponding actual errors here and in examples 1 and 2 (involving the same function), we see that the errors of the f.p. integral approximations are far better bounded. In those examples, the relative deviation of the error bound from the actual error is at most about 0,14 E+6 while here the maximum relative deviation of the error bound is $\approx 0,96 E+7$.

It thus seems that - at least as far as derivative-free error bounds are concerned - f.p. integral formulae behave better than their classical counterparts.

C O N C L U S I O N

We studied finite-part integrals which involve an algebraic singularity. We defined such integrals first by a regularization of a certain distribution and then generalized this definition so that we need not be restricted to test functions.

It was shown that the common rules for ordinary integration as far as they concern equalities are also valid for finite-part integrals. But we noticed that the standard rules concerning inequalities are not, in general, applicable. Furthermore we found the strange property that finite-part integrals with an integer exponent are not invariant under a scaling of their finite integration interval. This fact underlines the peculiarity of these integrals.

In order to derive a Gauss-type quadrature formula for the numerical evaluation of finite-part integrals we had to study a new class of orthogonal polynomials which are in a certain case elements of a pseudo-Euclidean space. The proof of the validity of the Christoffel-Darboux formula is the main result of our investigation concerning the optimal quadrature formula.

For the equispaced quadrature formula we gave two kinds of derivative-free error bounds. Their application to several examples yielded fairly good results.

In a further study of finite-part integrals, we shall investigate such integrals which involve a logarithmic or a trigonometric singularity. In particular, we shall focus attention on quadrature formulae for these kinds of finite-part integrals.

REFERENCES

- [1] BARRET, W. Convergence properties of Gaussian quadrature formulae, Comput. J. 3, p. 272-277, 1960.
- [2] COLLAR, A.R. On the reciprocal of a segment of a generalized Hilbert matrix, Proc. Cambridge Phil. Society, vol. 47, p. 11-17, 1951.
- [3] DAVIS, P.J. Interpolation and Approximation, Blaisdell Publishing Company, 1963.
- [4] DAVIS, P.J. Errors of numerical approximation for analytic functions, J. Rat. Mech. Anal. 2, p. 303-313, 1953.
- [5] FORSYTHE, G.E. & MOLER, C. Computer Solutions of Linear Algebraic Systems, Prentice Hall, 1967.
- [6] GAUSS, C.F. Methodus novus integralium valores per approximationem inveniendi, C.F. Gauss Werke, Göttingen: Königliche Gesellschaft der Wissenschaften, 3, p. 163-196, 1866.
- [7] GEL'FAND, I.M. & SHILOV, G.E. Generalized Functions Vol. I, Academic Press, New York and London, 1964
- [8] GREUB, W.H. Linear Algebra, Die Grundlehren der Mathematischen Wissenschaften in Einzeldarstellung, Band 97, Springer Verlag, 1963.
- [9] HADAMARD, J. Lectures on Cauchy's Problem in Linear Partial Differential Equations, Yale University Press, 1923.
- [10] HARDY, G.H. Divergent Series, Oxford University Press, 1949.
- [11] HÄMMERLIN, G. Über ableitungsfreie Schranken für Quadraturfehler, Num. Mathem. 5, p. 226-233, 1963.

- [12] KOPAL, Z. Numerical Analysis, Chapman & Hall Ltd., London, 1955.
- [13] KOWALEWSKI, G. Einführung in die Determinantentheorie, Walter de Gruyter and Company, Berlin, 1954.
- [14] KRYLOV, V.I. Approximate Calculation of Integrals, The MacMillan Company, New York, 1962.
- [15] KRYLOV, V.I., LUGIN, V.V. & YANOVICH. Tables for Numerical Integration of Functions with Power Singularities, Minsk: Izdat. Adad. Nauk BSSR, 1963
- [16] KUTT, H.R. The numerical evaluation of principal value integrals by finite-part integration, submitted to Num. Mathem. in January 1975.
- [17] KUTT, H.R. Routines for integer and rational arithmetics and linear system solving, CSIR Special Report, WISK 114, 1973.
- [18] KUTT, H.R. Quadrature formulae for finite-part integrals, CSIR Special Report, WISK 178, 1975.
- [19] LETHER, F.G. Error bounds for fully symmetric quadrature rules, SIAM J. Numer. Anal., Vol. 11, No. 1, March 1974.
- [20] LOBATTO, R. Lessen over de Integraal-Rekening, The Hague, 1852.
- [21] MANGLER, K.W. Improper integrals in theoretical aerodynamics, Royal Aircraft Establishment, Farnborough, Report No. 2424, June 1951.
- [22] MARKHOFF, A. Sur la méthode de Gauss par le calcul approché des intégrales, Math. Ann. Vol. 25, p. 427-432, 1885.
- [23] McNAMEE, J. Error bounds for the evaluation of integrals by the Euler-MacLaurin formula and by Gauss-type formulae, Math. Comput. 18, p. 368-381, 1964.

- [24] MORSE, P.M. & FESHBACH, H. Methods of Theoretical Physics
Part I, McGraw-Hill Book Company, Inc., 1953.
- [25] OSSICINI, A. Alcune formule di quadratura per il calcolo della
parte finita e del valore principale di integrali divergenti,
Rendiconti di Mathematica, Serie VI, Vol. 2, No. 3-4.
p. 385-403, 1969.
- [26] RADAU, R. Étude sur les formules d'approximation qui servent
à calculer la valeur numérique d'une intégral définie,
J. Math. Pures Appl. (3) Vol. 6, p. 283-336, 1880.
- [27] RÖSEL, R. Mathematical principles of aerodynamics (steady
plane subsonic potential flow), CSIR Special Report,
WISK 157, Pretoria, Dec. 1974.
- [28] SCHWARTZ, L. Théorie des Distributions, Vols I and II,
Hermann, Paris 1957-1959.
- [29] STENGER, F. Bounds on the error of Gauss-type quadratures,
Num. Mathem. 8, 150-160, 1966.
- [30] STROUD, A.H. & SECREST, D. Gaussian Quadrature Formulas,
Prentice Hall, Inc., Englewood Cliffs, N.Y., 1966.
- [31] SZEGÖ, G. Orthogonal Polynomials, American Mathematical
Society Colloquium Publications, Vol. XXIII, 1967.
- [32] TRUCKENBRODT, E. Das Geschwindigkeitspotential der tragenden
Fläche bei inkompressibler Strömung, ZAMM, Band 33, Heft 516,
Mai/Juni 1953.
- [33] WILF, H. Exactness conditions in numerical quadrature,
Num. Mathem. 6, 315-319, 1964.
- [34] ZURMÜHL, R. Matrizen, Springer Verlag, 3. Auflage 1961.

A PHYSICAL EXAMPLE ON THE NUMERICAL EVALUATION
OF FINITE-PART INTEGRALS

The following example arose in a project which is at present undertaken by the National Research Institute for Mathematical Sciences (NRIMS) of the CSIR, Pretoria. The main concerns of this project are potential problems occurring in electron optics. This physical example was the first where we practically applied the numerical quadrature of finite-part integrals and it was not available at the time the Ph.D. thesis [4] was submitted to the University of Stellenbosch.

Work upon this project is still in progress and it will presumably be finished during 1976. It is intended to publish the results.

The general physical problem

Given a rotationally symmetric electrode and an integrable surface charge density σ on it which does not depend on the rotation angle. Then the problem consists in finding the potential ϕ together with its first and second derivatives. Of particular interest are the values of these derivatives on the electrode itself. In order to compute them one has to introduce finite-part integrals.

Our present computer program calculates the potential and its first (partial) derivatives on the electrode. For testing purposes we chose the shape of the electrode such that the potential is analytically known, and we shall demonstrate essentially the numerical quadrature of finite-part integrals in this special case.

The special case

Given an infinite plane electrode containing a circular hole of radius 1,

suppose the electric fields above and below this electrode at infinity are constant and the potential is zero on the plate (electrode); see Fig. 1.

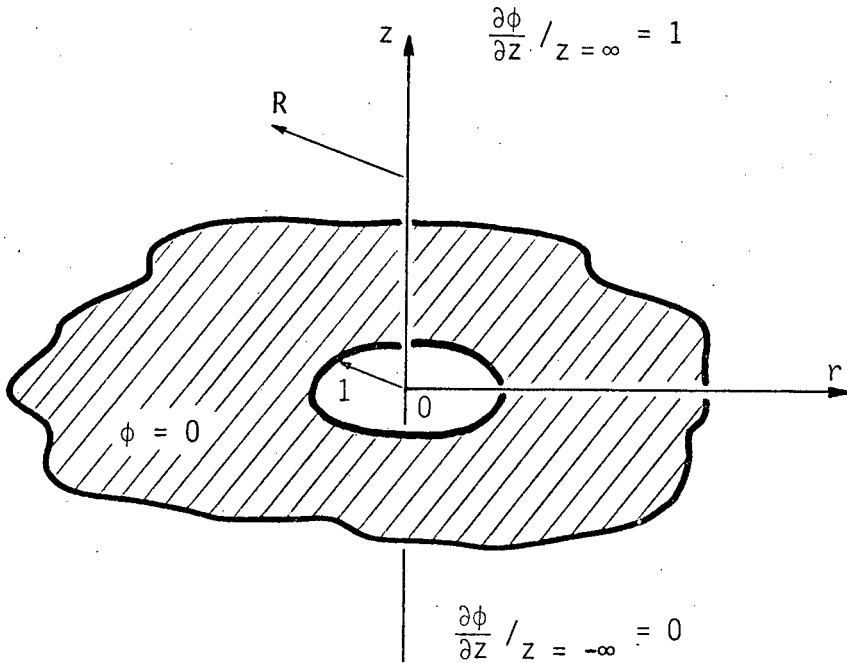


Fig. 1

From these assumptions, the potential ϕ and the surface charge density σ on the electrode can be analytically found by introducing cylindrical coordinates (see e.g. [1]) as

$$\phi(R,z) = \frac{z}{2} + \frac{z}{\pi} [\arctan(u) + 1/u] , \tag{1}$$

where
$$u = \sqrt{\frac{1}{2}(R^2+z^2-1) + \frac{1}{2}\sqrt{(R^2+z^2-1)^2 + 4z^2}} , R > 1$$

and
$$\sigma(r) = \frac{-1}{2\pi^2} [\arctan \sqrt{r^2-1} + 1/\sqrt{r^2-1}] , r > 1.$$

Example

We want to compute the first derivative of ϕ in tangential direction on

the electrode, i.e. $\lim_{z \rightarrow 0} \frac{\partial \phi}{\partial R} .$

In our case, ϕ represents the potential of a single layer. We know from potential theory that if a single layer is traversed in the normal direction the values of the potential and its derivatives in the tangential directions are continuous. This means that $\lim_{z \rightarrow 0^+} \frac{\partial \phi}{\partial R} = \lim_{z \rightarrow 0^-} \frac{\partial \phi}{\partial R} = \frac{\partial \phi}{\partial R} /_{z=0}$. From the analytic expression (1) for the potential it follows immediately that $\frac{\partial \phi}{\partial R} /_{z=0} = 0$.

In order to calculate numerically $\frac{\partial \phi}{\partial R} /_{z=0}$ we must also consider an upper electrode (to take into account the far field boundary condition $\frac{\partial \phi}{\partial z} /_{z=\infty} = 1$ in this case) the charge density on which is $\sigma_2 = -1/4\pi$. With this fictitious upper electrode we have

$$\frac{\partial \phi}{\partial R} /_{z=0} = \frac{\partial \phi_1}{\partial R} /_{z=0} + \frac{\partial \phi_2}{\partial R} /_{z=0}, \quad (3)$$

where ϕ_1 and ϕ_2 are the potentials produced by the surface charge densities $\sigma(r)$ and σ_2 . If we differentiate the integral representation of a potential $\phi(R,z)$ produced by a given charge density $\sigma(r)$ (see [2, 3]) with respect to R and let z tend to zero, we obtain

$$\frac{\partial \phi}{\partial R} /_{z=0} = 2 \int_1^{\infty} \frac{\sigma(r)r}{R(r+r)} \left[\frac{E(k)(r+R)}{r-R} - K(k) \right] dr, \quad R > 1 \quad (4)$$

where $K(k)$ is the complete elliptic integral of the first kind, $E(k)$ is the complete elliptic integral of the second kind,

$$\text{with } k^2 = \frac{4rR}{(r+R)^2} \quad (k \text{ the modulus}).$$

We remark that the elliptic integrals arise from the integration around the z -axis. The kernel of (4), i.e. the integrand without $\sigma(r)r$ represents a Green's function and is classically not integrable at the point $r = R$. We can, however, obtain the correct value of $\frac{\partial \phi}{\partial R} /_{z=0}$ by

taking the finite-part of the integral (symbol \int) in (4).

For $z = 0$ we can write

$$K(k) = K_1(k) + \ell n \left[\frac{(\sqrt{r} + \sqrt{R})^2}{|r-R|} \right] \tag{5}$$

where $K_1(k) = \int_0^{\pi/2} \sqrt{\frac{1-k \sin \alpha}{1+k \sin \alpha}} d\alpha$ is a regular integral.

Inserting the corresponding surface charge densities (2) and σ_2 respectively in (4) together with (5) we have for the lower electrode

$$\begin{aligned} \frac{\partial \phi_1}{\partial R} /_{z=0} &= \frac{-1}{\pi^2} \int_1^\infty [\arctan \sqrt{r^2-1} + 1/\sqrt{r^2-1}] \frac{E(k)r}{R(r-R)} dr + \\ &+ \frac{1}{\pi^2} \int_1^\infty [\arctan \sqrt{r^2-1} + 1/\sqrt{r^2-1}] [K_1(k) + \\ &+ \ell n \frac{(\sqrt{r} + \sqrt{R})^2}{|r-R|}] \frac{r}{R(r+R)} dr \end{aligned} \tag{6}$$

and for the upper electrode

$$\begin{aligned} \frac{\partial \phi_2}{\partial R} /_{z=0} &= \frac{-1}{2\pi} \int_0^\infty \frac{E(k)r}{R(r-R)} dr + \frac{1}{2\pi} \int_0^\infty \frac{r}{R(r+R)} [K_1(k) + \\ &+ \ell n \frac{(\sqrt{r} + \sqrt{R})^2}{|r-R|}] dr . \end{aligned} \tag{7}$$

By the substitution $r = 1/x$, the infinite integration interval of (6) may be transformed to $[0,1]$. Furthermore, if we split up the integrands we obtain

$$\frac{\partial \phi_1}{\partial R} /_{z=0} = -\frac{1}{\pi^2} \left\{ \int_0^1 \arctan \left(\frac{\sqrt{1-x^2}}{x} \right) \frac{E(k_1)}{R(1-Rx)} \frac{dx}{x^2} + \int_0^1 \frac{E(k_1) dx}{Rx(1-Rx)\sqrt{1-x^2}} - \right.$$

$$\begin{aligned}
 & - \int_0^1 \arctan\left(\frac{\sqrt{1-x^2}}{x}\right) \frac{K_1(k_1) + \ln(1+\sqrt{Rx})^2}{R(1+Rx)} \frac{dx}{x^2} - \\
 & - \int_0^1 \frac{K_1(k_1) + \ln(1+\sqrt{Rx})^2}{Rx(1+Rx)\sqrt{1-x^2}} dx - \int_0^1 \arctan\left(\frac{\sqrt{1-x^2}}{x}\right) \ln\frac{1}{|1-Rx|} \frac{dx}{Rx^2(1+Rx)} \\
 & - \int_0^1 \ln\frac{1}{|1-Rx|} \frac{dx}{Rx(1+Rx)\sqrt{1-x^2}} \} \tag{8}
 \end{aligned}$$

with $k_1^2 = \frac{4Rx}{(1+Rx)^2}$.

Separating [0,1] from the integration interval in (7) and applying the same substitution as before to the remaining (infinite) interval yields

$$\begin{aligned}
 \frac{\partial \phi_2}{\partial R} /_{z=0} &= - \frac{1}{2\pi} \left\{ \int_0^1 \frac{E(k)x}{R(x-R)} dx + \int_0^1 \frac{E(k_1)}{R(1-Rx)} \frac{dx}{x^2} - \right. \\
 & - \int_0^1 [K_1(k) + \ln\frac{(\sqrt{x} + \sqrt{R})^2}{|x-R|}] \frac{x}{R(x+R)} dx - \\
 & \left. - \int_0^1 \frac{K_1(k_1) + \ln(1+\sqrt{Rx})^2}{R(1+Rx)} \frac{dx}{x^2} - \int_0^1 \ln\frac{1}{|1-Rx|} \frac{dx}{Rx^2(1+Rx)} \right\}. \tag{9}
 \end{aligned}$$

We note that all integrals in (8) except the last must be taken in the sense of finite-part otherwise they are meaningless.

The last integral in (8) is only apparently singular at $x = 0$. This is easily seen if we write it in the form $\int_0^1 f(x) \frac{dx}{x}$ and consider $f(x)/_{x=0}$. Since $f(0) = 0$ the constant term of the Taylor series of $f(x)$ vanishes and thus that integral is integrable at $x = 0$.

In (9), there are three finite-part integrals, the other integrals exist classically.

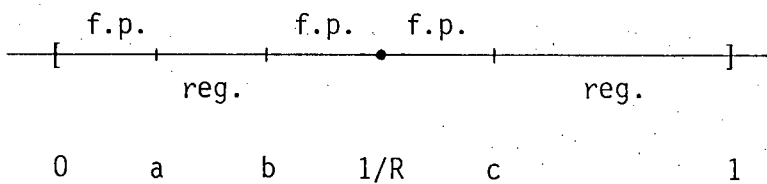
We recognize two singular locations in the finite-part integrals of (8) and (9): the origin and the point $x = 1/R$. The first singularity originates from the unbounded interval in (6) and (7) (see [4, page 52]), it corresponds to the point $r = \infty$ before the transformation and is merely due to the fact that the electrode is infinite, whereas the second was already located at the finite point $r = R$ before the change of the integration variable. We remember that this singularity is due to the kernel of the integral in (4) and must be expected.

Besides these singularities at which the integrand is not classically integrable there are integrable singular points at $x = 1/R$ and at $x = 1$. The former represents the logarithmic singularity of the term $\ln \frac{1}{|1-Rx|}$ and the latter is a singularity of $1/\sqrt{1-x^2}$ which stems from $\sigma(r)$.

Altogether we have four singularities located at three different points. Thus for the numerical evaluation of each integral in (8) and (9) we have to split up the integration interval $[0,1]$ in a suitable way. We shall illustrate this only by the first integral in (8), viz

$$\int_0^1 \arctan \left(\frac{\sqrt{1-x^2}}{x} \right) \frac{E(k_1)}{R(1-Rx)} \frac{dx}{x^2} \tag{10}$$

In order to compute this integral we divide $[0,1]$ as follows.



Thus (10) can be written as (omitting the integrand)

$$\int_0^a + \int_a^b + \int_b^{1/R} + \int_{1/R}^c + \int_c^1 ,$$

a sum of three finite-part integrals and two regular integrals.

Splitting up the interval of all singular integrals in (8) and (9) in a similar way we obtain 14 finite-part integrals. Then the remaining 32 integrals are either regular or are improper integrals of the first kind (unbounded integrand).

Our program computes each finite-part integral by the interpolatory quadrature formula with equispaced stations. The integrals involving a logarithmic singularity are numerically evaluated by the special Gaussian-type formula¹ and all other integrals by the standard Gauss-Legendre formula.

We performed several runs where R varied between 1,5 and 10 and obtained for the total sum $\Sigma := \frac{\partial \phi}{\partial R} / z=0$ of the above-mentioned 46 integrals values whose order of magnitude is 10^{-6} , i.e. six correct significant digits. In these runs, we took 32 stations for the Gaussian type formulae and 16 equispaced stations for each finite-part integral. In order to check the quality of the finite-part quadrature, we repeated some runs using the 8-, 12- and 20-point formulae. With the 12-point formula, Σ was still correct up to six significant digits, whereas the 8- and 20-point formulae yielded for Σ two significant digits less. One would expect a loss of digits with these formulae since the accuracy of the former is too low (compared with the complicate integrand) and the weights of the latter are very large (see also the remark in [4, page 76]).

Before concluding this example we briefly comment the problem of an error bound. In order to apply the derivative-free error bound given in [4] to a finite-part integral one needs the Taylor coefficients a_j of the

1 This formula approximates $\int_0^1 \ln\left(\frac{1}{x}\right) f(x) dx$ (see e.g. [5])

integrand function involved or at least a bound of $\sum_{i=0}^{\infty} |a_i|$ or $\left\{ \sum_{i=0}^{\infty} a_i^2 \right\}^{\frac{1}{2}}$.

But for this example both, the coefficients themselves or the bound of one of those series, are (unfortunately) practically not obtainable.

Therefore the numerical evaluation of the error bound expression becomes so unwieldy as to make the error bound illusory.

References

- [1] EL-KAREH, A.B. & EL-KAREH, J.C.J. Electron beams, lenses and optics. Academic Press, 1970.
- [2] BECKER, R. & SAUTER, F. Theorie der Elektrizität I. Teubner Verlag Stuttgart, 1962, pp. 50-61.
- [3] KNESCHKE, A. Differentialgleichungen und Randwertprobleme II. Teubner Verlag, Leipzig, 1961, pp. 149-157.
- [4] KUTT, H.R. On the numerical evaluation of finite-part integrals involving an algebraic singularity. Ph.D. Thesis submitted to the University of Stellenbosch, South Africa, September 1975.
- [5] STROUD, A.H. & SECREST, D. Gaussian Quadrature Formulas. Prentice-Hall, Inc., Englewood Cliffs, N.Y., 1966.