Maybe some appendix of
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A

Quadrature Rules

A quadrature rule Q is defined as

$$\int_a^b F(s)\,ds = \sum_{j=1}^{n+1} w_j\,F(s_j) + E(F), \tag{A.1.1}$$

where w_j are the weights (or coefficients) and s_j are the quadrature points (also called base points or nodes). The interval $[a,b]$ is a finite or infinite interval of integration. The error term $E(F) = 0$ iff $F(x)$ is a polynomial of degree $\leq n$.

A.1. Newton–Cotes Quadratures

Let the interval $[a,b]$ be finite and partitioned by n equally spaced points

$$s_1 = a, \quad s_2 = a+\frac{b-a}{n}, \ldots, \; s_n = a+(n-1)\frac{b-a}{n} = b-\frac{b-a}{n}, \; s_{n+1} = a.$$

Some frequently used quadrature rules are as follows:

Q_1: Repeated rectangle rule: $\displaystyle\int_a^b F(s)\,ds = \frac{b-a}{n}\sum_{j=1}^{n+1} F(s_j)\,.$

Q_2: Repeated trapezoidal rule: $\displaystyle\int_a^b F(s)\,ds = \frac{b-a}{2n}\sum_{j=1}^{n+1}{}'' \left\{2F(s_j)\right\},$

where the double primes on the summation indicate that the first and the last terms are halved.

Q_3: Repeated midpoint rule:

$$\int_a^b F(s)\,ds = h\sum_{j=0}^{n-1} F\left(a+(j+1/2)h\right), \quad h=\frac{b-a}{n}.$$

Q_4: Repeated Simpson's rule:

$$\int_a^b F(s)\,ds = \frac{b-a}{3n}\Big[F(s_1)+4\,F(s_2)+2\,F(s_3)+4\,F(s_4) + 2\,F(s_5)+\cdots+2\,F(s_{n-1})+4\,F(s_n)+F(s_{n+1})\Big].$$

Q_5: Repeated Weddle's rule:

$$\int_a^b F(s)\,ds = \frac{3(b-a)}{10n}\Big[F(s_1)+5\,F(s_2)+F(s_3)+6\,F(s_4)+F(s_5)+5\,F(s_6) + 2\,F(s_7)+5\,F(s_8)+F(s_9)+6\,F(s_{10}) + F(s_{11})+\cdots+F(s_{n-1})+5\,F(s_n)+F(s_{n+1})\Big].$$

For $n=7$ it reduces to the simple Weddle's rule.

Q_6: Newton–Cotes (N–C) rule:

$$\int_a^b F(s)\,ds = (b-a)\sum_{j=1}^{n+1} w_j\,F(s_j),$$

where $\sum_{j=1}^{n+1} w_j = 1$. The weights w_j for $n=1,2,\dots,6$ are given in Table A.1.1.

For $n=1$ this formula gives the simplest rectangle rule; for $n=2$ it gives Simpson's two-strip rule:

$$\int_a^b F(s)\,ds = \frac{b-a}{6}\left[F(s_1)+4F(s_2)+F(s_3)\right];$$

for $n = 3$ it gives Simpson's 3/8–rule:

$$\int_a^b F(s)\,ds = \frac{b-a}{8}\left[F(s_1) + 3F(s_2) + 3F(s_3) + F(s_4)\right];$$

for $n = 4$ it gives the four-strip rule:

$$\int_a^b F(s)\,ds = \frac{b-a}{90}\left[7F(s_1) + 32F(s_2) + 12F(s_3) + 32F(s_4) + 7F(s_5)\right];$$

similarly, for $n = 5$ it gives the five-strip rule and for $n = 6$ the six-strip rule, and so on; these rules can be written from Table A.1.1. A simple guideline to use this rule is as follows: When n is even (i.e., when there is an even number of subintervals or an odd number of base points), this rule is exact when $F(x)$ is a polynomials of degree $n+1$ or less; when n is odd, this rule is exact for polynomials of degree n or less; conversely, a polynomial of degree n is integrated exactly by choosing $n+1$ base points.

Table A.1.1. Weights for Newton–Cotes rule

n	w_1	w_2	w_3	w_4	w_5	w_6	w_7
1	1/2	1/2					
2	1/6	4/6	1/6				
3	1/8	3/8	3/8	1/8			
4	7/90	32/90	12/90	32/90	7/90		
5	19/288	75/288	50/288	50/288	75/288	19/288	
6	41/840	216/840	27/840	272/840	27/840	216/840	41/840

Q_7: Tangential rule:

$$\int_a^b F(s)\,ds = \frac{b-a}{n}\sum_{j=1}^{n+1} F(s_j),$$

where $s_1 = a,\quad s_2 = a + \dfrac{b-a}{2n},\quad s_3 = a + 3\dfrac{b-a}{2n}, \dots, s_{n+1} = b.$

Notes: (i) N–C rules are Riemann sums; thus, if $n \to \infty$, they converge to the exact value of the integral. (ii) Trapezoidal rule Q_2 is sometimes modified to Romberg's scheme (see Davis and Rabinowitz 1967, p.434) or Gregory's scheme (see Section 4.4, and Baker 1978, p.120). These schemes provide modifications of this rule with an end correction.

If we use the step size $h = (b-a)/n$, then the approximation formula (A.1.1) becomes

$$\int_0^{mh} F(s)\,ds = \sum_{j=0}^{m} W_{mj}\,F(jh), \quad m = 1, 2, \dots, n. \tag{A.1.2}$$

Weights W_{mj} for some useful quadrature rules are given in following tables.

Table A.1.2. Weights for a single trapezoidal rule and repeated Simpson's rule*

$m \backslash j$	0	1	2	3	4	5
1	$h/2$	$h/2$				
2	$h/3$	$4h/3$	$h/3$			
3	$h/2$	$5h/6$	$4h/3$	$h/3$		
4	$h/3$	$4h/3$	$2h/3$	$4h/3$	$h/3$	
5	$h/2$	$5h/6$	$4h/3$	$2h/3$	$4h/3$	$h/3$

Table A.1.3. Weights for repeated Simpson's rule and a single trapezoidalrule

$m \backslash j$	0	1	2	3	4	5
1	$h/2$	$h/2$				
2	$h/3$	$4h/3$	$h/3$			
3	$h/3$	$4h/3$	$5h/6$	$h/2$		
4	$h/3$	$4h/3$	$2h/3$	$4h/3$	$h/3$	
5	$h/3$	$4h/3$	$2h/3$	$4h/3$	$5h/6$	$h/2$

Table A.1.4. Weights for a single 3/8-rule and repeated Simpson's rule

$m \backslash j$	0	1	2	3	4	5	6
1	$h/2$	$h/2$					
2	$h/3$	$4h/3$	$h/3$				
3	$3h/8$	$9h/8$	$9h/8$	$3h/8$			
4	$h/3$	$4h/3$	$2h/3$	$4h/3$	$h/3$		
5	$3h/8$	$9h/8$	$9h/8$	$17h/24$	$4h/3$	$h/3$	
6	$h/3$	$4h/3$	$2h/3$	$4h/3$	$2h/3$	$4h/3$	$h/3$

*Trapezoidal rule is used for integral $\int_0^h$ and Simpson's rule for the remainder of the integral.

Table A.1.5. Weights for repeated Simpson's rule and a single 3/8-rule

$m \backslash j$	0	1	2	3	4	5	6	7
1	$h/2$	$h/2$						
2	$h/3$	$4h/3$	$h/3$					
3	$3h/8$	$9h/8$	$9h/8$	$3h/8$				
4	$h/3$	$4h/3$	$2h/3$	$4h/3$	$h/3$			
5*	$h/3$	$4h/3$	$17h/24$	$9h/8$	$9h/8$	$3h/8$		
6	$h/3$	$4h/3$	$2h/3$	$4h/3$	$2h/3$	$4h/3$	$h/3$	
7*	$h/3$	$4h/3$	$2h/3$	$4h/3$	$17h/24$	$9h/8$	$9h/8$	$3h/8$

The asterisk (*) indicates values that differ from corresponding values in Table A.1.4. This table has practical advantages over the previous table.

A.2. Gaussian Quadrature

Q_8: Gauss–Legendre rule:

$$\int_a^b F(s)\,ds = \sum_{j=1}^{n} w_j\, F(s_j)\,,$$

where

$$s_j = \frac{a+b+(b-a)\,\xi_j}{2}, \quad w_j = \frac{b-a}{\left(1-\xi_j\right)^2 \left[P_n'(\xi_j)\right]^2};$$

here ξ_j are the Gauss points for the interval $[-1,1]$ which are the zeros of the Legendre polynomials $P_n(x)$ in the interval $(-1,1)$. Although tables for the Gauss points ξ_j and weights w_j are readily available (see, e.g., Abramowitz and Stegun (1968)), they can be easily computed by Mathematica for any n (see, e.g., `gausspoints.nb` where they are also computed for the interval $(0,1)$). These rules can always be transformed to the interval $(-1,1)$ as follows:

$$\int_{-1}^{1} F(s)\,ds = \sum_{j=1}^{n} w_j\, f(s_j), \tag{A.2.1}$$

where w_j are the weights and x_j the zeros of $P_n(x)$ such that

$$w_j = \frac{1}{P_n'(x_j)} \int_{-1}^{1} \frac{P_n(x)}{(x-x_j)}\,dx. \tag{A.2.2}$$

A MODIFICATION OF GAUSS QUADRATURE is as follows: For its application to the numerical inversion of the Laplace transform, we need to modify the quadrature formula to the interval $(0, 1)$. In order to accomplish this, we make the substitution $x = 2r - 1$, $dx = 2dr$, which gives

$$\int_{-1}^{1} f(x)\,dx = \int_{0}^{1} f(2r-1)2\,dr = \sum_{j=1}^{N} w_j\, f(2r_j - 1)$$

or

$$\int_{0}^{1} f(2r-1)\,dr = \sum_{j=1}^{n} \frac{w_j}{2}\, f(2r_j - 1). \tag{A.2.3}$$

Now, if we define $f(2r-1) = \phi(r)$, then the quadrature rule reduces to

$$\int_{0}^{1} \phi(r)dr = \sum_{j=1}^{n} w'_j\, \phi(r_j), \tag{A.2.4}$$

where $r_j = \dfrac{x_j + 1}{2}$, $w'_j = \dfrac{w_j}{2}$, and r_j are the zeros of the shifted Legendre polynomials $P^*_n(r) = P_n(2r-1)$.

Q_9: Chebyshev* rule:

$$\int_{a}^{b} F(s)\,ds = h \sum_{j=1}^{n} F(s_j),$$

where $h = \dfrac{b-a}{n}$, and $s_j = \dfrac{b-a}{2} + \dfrac{b-a}{2}\xi_j$; here ξ_j denote the Chebyshev points that are the zeros of the Chebyshev polynomials $T_n(x)$, i.e., $\xi_j = \cos\dfrac{(2j-1)\pi}{2n}$, $j = 1, 2, \dots$. An advantage in using this rule is that the weights are all equal to h. See `chebyshevpoints.nb` for computing ξ_j for the intervals $(-1, 1)$ and $(0, 1)$ since they are not readily available.

Q_{10}: Clenshaw–Curtis rule:

$$\int_{-1}^{1} F(s)\,ds = \sum_{j=0}^{n} w_j\, F\Big(\cos\frac{j\pi}{n}\Big),$$

*'Chebyshev' is a transliteration from the Russian name Qebyxev ; another spelling, Tschebyscheff, is sometimes used.

where

$$w_j = \frac{4}{n} \sum_{m=0}^{[n/2]} \frac{\cos(2jm\pi/n)}{1-4m^2}, \quad j \neq 0, n; \quad w_0 = w_n = \frac{1}{n^2-1}.$$

This rule requires $(n+1)^2$ multiplications and additions, and thus it takes longer to compute. However, the weights w_j can be regarded as discrete Fourier cosine transform and computed directly with $O\,(n \ln\, n)$ operations (see Clenshaw and Curtis 1960).

Q_{11}: Cubic spline rule:

$$\int_a^b F(s)\,ds = \frac{h}{2} \sum_{j=1}^{n+1}{}'' \,(2F_j) - \frac{h^3}{4!} \sum_{j=1}^{n+1}{}'' \,(2m_j),$$

where $h = \dfrac{b-a}{n}$, $F_j = F\,(s_j)$, and $m_j = F''\,(s_j)$ for $j = 1, \dots, n+1$ (see King 1984, p. 175).

Q_{12}: One-point Gauss quadrature:

$$\int_a^b f(s)\,g(s)\,ds = w_1\,g(s_1), \tag{A.2.5}$$

where the quantities w_1 and s_1 are determined in terms of $f(s)$ as follows: Require that Eq (A.2.5) be exact for $g(s) = s^m$, $m = 0, 1$. Thus,

$$\int_a^b f(s)\,ds = w_1, \quad \int_a^b s\,f(s)\,ds = w_1 t_1, \tag{A.2.6}$$

which determine both w_1 and s_1.

Note that the built-in Mathematica object `NIntegrate` uses an adaptive algorithm, which recursively divides the interval of integration as needed; the Gauss points specify the number of initial points to choose. If an explicit setting for maximum points is given, `NIntegrate` also uses quasi-Monte Carlo methods to get an estimate of the result, sampling at most the numbers specified (see Wolfram, *The Mathematica Book*, 1996, p.1145).

The error estimate $E_x(F)$ for the above quadrature rules Q_j of degree p is bounded by

$$\left|E_x(F)\right| = \left| \int_a^b F(s)\,ds - \sum_{j=1}^{n} w_j\,F\,(s_j) \right| \leq C(F)\,n^{-p}, \tag{A.2.7}$$

where the constant $C(F)$ depends on the function $F(x)$. The degree p is called the *order* of convergence. The above inequality implies that $\lim_{n\to\infty} \left|E_x(F)\right| = 0$ for any sequence $\{Q_j\}$ of quadrature rules. This condition is met by any n-panel Newton–Cotes rules of degree p for any fixed p and increasing n, and also Gauss–Legendre and Chebyshev n-point rules for increasing n. But this condition is not met by n-panel Newton–Cotes rules for any fixed n and increasing p. We should avoid this situation. Thus, in practice repeated trapezoidal or Simpson's rule and one-panel Gauss–Legendre or Chebyshev rules make the best choice since these rules guarantee not only convergence but also a fast rate of convergence.

In some cases the Gauss–Legendre quadrature formulas become unstable for large n, say $n > 20$. This arises because of the fact that the points and weights are rational numbers and, therefore, must be rounded off. In general, this quadrature rule is superior to most other rules with the same number of points. However, for some integrals it is not true that a Gauss rule is always the best one. For example, the n-point trapezoidal rule is much better than the n-point Gauss–Legendre rule for the integral

$$\int_0^1 \frac{2}{2+\sin(10\pi x)}\, dx,$$

as the following results show: Exact value $= 2/\sqrt{3} \approx 1.1547$; 4-point trapezoidal rule gives 1.91667, while 4-point Gauss–Legendre rule gives 2.53883; 12-point trapezoidal rule gives 2.1594, while 12-point Gauss–Legendre rule gives 2.25809. For computational details, see `app1.nb`.

A.3. Integration of Products

We shall construct a quadrature rule for an integral with an integrand that is the product of any two functions $w(x)$ and $F(x)$ over an interval $[a, b]$. Such a rule is of the form

$$\int_a^b w(s)F(s)\, ds = \sum_{j=0}^{n} v_j\, F(s_j), \tag{A.3.1}$$

where s_j are the quadrature points, $a \le s_j \le b$, and the weights v_j depend on a, b as well as the function $w(x)$. If the function $w \equiv 1$, the rule (A.3.1) reduces to the quadrature rules presented in Section A.1–A.2. We discuss two cases:

CASE 1. If the function $F(x)$ is "badly behaved", e.g., $F(x)$ behaves like $(x-s)^{-1/2}$ near $x=s$ but is continuous everywhere else, we can find a function $g(x)$ such that $F(x)=g(x)(x-s)^{-1/2}$. In general, if we approximate $F(x)$ by using a polynomial interpolant

$$I(x)=\sum_{j=0}^{n} l_j(x)\,F(s_j),$$

where

$$l_j(x)=\prod_{\substack{i=0\\ i\neq j}}\frac{x-s_i}{s_j-s_i},$$

which agrees with $F(x)$ at the quadrature points $s_j, j=0,1,\ldots,n$, then

$$\int_a^b w(s)I(s)\,ds=\sum_{j=0}^{n} v_jF(s_j),$$

where

$$v_j=\int_a^b w(s)\,l_j(s)\,ds.$$

Since $F\in C[a,b]$, we can choose the quadrature points $s_0,s_1,\ldots,s_n$ such that $I(x)$ is a reasonable approximation of $F(x)$.

EXAMPLE A.3.1. Suppose $s_0=a$, $s_1=b$, and $F''\in C[a,b]$. Then $l_0(x)=\dfrac{b-x}{b-a}$ and $l_1(x)=\dfrac{x-a}{b-a}$, which gives $I(x)=\dfrac{b-x}{b-a}F(a)+\dfrac{x-a}{b-a}F(b)$, and $\displaystyle\int_a^b w(s)F(s)\,ds=v_0F(a)+v_1F(b)$, where

$$v_0=\int_a^b\frac{b-s}{b-a}w(s)\,ds,\quad v_1=\int_a^b\frac{s-a}{b-a}w(s)\,ds. \blacksquare$$

Formulas of the form (A.3.1) that are exact when $F(x)$ is a polynomial of degree $(2n+1)$ are known as Gauss-type quadrature rules. In particular, for $a=0, b=\infty, w(x)=e^{-x}$, we have the Gauss–Laguerre rule; for $a=-\infty, b=\infty$, $w(x)=e^{-x^2}$, we have the Gauss–Hermite rule; and for $a=-1, b=1$, $w(x)=\left(1-x^2\right)^{-1/2}$, we have the Gauss–Chebyshev rule.

CASE 2. Since integral equations involve integrals of the form $\int_a^b k(x,s)\phi(s)\, ds$, we keep x fixed, write $w(s) = k(x,s)$, and have an integral of the form (A.3.1), where the function $w(x)$ may be well behaved, or it may be badly behaved as, e.g., in the case of weakly singular integral equations where $w(s)$ may be of the form $|x-s|^{-\alpha}\, g(x,s), 0 < \alpha < 1$. If $\phi \in C^{n+1}[a,b]$, and $a \le s_i \le b, i = 0, 1, \dots, n$, then there is a value ξ depending on a such that

$$\phi(x) - I(x) = \frac{\phi^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n} (x - s_i)\,.$$

Hence, in the case when a and b are finite,

$$\int_a^b w(s)\phi(s)\, ds - \int_a^b w(s) I(s)\, ds = \int_a^b w(s)\, \frac{\phi^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n} (s - s_i)\, ds,$$

where $\xi = \xi(s)$. If in (A.3.1) we set

$$v_j = \int_a^b w(s) \prod_{i \ne j} \frac{s - s_i}{s_j - s_i}\, ds,$$

then the error in the above approximation is bounded by

$$\left\| \phi^{(n+1)(x)} \right\|_\infty \int_a^b \left| w(s) \prod_{i \ne j} \frac{s - s_i}{s_j - s_i} \right| ds, \tag{A.3.2}$$

provided $\displaystyle\int_a^b |w(s)|\, ds < \infty$. This leads to the quadrature rule

$$\int_a^b k(x,s)\, \phi(s)\, ds = \sum_{j=0}^{n} v_j \phi\left(s_j\right), \tag{A.3.3}$$

which is exact when $\phi(x)$ is a polynomial of degree n.

To obtain an improved approximation, we partition $[a,b]$ at the points s_j, $j = 0, 1, \dots, n$, by $a = s_0 < s_1 < \dots < s_n = b$, and write

$$\int_a^b w(s) F(s)\, ds = \sum_{j=0}^{n-1} \int_{s_j}^{s_{j+1}} w(s) F(s)\, ds = \sum_{j=0}^{n-1} \left\{ v_0^{(j)} F\left(s_j\right) + v_1^{(j)} F\left(s_{j+1}\right) \right\}, \tag{A.3.4}$$

where

$$
\begin{aligned}
v_0^{(j)} &= \int_{s_j}^{s_{j+1}} \frac{s_{j+1}-s}{s_{j+1}-s_j}\, w(s)\, ds, \\
v_1^{(j)} &= \int_{s_j}^{s_{j+1}} \frac{s-s_j}{s_{j+1}-s_j}\, w(s)\, ds.
\end{aligned} \tag{A.3.5}
$$

The approximation is still of the form (A.3.1), and the error is bounded by

$$
\frac{1}{2} \left\| F''(x) \right\|_\infty \sum_{j=0}^{n} \int_{s_j}^{s_{j+1}} \left| w(s)\,(s-s_j)\,(s-s_{j+1}) \right| ds,
$$

which is of the order $O\left(h^2\right)$ for $s_j = a + j\,h$, where $h = (b-a)/n$ is the step size, provided $\int_a^b |w(s)|\, ds < \infty$. This quadrature is known as the GENERALIZED TRAPEZOIDAL RULE since it is an extension of the repeated trapezoidal rule. A GENERALIZED MIDPOINT RULE is obtained by taking n even and setting $s_j = a + j\,h$ as above, with $v_0 = v_2 = v_4 = \ldots = 0$, and $v_{2m+1} = \int_{s_{2m}}^{s_{2m+2}} w(s)F(s)\, ds$ for $m = 0, 1, \ldots$. This rule is exact if $F(x)$ is piecewise-constant, i.e., constant in each subinterval $[s_{2m}, s_{2m+2}]$.

An extension of Simpson's rule is obtained for even n by setting $s_j = a + j\,h$, as above. Then in the subinterval $[s_{2m}, s_{2m+2}]$ the function $F(x)$ is approximated by the interpolant

$$
\begin{aligned}
I(x) = \frac{1}{h^2} \Big[&\frac{1}{2}\,(x - s_{2m+1})\,(x - s_{2m+2})\; F(s_{2m}) + (x - s_{2m})\,(x - s_{2m+2}) \\
&\times F(s_{2m+1}) + \frac{1}{2}\,(x - s_{2m})\,(x - s_{2m+1})\; F(s_{2m+2}) \Big].
\end{aligned}
$$

This gives the GENERALIZED SIMPSON'S RULE:

$$
\int_a^b w(s)F(s)\, ds = \sum_{m=0}^{n/2-1} \int_{s_{2m}}^{s_{2m+2}} w(s)I(s)\, ds = \sum_{j=0}^{n} v_j\, F(s_j)\,, \tag{A.3.6}
$$

where

$$
\begin{aligned}
v_0 &= \frac{1}{2h^2}\int_a^{a+2h} (s-s_1)\,(s-s_2)\,w(s)\,ds,\\
v_{2j+1} &= -\frac{1}{h^2}\int_{s_{2j}}^{s_{2j+2}} (s-s_{2j})\,(s-s_{2j+2})\,w(s)\,ds,\\
v_{2j} &= \frac{1}{2h^2}\left\{\int_{s_{2j-2}}^{s_{2j}} (s-s_{2j-2})\,(s-s_{2j-1})\,w(s)\,ds,\right.\\
&\quad\left. + \int_{s_{2j}}^{s_{2j+2}} (s-s_{2j+1})\,(s-s_{2j+2})\,w(s)\,ds\right\}, \quad j \neq 0 \text{ or } m,\\
v_n &= \frac{1}{2h^2}\int_{b-h}^{b} (s-s_{2m-2})\,(s-s_{2m-1})\,w(s)\,ds.
\end{aligned}
\tag{A.3.7}
$$

If $F''(x) \in C[a,b]$, then the error in this rule is of the order $O\left(h^3\right)$. Note that the error may not be of the order $O\left(h^4\right)$ even if $F^{(4)}(x) \in C[a,b]$ unless $w(x) \equiv 1$ (see Wang 1976).

If the function $w(x)$ is of the form $(x-s)^{-\alpha} g(x,s)$, then the generalized trapezoidal rule is obtained by taking $\alpha = 1/2$, $s_j = a + j\,h$, as above, $g(x,s) = 1$, and $x = s_m$, $m = 0, 1, \dots, n$. Then

$$
\int_a^b (s_m - s)^{-1/2}\, F(s)\,ds = \sum_{j=0}^{n-1} \left[v_{0,m}^{(j)}\, F(s_j) + v_{1,m}^{(j)}\, F(s_{j+1}) \right], \tag{A.3.8}
$$

where

$$
\begin{aligned}
v_{0,m}^{(j)} &= \frac{1}{h}\int_{s_j}^{s_{j+1}} (s_{j+1}-s)\,(s_m-s)^{-1/2}\,ds,\\
v_{1,m}^{(j)} &= \frac{1}{h}\int_{s_j}^{s_{j+1}} (s-s_j)\,(s_m-s)^{-1/2}\,ds.
\end{aligned}
\tag{A.3.9}
$$

Alternatively, if we set

$$
\begin{aligned}
\psi_0(r) &= \int_0^a (1-s)|r-s|^{-1/2}\,ds,\\
\psi_1(r) &= \int_0^a s|r-s|^{-1/2}\,ds,
\end{aligned}
$$

then

$$
\begin{aligned}
v_{0,m}^{(j)} &= \sqrt{h}\,\psi_0(m-j),\\
v_{1,m}^{(j)} &= \sqrt{h}\,\psi_1(m-j),
\end{aligned}
\tag{A.3.10}
$$

where

$$\begin{aligned}
\psi_0(r) &= \psi_2(r) - \psi_1(r), \\
\psi_1(r) &= \frac{2}{3}\left[\frac{(r-1)^2}{|r-1|^{1/2}} - \frac{r^2}{|r|^{1/2}}\right] + r\psi_2(r), \\
\psi_2(r) &= 2\left[\frac{r}{|r|^{1/2}} - \frac{r-1}{|r-1|^{1/2}}\right].
\end{aligned}$$

Further, the quadrature rule for $w(s) = \ln\left|s_m - s\right|$ is given by

$$\int_a^b \ln\left|s_m - s\right| F(s)\,ds = \sum_{j=0}^{n-1}\left[\hat{v}_{0,m}^{(j)}\,F\left(s_j\right) + \hat{v}_{1,m}^{(j)}\,F\left(s_{j+1}\right)\right], \tag{A.3.11}$$

where by setting

$$\begin{aligned}
\hat{\psi}_0(r) &= \int_0^a (1-s)\ln|r-s|\,ds, \\
\hat{\psi}_1(r) &= \int_0^a s\ln|r-s|\,ds,
\end{aligned}$$

we have

$$\begin{aligned}
\hat{v}_{0,m}^{(j)} &= \frac{1}{2}h\,\ln h + h\,\hat{\psi}_0(m-j), \\
\hat{v}_{1,m}^{(j)} &= \frac{1}{2}h\,\ln h + h\,\hat{\psi}_1(m-i);
\end{aligned} \tag{A.3.12}$$

or, alternatively, $\hat{\psi}_0(r) = \hat{\psi}_2(r) - \hat{\psi}_1(r)$, where

$$\begin{aligned}
\hat{\psi}_1(r) &= \frac{1}{2}\left\{(r-1)^2\,\ln|r-1| - r^2\,\ln|r| + \frac{1}{4}\left[r^2 - (r-1)^2\right]\right\} + r\hat{\psi}_2(r), \\
\hat{\psi}_2(r) &= r\,\ln|r| = (r-1)\,\ln|r-1| - 1.
\end{aligned}$$

A word of caution: While computing above formulas for $v_{0,m}^{(j)}$ and $\hat{v}_{1,m}^{(j)}$, to avoid cancellation error take the limit values as $r \to 0$ or $r \to 1$. Also, note the following GENERALIZATIONS OF THE MIDPOINT RULE for even n:

$$\int_a^b \left|s_m - s\right|^{-1/2} F(s)\,ds = \sum_{j=0}^{n/2-1} w_m^{2j+1}\,F\left(a + (2j+1)h\right) \tag{A.3.13}$$

and

$$\int_a^b \ln\left|s_m - s\right| F(s)\,ds = \sum_{j=0}^{n/2-1} \hat{w}_m^{2j+1}\,F\left(a + (2j+1)h\right), \tag{A.3.14}$$

where

$$w_m^{2j+1} = v_{0,m}^{(2j)} + v_{1,m}^{(2j)} + v_{0,m}^{(2j+1)} + v_{1,m}^{(2j+1)},$$
$$\hat{w}_m^{2j+1} = \hat{v}_{0,m}^{(2j)} + \hat{v}_{1,m}^{(2j)} + \hat{v}_{0,m}^{(2j+1)} + \hat{v}_{1,m}^{(2j+1)}.$$

Thus,

$$w_m^{(2j+1)} = 2\sqrt{h}\left[\frac{m-2j}{|m-2j|^{1/2}} - \frac{m-2j-2}{|m-2j-2|^{1/2}}\right],$$

whence by taking the limit values we get

$$w_{2j+2}^{(2j+1)} = w_{2j}^{(2j+1)} = 2\sqrt{2h}.$$

Another MODIFICATION OF THE QUADRATURE METHOD in the case when the kernel $k(x,s)$ is badly behaved at $x = s$, i.e., when it is discontinuous or when one of its derivatives is discontinuous at $x = s$, consists of writing the FK2 of the form (1.2.2) as

$$\phi(x) - \lambda\,\phi(x)\int_a^b k(x,s)\,[\phi(s) - \phi(x)]\,ds = f(x), \tag{A.3.15}$$

and using a quadrature rule to obtain

$$\{1 - \lambda\,A(x)\}\,\tilde{\phi}(x) - \lambda\sum_{j=0}^{n} w_j\,k(x,s_j)\,\{\tilde{\phi}(s_j) - \tilde{\phi}(x)\} = f(x), \tag{A.3.16}$$

where

$$A(x) = \int_a^b k(x,s)\,ds. \tag{A.3.17}$$

If we use the notation

$$\Delta(x) = \sum_{j=0}^{n} w_j\,k(x,s_j) - A(x), \tag{A.3.18}$$

we obtain from (A.3.16)

$$\{1 + \lambda\,\Delta(x)\}\,\tilde{\phi}(x) - \lambda\sum_{j=0}^{n} w_j\,k(x,s_j)\,\tilde{\phi}(s_j) = f(x). \tag{A.3.19}$$

If we set $x = x_i$, $i = 0, 1, \dots, n$, in (A.3.19), we have the MODIFIED QUADRATURE RULE

$$\{1 + \lambda\,\Delta(x_i)\}\,\tilde{\phi}(x) - \lambda\sum_{j=0}^{n} w_j\,k(x_i,s_j)\,\tilde{\phi}(s_j) = f(x_i), \tag{A.3.20}$$

which in matrix notation is

$$\left(\mathbf{I}+\lambda\left(\boldsymbol{\Delta}-\mathbf{KD}\right)\right)\tilde{\Phi}=\mathbf{f}, \tag{A.3.21}$$

where $\mathbf{I}$ is the identity matrix, $\mathbf{k}=\left(k\left(x_i,s_j\right)\right)_{ij}$, $\boldsymbol{\Delta}=\operatorname{diag}\{\Delta\left(x_0\right),\Delta\left(x_1\right),\dots,\Delta\left(x_n\right)\}$, and $\mathbf{D}=\operatorname{diag}\{w_0,w_1,\dots,w_n\}$. Note that the integral $A(x)$ needs be computed accurately, either analytically or numerically, for this method.

Lastly, the generalized rules can be extended to the case when $F(x)$ is the polynomial interpolant. For example, let $h=(b-a)/n$, and $n=Nm$, where N and m are integers; set $s_j=a+j\,h$, $j=,1,\dots,n$. For $s_{lm}\le x\le s_{lm+m}$ approximate $F(x)$ by the interpolant $I(x)\equiv P_{lm,lm+1,\dots,lm+m}(x)$ of degree m such that $I(x)$ agrees with $F(x)$ at the points $s_{lm},s_{lm+1},\dots,s_{lm+m}$. Then

$$\int_a^b w(s)F(s)\,ds=\sum_{l=0}^{N-1}\int_{s_{lm}}^{s_{lm+m}} s(s)I(s)\,ds=\sum_{j=0}^{n} v_j\,F\left(s_j\right), \tag{A.3.22}$$

where

$$v_j=\begin{cases} v_{lm+i}=\int_{s_{lm}}^{s_{lm+m}}\prod_{\substack{j=lm\\ j\neq lm+i}}\dfrac{s-s_j}{s_{lm+i}-s_j}\,w(s)\,ds & \text{if } j=lm+i,\ i\neq 0,\\ v_{lm}=\int_{s_{lm}}^{s_{lm+m}}\prod_{lm+1}^{lm+m}\dfrac{s-s_j}{s_{lm}-s_j}\,w(s)\,ds & \\ \qquad+\int_{s_{lm-m}}^{s_{lm}}\prod_{lm-m}^{lm-1}\dfrac{s-s_j}{s_{lm+i}-s_j}\,w(s)\,ds & \text{if } j=lm. \end{cases} \tag{A.3.23}$$

A.4. Singular Integrals

Sometimes we shall encounter singular integrals of the form $\int_a^b w(x)\,F(x)\,dx$. In such integrals the integrand is not easy to handle because of the following features:

(i) A singularity occurs in the integrand, or the integrand has a low-order derivative;
(ii) The integrand is discontinuous, or has a low-order derivative; and
(iii) The integrand oscillates rapidly.

Integrals of type (i) are usually found in the study of integral equations; those of type (ii) can be integrated piecewise over the subintervals where the integrand is continuous; and those of type (iii) are not discussed here.

To compute type (i) integrals there are four methods:

(1). It is often possible to factor the singularity out of the integrand so that only $w(x)$ becomes singular and $F(x)$ becomes regular. In such cases we can then use a Gauss rule for the weight function $w(x)$ provided one is available (see Stroud and Secrest 1966).

(2). A Chebyshev or Clenshaw–Curtis rule may be used, provided that, e.g., $F(x)$ has the Chebyshev expansion

$$F(x) = \sum_{i=0}^{\infty}{}' a_i \, T_i(x), \tag{A.4.1}$$

where the prime over the summation indicates that the first term is halved. Then

$$\int_a^b w(x)\, F(x)\, dx = \sum_{i=0}^{\infty}{}' a_i \int_{-1}^{1} w(x)\, T_i(x)\, dx = \sum_{i=0}^{\infty}{}' a_i \, m_i, \tag{A.4.2}$$

provided that the moments m_i are available. Generally, we truncate the series (A.4.1) at $i = n$ and replace a_i by approximations in terms of the known values of $F\big(\cos \frac{j\pi}{n}\big)$, $j = 0, 1, \dots, n$.

(3). If the singularity in $F(x)$ can be subtracted out, i.e., if it is possible to write the integral at a singularity x_0 in the form

$$\begin{aligned}\int_a^b w(x)\, F(x)\, dx &= \int_a^b w(x) \left[F(x) - F(x_0)\right] dx + F(x_0) \int_a^b w(x)\, dx \\ &= \int_a^b w(x)\, g(x)\, dx + F(x_0)\, m_0,\end{aligned} \tag{A.4.3}$$

the integral $\int_a^b w(x) g(x)\, dx$ can then be estimated provided that the moment $m_0 = \int_a^b w(x)\, dx$ is known. For example, let $w(x) = x^{-1/2}$, and consider $\int_0^1 x^{-1/2}\, F(x)\, dx$, which has singularity at $x_0 = 0$. Then the subtraction method gives

$$\begin{aligned}\int_0^1 x^{-1/2}\, F(x)\, dx &= \int_0^1 x^{-1/2} \left[F(x) - F(0)\right] dx + F(0) \int_0^1 x^{-1/2}\, dx \\ &= \int_0^1 x^{-1/2} \left[F(x) - F(0)\right] dx + 2F(0).\end{aligned}$$

Since in most cases $\lim_{x \to 0} \left[F(x) - F(x_0) \right] = 0$, the integrand $x^{-1/2} \left[F(x) - F(0) \right]$ will be finite (in fact, zero) at $x = 0$. Thus, this integral is easier to compute as an improper integral. In some cases this subtraction method can be repeated successively until the singularity is weakened (consider, e.g., $\int_0^1 x^{-5/2} F(x)\, dx$).

(4). If the singularity is weak, it can be ignored. In fact, integrands that are regular everywhere but have singular derivatives of some low order only make the convergence slower. In many cases, if the integrand is singular at x_0, we can choose quadrature rules that avoid the point x_0 as an abscissa and thus they converge rapidly to 'exact' results. See Davis and Rabinowitz (1975, Section 2.12) for details on this method.

A.5. Infinite-Range Integrals

We shall encounter infinite-range integrals, which have the general forms

$$I_1 = \int_a^\infty w(x)\, F(x)\, dx, \quad I_2 = \int_{-\infty}^\infty w(x)\, F(x)\, dx, \tag{A.5.1}$$

where the integrand usually vanishes near the infinite ends of the interval. If this is the case, then we take

$$\begin{aligned} I_1 &= \lim_{R \to \infty} \int_0^R w(x)\, F(x)\, dx = \lim_{R \to \infty} I_1(R), \\ I_2 &= \lim_{R \to \infty} \int_{-R}^R w(x)\, F(x)\, dx = \lim_{R \to \infty} I_2(R), \end{aligned} \tag{A.5.2}$$

i.e., we solve the infinite-range integrals by truncating the range to some large $R > 0$; the slower the decay of the integrand, the large the value of R is chosen.

The infinite-range Gauss–Laguerre quadrature rule is

$$\int_0^\infty e^{-x}\, F(x)\, dx = \sum_{j=1}^n w_j\, F(\xi_j), \tag{A.5.3}$$

where ξ_j are the zeros of the Laguerre polynomial $L_n(x)$ and

$$w_j = \frac{(n!)^2}{\xi_j \left[L_n'(\xi_j) \right]^2}, \quad j = 1, \dots, n.$$

The infinite-range Gauss–Hermite rule is

$$\int_{-\infty}^{\infty} e^{-x^2} F(x)\, dx = \sum_{j=1}^{n} w_j\, F(\xi_j), \tag{A.5.4}$$

where ξ_j are the zeros of the Hermite polynomial $H_n(x)$ and

$$w_j = \frac{2^{n+1}\, n!\, \sqrt{\pi}}{\left[H_n'(\xi_j)\right]^2}, \quad j = 1, \dots, n.$$

A.6. Linear Transformation of Quadratures

Under the transformation

$$\begin{gathered} x = \gamma\, u, \quad u = \frac{1}{\gamma}(x - \beta), \\ dx = \gamma\, du, \quad \gamma = \frac{b-a}{d-c}, \quad \beta = \frac{ad - bc}{d-c}, \end{gathered} \tag{A.6.1}$$

the interval $a \le x \le b$ is transformed into the interval $c \le u \le d$. Hence,

$$\int_a^b w(x)\, F(x)\, dx = \int_c^d w^*(u)\, G(u)\, du, \tag{A.6.2}$$

where

$$G(u) \equiv F(\gamma\, u + \beta), \quad w^*(u) \equiv w(\gamma\, u + \beta). \tag{A.6.3}$$

Then under the linear transformation (A.6.1) the quadrature formula

$$\int_a^b w(x)\, F(x)\, dx = \sum_{j=1}^{n} w_j\, F(x_j) + E(F) \tag{A.6.4}$$

transforms into

$$\int_a^b w^*(u)\, G(u)\, dx = \sum_{j=1}^{n} w_j^*\, G(u_j) + E^*(G), \tag{A.6.5}$$

where

$$u_k = \frac{1}{\gamma}\,(x_k - \beta)\,, \quad w_k^* = \frac{1}{\gamma}\,w_k \quad (k = 1, \dots, n),$$
$$E^*(G) = \frac{1}{\gamma}\,E(F). \tag{A.6.6}$$

EXAMPLE A.1. The 4-point N–C formula, known as Simpson's $\frac{3}{8}$-rule, is

$$\int_a^b F(x)\,dx = \frac{3h}{8}\,F(a) + \frac{9h}{8}\,F(a+h) + \frac{9h}{8}\,F(a+2h) + \frac{3h}{8}\,F(b), \tag{A.6.7}$$

where $h = (b-a)/3$. To transform this onto the interval $[-1, 1]$, we have $c = -1$, $d = 1$, $\gamma = \dfrac{b-a}{2}$, and $\beta = \dfrac{a+b}{2}$. Also,

$$x = a \longrightarrow u = -1, \qquad x = a + h \longrightarrow u = -\frac{1}{3},$$
$$x = a + 2h \longrightarrow u = \frac{1}{3}, \qquad x = b \longrightarrow u = 1.$$

Thus, $F(a) = G(-1), F(a+h) = G(-1/3), F(a+2h) = G(1/3), F(b) = G(1)$, and the weights become $w_1^* = \frac{1}{4} = w_4^*, w_2^* = \frac{3}{4} = w_3^*$. Hence the formula (A.6.7) is transformed into

$$\int_{-1}^1 G(u)\,du = \frac{1}{4}\,G(-1) + \frac{3}{4}\,G\left(-\frac{1}{3}\right) + \frac{3}{4}\,G\left(\frac{1}{3}\right) + \frac{1}{4}\,G(1),$$

where $G(u) = F\left(\dfrac{b-a}{2}\,u + \dfrac{a+b}{2}\right)$, and the error term becomes $E^*(G) = \dfrac{2E(F)}{b-a}$. ■

A.7. Trigonometric Polynomials

Let $F(x)$ be a trigonometric polynomial of degree m defined as a linear combination of the following functions: $1,\ \cos x,\ \sin x,\ \cos^2 x,\ \cos x \sin x,\ \sin^2 x,\ \dots,\ \cos^m x,\ \cos^{m-1} x\ \sin x, \dots,\ \sin^m x$, or, equivalently, a linear combination of the functions

$$1, \quad \cos x, \quad \sin x, \quad \cos 2x, \quad \sin 2x, \dots, \cos mx, \quad \sin mx.$$

Then the approximation

$$\int_0^{2\pi} F(x)\,dx \approx \sum_{j=1}^{n+1} w_j\, F(x_j) \tag{A.7.1}$$

cannot be exact for all trigonometric polynomials of degree m no matter how we choose w_k and x_k for $k = 1, \dots, n+1$. However, if all the points x_k in (A.7.1) are chosen as equally spaced and all w_k as equal, then we obtain a formula of degree n which is the highest degree possible. Thus, define the step size $h = \dfrac{2\pi}{n}$, and let β be any real number such that $0 \le \beta < h$. Also define x_k and w_k by

$$x_m = \beta + (m-1)h, \quad w_m = h, \quad m = 1, \dots, n+1. \tag{A.7.2}$$

Then the quadrature rule (A.7.1) is exact for all trigonometric polynomials of degree $\le n$. This choice of x_m and w_m is known as the REPEATED MIDPOINT FORMULA. Thus, e.g., the $(n+1)$-point repeated trapezoidal rule is

$$\int_0^{2\pi} F(x)\,dx \approx \frac{h}{2}\, F(0) + h\, F(h) + h\, F(2h) + \cdots + h\, F(nh) + \frac{h}{2}\, F(2\pi). \tag{A.7.3}$$

If $F(x)$ is a periodic function with period 2π, then $F(0) = F(2\pi)$, and the rule (A.7.3) becomes

$$\int_0^{2\pi} F(x)\,dx \approx h \sum_{j=1}^{n+1} F(jh). \tag{A.7.4}$$

A.8. Condition Number

A quadrature rule reduces the problem of finding the solution of an integral equation, or that of an eigenvalue problem, to solving a system of algebraic equations of the form $\mathbf{A}\tilde{\mathbf{\Phi}} = \mathbf{f}$, or

$$\sum_{j=0}^{n} A_{ij}\, \tilde{\phi}_j = f_i, \quad i = 0, 1, \dots, n, \tag{A.8.1}$$

where $\det \left| (A_{ij}) \right| \neq 0$. The solution of this system may be obtained by Gaussian elimination with partial pivoting or total condensation. In practice, we work with the augmented matrix $[\mathbf{A} \mid \mathbf{f}]$ and interchange rows. Also, if we interchange the columns of $\mathbf{A}$ and rearrange the elements $\{\tilde{\phi}_i\}$, we obtain complete pivoting. In either case, the basic idea of pivoting is to restrict the effects of roundoff error, because even though $\det \left| (A_{ij}) \right|$ may be large, the solution may become sensitive to roundoff error. In such cases we say that the system (A.8.1) is ill conditioned, and the degree of ill-conditioning is measured by the *condition number* $\rho(\mathbf{A})$ of the matrix $\mathbf{A}$, which is generally defined as $\rho(\mathbf{A}) = \|\mathbf{A}\| \, \|\mathbf{A}\|^{-1}$, where $\mathbf{A}$ is a square nonsingular matrix and $\| \ \|$ denotes the matrix norm. Thus,

(i) $\rho(\mathbf{A})$ is undefined if $\mathbf{A}$ is singular.
(ii) The system (A.8.1) is said to be ill conditioned if $\rho(\mathbf{A})$ is "large" which depends on the choice of norm.

In fact, an error analysis shows that if $\mathbf{A}\tilde{\Phi} = \mathbf{f}$, and $(\mathbf{A} + \delta\mathbf{A})\left(\tilde{\Phi} + \delta\tilde{\Phi}\right) = \mathbf{f} + \delta\mathbf{f}$, where $\mathbf{A}$ is nonsingular and the perturbation $\delta\mathbf{A}$ is relatively small, then $\dfrac{\|\delta\tilde{\Phi}\|}{\|\tilde{\Phi}\|}$ can be bounded in terms of $\dfrac{\|\delta\Phi\|}{\|\tilde{\Phi}\|}$ and $\dfrac{\|\delta\mathbf{f}\|}{\|\mathbf{f}\|}$ by a quantity that is large when $\rho(\mathbf{A})$ is large. Large condition numbers imply possible ill-conditioning.

For example, consider the FK2 $(K\phi)(x) = f(x)$, where

$$k(x,s) = \begin{cases} x(1-s) & \text{if } x \le s, \\ s(1-x) & \text{if } x \ge s, \end{cases}$$

and $a = 0, b = 1$. There exists a solution of this equation if $f(0) = f(1) = 0$ and $f''(x)$ exists. This solution $\phi(x) = -f''(x)$ is then continuous if $f'' \in C[0,1]$. If we solve this equation by the repeated trapezoidal rule, and take $s_i = ih$, $h = 1/n$, then $k(0,s) = k(1,s) = k(x,0) = k(x,1) = 0$ for $0 \le x, s \le 1$, and this equation reduces to the system

$$\sum_{j=1}^{n-1} h\, k\,(ih, jh)\; \tilde{\phi}(jh) = h\,(ih)\,, \quad i = 0, 1, \dots, n, \tag{A.8.2}$$

where $i = 0$ and $i = n$ correspond to $f(0)$ and $f(1)$, respectively. An explicit solution of the system (A.8.2) is

$$\begin{Bmatrix} \tilde{\phi}(h) \\ \tilde{\phi}(2h) \\ \tilde{\phi}(3h) \\ \vdots \\ \tilde{\phi}(1-h) \end{Bmatrix} = -\frac{1}{h^2} \begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & \cdots & \cdots & \cdots & \\ & & & 1 & -2 \end{bmatrix} \begin{Bmatrix} f(h) \\ f(2h) \\ f(3h) \\ \vdots \\ f(1-h) \end{Bmatrix}, \tag{A.8.3}$$

where

$$\tilde{\phi}(ih) = -\frac{f((i-1)h) - 2f(ih) + f((i+1)h)}{h^2}, \quad f(0) = f(1) = 0.$$

If we proceed with Simpson's rule instead, we obtain the solution of the system (A.8.2) as

$$\left\{\begin{matrix} \frac{4}{3}\tilde{\phi}(h) \\ \frac{2}{3}\tilde{\phi}(2h) \\ \frac{4}{3}\tilde{\phi}(3h) \\ \vdots \\ \frac{4}{3}\tilde{\phi}(1-h) \end{matrix}\right\} = -\frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \cdots & \cdots & \cdots \\ & & & 1 & -2 \end{bmatrix}\left\{\begin{matrix} f(h) \\ f(2h) \\ f(3h) \\ \vdots \\ f(1-h) \end{matrix}\right\}. \tag{A.8.4}$$

Note that both these quadrature rules produce a system of the form $h\,\mathbf{K}\tilde{\Phi} = \mathbf{f}$ with $\tilde{\Phi} = \left[\tilde{\phi}(h), \tilde{\phi}(2h), \dots, \tilde{\phi}(1-h)\right]^T$, $\mathbf{f} = \left[f(h), f(2h), \dots, f(1-h)\right]^T$, where $\left[h\,\mathbf{K}\right]^{-1}$ is a tridiagonal matrix $-h^{-2}\,\mathbf{T}$ with the diagonal elements as -2 and codiagonal elements as 1. Thus, a condition number of $\left[h\,\mathbf{K}\right]$ is given by $\rho\,(h\,\mathbf{K}) = \|h\,\mathbf{K}\|_\infty\, \|h^{-2}\,\mathbf{T}\|_\infty$. But $\|h\,\mathbf{K}\|_\infty \to \|\mathbf{K}\|_\infty$ as $h \to 0$, whereas $\|h^{-2}\,\mathbf{T}\|_\infty = \dfrac{4}{h^2} \to \infty$ as $h \to 0$; hence, this condition number increases like h^{-2} as $h \to 0$.

However, in the case of an eigenvalue problem $(K\phi)\,(x) = \mu\, f$, the condition number

$$\rho \equiv \rho(\mu) = \frac{\left|\langle \phi, f\rangle\right|}{\|\phi\|_2\,\|f\|_2} \tag{A.8.5}$$

indicates the sensitivity of the characteristic value μ to a perturbation of the eigenvalue problem, and the smaller the value of μ is, the more difficult the computation of the approximate value $\tilde{\mu}$ is, since $0 < \rho \le 1$. If μ is not a simple characteristic value, the ill-conditioning gets more complicated; in general, a multiple characteristic value of a non-Hermitian kernel is likely to be ill conditioned. The situation reverses for the eigenvalue $\lambda = 1/\mu$.

Geometrically, the definition (A.8.5) may be regarded as "the 'cosine' of the angle between corresponding left and right eigenfunctions" (Baker 1978, p.173). In practice, it is not possible to compute $\rho(\mu)$ although we can estimate this number if we compute the left and right eigenfunctions and find the cosine of the angle between them.

The condition number of a matrix A is sometimes defined in some linear algebra books as the ratio of the largest eigenvalue to the smallest of eigenvalues of the matrix, which is the product of A with its transpose A^T. While the two different definitions will give different condition numbers, they will both be large or small together.

The Mathematica Book (Wolfram 1996, p.851) defines the condition number as the ratio of the largest singular value of a matrix to the smallest one. This ratio determines, e.g., the accuracy of numerical matrix inverses. Note that very small singular values are usually numerically meaningless. The built-in Mathematica object `SingularValues` removes any singular values of a matrix that are smaller than a preassigned tolerance multiplied by its largest singular value. The option `Tolerance` specifies the preassigned tolerance to be used in such computations.

A.9. Quadrature Tables

Various tables are available for quadrature, and still many others can be made through computational techniques. If Mathematica is accessible, there is no need to collect published quadrature tables. Any required table can be produced using Mathematica.

However, if Mathematica is not accessible, there are some important published tables which contain certain quadrature formulas and tables. Of such literature the following description explains the contents and extent of such tables.

(1) *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables* by Abramowitz and Stegun (1968) contains formulas and tables on numerical integration in Ch. 25. The details are as follows:

§25.4.1: Trapezoidal rule
§25.4.2: Extended trapezoidal rule
§25.4.4: Modified trapezoidal rule
§25.4.5: Simpson's rule
§25.4.6: Extended Simpson's rule
§25.4.7: Euler–Maclaurin summation formula
§25.4.8: Lagrange formula
§25.4.11: Equally spaced abscissas
§25.4.13: Simpson's 3/8-rule
§25.4.14: Bode's rule
§25.4.13–20: Newton–Cotes formulas (closed type)

§25.4.21–26: Newton–Cotes formulas (open type)
§25.4.28: Chebyshev's equal weight integration formula
§25.4.29–46: Gaussian-type integration formula
§25.4.29: Gauss' formula on the interval $[-1, 1]$
§25.4.30: Gauss' formula on arbitrary interval
§25.4.31: Radau's formula on the interval $[-1, 1]$
§25.4.32: Lobatto's formula on the interval $[-1, 1]$
§25.4.47: Filon's formula
Table 25.4, pp.916–919: Abscissas and weights for Gaussian integration on the interval $[-1, 1]$ for $n = 2(1)10, 12(4)24(8)48(16)96$
Table 25.5, p.920: Abscissas for equal weight Chebyshev integration on the interval $[-1, 1]$ for $n = 2(1)7, 9$
Table 25.6, p.920: Abscissas and weights for Labato integration on the interval $[-1, 1]$ for $n = 3(1)7, 10$
Table 25.7, p.920: Abscissas and weights for Gaussian integration for integrands with a logarithmic singularity on the interval $[0, 1]$ for $n = 2(1)4$.
Table 25.8, pp.921–922: Abscissas and weights for Gaussian integration of moments on the interval $[0, 1]$ for $n = 1(1)8$ and $k = 1(1)5$
Table 25.9, p.923: Abscissas and weights for Laguerre integration on the interval $[0, \infty)$ for $n = 2(1)10, 12, 15$
Table 25.10, p.924: Abscissas and weights for Hermite integration on the interval $[-\infty, \infty)$ for $n = 2(1)10, 12(4)20$
Table 25.11, p.924: Coefficients for Filon's quadrature

(2) The *Index of Mathematical Tables* by Fletcher, Miller, Rosenhead and Comrie (1962) contains:

§23.5	Numerical integration
§23.51	Cotes formulae
§23.512	Sard's formulae
§23.515	Other formulae with equal intervals
§23.518	Integration of linear sums of exponential functions
§23.52	Part-range formulae and others
§23.53	Formulae for forward integration
§23.54	Steffensen's formulae
§23.55	Maclauren's formulae
§23.56	Filon's formulae
§23.57	Chebyshev's formulae
§23.575	Other formulae with equal coefficients
§23.58	Formulae with unequal intervals and coefficients
§23.581	Gaussian quadrature formulae
§23.5815	Radau's quadrature formulae

§23.582	Gauss–Laguerre quadrature formulae
§23.583	Generalized Gauss–Laguerre quadrature formulae
§23.584	Gauss–Hermite quadrature formulae
§23.585	Other quadrature formulae with unequal intervals and coefficients
§23.588	A formula for repeated integration
§23.59	Lagrangian integration polynomials
§23.6	Integration and summation, using differences
§23.61	Single integrals anywhere in the interval
§23.62	Repeated integrals anywhere in the interval
§23.67	Osculatory quadrature formulae
§23.68	$J = 1/(nw) \int_0^{nw} f(x)\,dx$ in terms of differences
§23.69	Lubbock coefficients
§23.695	Summation of slowly convergent series
§23.7	Double integrals

(3) The *NBS Handbook* (1964) contains:

pp.886–887 Newton–Cotes formulas (closed type), $n = 2(1)11$
p.887 Newton–Cotes formulas (open type), $n = 2(1)7$
p.915 Lagrangian integration coefficients $\int_{x_m}^{x_{m+1}} f(x)\,dx \approx \frac{1}{h} \sum_i A_i(m)\, f(x_i)$, $n = 3(1)10$
pp.916–919 Abscissas and weights for Gaussian integration, $n = 2(1)12(4)24(8)48(16)96$
p.920 Abscissas for equal weight Chebyshev integration $\int_{-1}^{1} f(x)\,dx \approx \frac{2}{n} \sum_{i=1}^{n} f(x_i)$, $n = 2(1)7, 9$
p.920 Abscissas and weights for Lobatto integration, $n = 3(1)10$
p.920 Abscissas and weights for Gaussian integration for integrands with logarithmic singularity, $n = 2(1)12$
pp.921–922 Abscissas and weights for Gaussian integration of moments $\int_0^1 x^m f(x)\,dx \approx \sum_{i=1}^{n} w_i\, f(x_i)$, $m = 0(1)5, n = 1(1)8$
p.923 Abscissas and weights for Laguerre integration, $n = 2(1)10, 12, 15$
p.924 Abscissas and weights for Hermite integration, $n = 2(1)10, 12, 15$
p.924 Coefficients for Filon's quadrature formula, n = number of quadrature points

(4) *Gaussian Quadrature Formulas* by Stroud and Secrest (1966) contains integration formulas to 30 significant figures:

$$\int_{-1}^{1} f(x)\,dx \approx \sum_{i=1}^{n} w_i\, f(x_i) \text{ (Gauss)}, \quad n = 2(1)64(4)96(8)168, 256, 384, 512.$$

$\int_{-1}^{1} \left(1-x^2\right)^{\alpha} f(x)\,dx \approx \sum_{i=1}^{n} w_i\, f\left(x_i\right)$ $n = 2(1)20$; $\alpha = -0.5, 0.5, 1, 1.5$.

$\int_{-1}^{1} (1+x)^{\beta} f(x)\,dx \approx \sum_{i=1}^{n} w_i\, f\left(x_i\right)$ $n = 2(1)30$ for $\beta = 1$; $n = 2(10)20$ for $\beta = 2, 3, 4$.

$\int_{-1}^{1} |x|^{\alpha} f(x)\,dx \approx \sum_{i=1}^{n} w_i\, f\left(x_i\right)$ $n = 2(1)20$; $\alpha = 1, 2, 3, 4$.

$\int_{-\infty}^{\infty} e^{-x^2} f(x)\,dx \approx \sum_{i=1}^{n} w_i\, f\left(x_i\right)$ (Hermite), $n = 2(1)64(4)96(8)136$.

$\int_{-\infty}^{\infty} e^{-x} f(x)\,dx \approx \sum_{i=1}^{n} w_i\, f\left(x_i\right)$ (Laguerre), $n = 2(1)32(4)68$.

$\int_{-\infty}^{\infty} |x|^{\alpha} e^{-x^2} f(x)\,dx \approx \sum_{i=1}^{n} w_i\, f\left(x_i\right)$, $n = 2(1)20$; $\alpha = 1, 2, 3$.

$\int_{-\infty}^{\infty} |x|^{\alpha} e^{-|x|} f(x)\,dx \approx \sum_{i=1}^{n} w_i\, f\left(x_i\right)$, $n = 2(1)20$; $\alpha = 1, 2, 3$.

$\int_{0}^{1} \ln(1/x) f(x)\,dx \approx \sum_{i=1}^{n} w_i\, f\left(x_i\right)$ $n = 2(1)16$.

$\frac{1}{2i\pi} \int_{c-i\infty}^{c+i\infty} p^{-1} e^{p}\, F(p)\,dp \approx \sum_{i=1}^{n} w_i\, F\left(p_i\right)$, $n = 2(1)24$.

$\int_{-1}^{1} f(x)\,dx \approx A f(-1) + \sum_{i=1}^{n} A_i\, f\left(x_i\right) + A f(1)$ (Lobatto), $n = 2(1)32(4)96$.

$\int_{-1}^{1} f(x)\,dx \approx A f(-1) + \sum_{i=1}^{n} A_i\, f\left(x_i\right)$ (Radau), $n = 2(1)19(4)47$.

$\int_{-1}^{1} f(x)\,dx \approx \sum_{i=1}^{n} A_i\, f\left(x_i\right) + \sum_{j=0}^{m} B_{2j}\, f^{2j}(0)$ (Lobatto), $n = 2(2)16$; $m = 1, 2, 3$.

$\int_{-1}^{1} e^{-x^2} f(x)\,dx \approx \sum_{i=1}^{n} A_i\, f\left(x_i\right) + \sum_{j=0}^{m} B_{2j}\, f^{2j}(0)$ (Lobatto), $n = 2(2)16$; $m = 1, 2, 3$.

(5) Boujot and Maroni (1968) provide tables of Gauss formulas for $n = 2(1)12, 12$ for the following weights:

$x^{\alpha-1} \left(1-x\right)^{\beta}$, $\alpha, \beta > 0$, over the interval $[0, 1]$.
$x^{\alpha-1} \left(1 \log 1/x\right)^{\beta}$, $\alpha, \beta > 0$, over the interval $[0, 1]$.
$e^{-x} x^{\alpha-1}$, $\alpha > 0$, over the interval $[0, \infty)$.

$w(x)/x$ and $w(x)/x(1-x)$ over the interval $[0,1]$, where

$$w(x) = \frac{1}{\pi^2 + \log^2\left(\dfrac{1-x}{x}\right)}.$$

(6) Krylov and Pal'tsev (1974) have tabulated Gauss formulas for $n = 1(1)10, 15S$*
for the following weights:

$x^\alpha \log e/x, \quad \alpha = -0.9(0.01)0(0.1)5$, over the interval $[0,1]$.
$x^\beta \log e/x \log\left(e/(1-x)\right), \quad \beta = 0(1)5$, over the interval $[0,1]$.
$\log(1/x)$ over the interval $[0,1]$.
$x^\beta e^{-x} \log(1+1/x), \quad \beta = 0(1)5$, over the interval $[0,\infty)$.

(7) Berger (1969a,b) has tabulated zeros and weights for Gauss–Laguerre quadrature to 23–24S for $n = 100, 150, 200(100)900$, and for Gauss–Hermite quadrature to 26–27S for $n = 200(200)1000, 2000$.

(8) Piessens and Branders (1975) have tabulated Gauss formulas for selected values of n to $25S$ for the following weights:

$x^\alpha e^{-ax}$, $\alpha = -0.5, 0, 0.5$; $a = 1, 2, 5$, over the interval $[-1,1]$.
$e^{-ax^3}, \quad a = 1, 2, 5, 10$, over the interval $[-1,1]$.
$x^{-\alpha} \log(1/x)$, $\alpha = -1/2, -1/3, 1/5, 1/4, 1/3, 1/2$, over the interval $[-1,1]$.
$(1-x)^{-\alpha} x^{-\beta} \log(1/x), \quad \alpha, \beta = -1/2, -1/3, 1/5, 1/4, 1/3, 1/2$,
over the interval $[0,1]$.
$\cos x$, over the interval $[-\pi,\pi]$.
$\sin x$, over the interval $[-\pi,\pi]$.
$e^{-ax^2}, \quad a = 1, 2, 5, 10$, over the interval $[-1,1]$.
$(x+a)^{-\alpha}, \quad a = 1.001, 1.01$; $\alpha = 1/2, 1, 2$, over the interval $[-1,1]$.
$\left(x^2+a^2\right)^{-\alpha}$, $a = 0.001, 0.01, 0.1, 1$; $\alpha = 1/2, 1, 2$, over the interval $[-1,1]$.

(9) Miller (1960) in *Quadrature in terms of equally spaced Function values* has given almost every formula developed up to that date which expresses an integral as a weighted sum of equally spaced values of the integrand; both finite difference formulas and formulas in terms of equally spaced function values are available. A number of special formulas are also given. In many formulas the coefficients are given both as exact fractions and in decimal form. Error coefficients are given both for truncation and roundoff errors.

(10) Aizenshtat, Krylov and Metleskii (1962) in *Tables for calculating Laplace transforms and integrals of the form* $\int_0^\infty x^s e^{-x} f(x)\, dx$ give x_i, w_i, and $w_i e^{x_i}$

*Here, and in the sequel, S means "significant digits."

for $s = -0.9(0.02)0, 0.55(0.05)3, -\frac{3}{4}, -\frac{1}{4}, m + j/3, \quad m = -1(1)2, \quad j = 1, 2, \quad n = 1(1)15, 8S$.

(11) Shao, Chen and Frank (1964) in *Tables of zeros and Gaussian weights of certain associated Laguerre polynomials and the related generalized Hermite polynomials* give x_i, w_i for generalized Laguerre integration for $\alpha = -0.5(0.5)10$, $n = 4, 8(8)32(16)64(32)128$, and for generalized Hermite integration for $\lambda = 0(1)10, n = 8(8)32(16)64(32)128(64)256$ to $25S$.

(12) Kronrod (1965) in *Nodes and Weights of Quadrature Formulas* gives tables in both decimal and octal forms for $n = 1(1)40$ to $16S$, arranging decimal forms on even-numbered and octal forms on odd-numbered pages.

REFERENCES USED: Abramowitz and Stegun (1968), Aizenshtat, Krylov and Metleskii (1962), Baker (1978), Berger (1969), Boujot and Maroni (1968), Clenshaw and Curtis (1960), Davis and Rabinowitz (1967, 1975), Fletcher, Miller, Rosenhead and Comrie (1962), Golub and Welsh (1967), Henrici (1964), Hornback (1975), Isaacson and Keller (1966), King (1984), Kronrod (1965), Krylov (1962), Krylov and Pal'tsev (1974), Kuo (1972), Miller (1960), NBS Handbook (1964), Piessens and Branders (1975), Shao, Chen, and Frank (1964), Squire (1970), Stroud (1974), Stroud and Secrest (1966), Wang (1976), Wolfram (1996).

B

Orthogonal Polynomials

A set of of polynomials $\{f_i\}$ with degree i and such that $\langle f_i, f_j \rangle = 0$ for $i \neq j$ is called a set of orthogonal polynomials with respect to the inner product $\langle f_i, f_j \rangle$. Let $w(x)$ be an admissible weight function on a finite or infinite interval $[a, b]$. If we orthonormalize the powers $1, x, x^2, \ldots$, we obtain a unique set of polynomials $p_n(x)$ of degree n and leading coefficient positive, such that

$$\int_a^b w(x)p_n(x)p_m(x)\,dx = \delta_{mn} = \begin{cases} 0 & \text{if } m \neq n, \\ 1 & \text{if } m = n, \end{cases} \tag{B.1}$$

where δ_{mn} is known as the Kronecker delta. Table B.1 gives the classical polynomials corresponding to their specific weights and intervals.

Table B.1

Name	Symbol	Interval	$w(x)$
Chebyshev, 1st kind	$T_n(x)$	$[-1, 1]$	$(1 - x^2)^{-1/2}$
Chebyshev, 2nd kind	$U_n(x)$	$[-1, 1]$	$(1 - x^2)^{1/2}$
Gegenbauer (ultraspherical)	$C_n^\mu(x)$	$[-1, 1]$	$(1 - x^2)^{\mu - 1/2}$, $\mu > -1/2$
Hermite	$H_n(x)$	$(-\infty, \infty)$	e^{-x^2}
Jacobi	$P_n^{(\alpha,\beta)}(x)$	$[-1, 1]$	$(1 - x)^\alpha (1 + x)^\beta$, $\alpha, \beta > 1$
Laguerre	$L_n(x)$	$[0, \infty)$	e^{-x}
Generalized Laguerre	$L_n^{(\alpha)}$	$[0, \infty)$	$x^\alpha e^{-x}$, $\alpha > 1$
Legendre	$P_n(x)$	$[-1, 1]$	1

Orthogonal polynomials with respect to the above inner product satisfy another type of orthogonality, known as "discrete" orthogonality. Let $\mathcal{P}_n$ denote the class of all polynomials $p_i(x)$, $i = 1, \ldots, n+1$, such that

$$p_n(x_i) = \alpha_i, \quad i = 1, \ldots, n+1, \tag{B.2}$$

where $x_1 < x_2 < \cdots < x_{n+1}$ are $(n+1)$ distinct points and $\alpha_1, \ldots, \alpha_{n+1}$ arbitrary numbers.

Let $p_0(x), p_1(x), \ldots, p_n(x), p_{n+1}(x)$ be orthonormal polynomials with the weight function $w(x)$ on $[a, b]$. Let $x_1 \ldots, x_{n+1}$ be $(n+1)$ zeros of $p_{n+1}(x)$ and let $w_1, \ldots, w_{n+1}$ be the respective Gaussian weights. Then, in view of Gaussian integration (see $Q7$, Appendix A)

$$\int_a^b w(x) f(x)\, dx = \sum_{i=1}^{n+1} w_i\, f(x_i) \tag{B.3}$$

for all $f \in \mathcal{P}_{2n+1}$. Now, since $p_j(x)p_k(x) \in \mathcal{P}_{2n+1}$ for $j, k \le n$, we have

$$\sum_{i=1}^{n+1} w_i p_j(x_i)\, p_k(x_i) = \int_a^b w(x) p_j(x) p_k(x)\, dx = \delta_{jk}. \tag{B.4}$$

Thus, $p_0, p_1, \ldots, p_n$ are orthonormal on the zeros of p_{n+1} with respect to the above inner product. This means that if we start with the monomials $1, x, x^2, \ldots, x^n$ and orthonormalize them with respect to the discrete inner product $\langle f, g \rangle = \int_a^b w(x) f(x) g(x)\, dx$, we shall obtain orthonormal polynomials with respect to the continuous inner product defined above. Also, if $p_0(x), p_1(x), \ldots$ are polynomials with $p_n(x) = c_n x^n + \cdots$, $c_n > 0$, which are orthogonal with respect to the inner product $\langle f, g \rangle$, then we have the recurrence relation

$$p_{n+1}(x) = (\gamma_n x - a_{mn})\, p_n(x) - a_{n,n-1} p_{n-1}(x) - \cdots - a_{n0} p_0(x), \tag{B.5}$$

for $n = 0, 1, \ldots$, where

$$p_0(x) \equiv c_0, \quad \gamma_n = \frac{c_{n+1}}{c_n},$$

$$a_{nk} = \frac{\gamma_n \langle x p_n, p_k \rangle}{\langle p_k, p_k \rangle}, \quad k = 0, 1, \ldots, n.$$

Moreover, if the above inner product satisfies the further condition $\langle xf, g \rangle = \langle f, xg \rangle$, then the recurrence relation (B.5) reduces to the three-term recurrence relation

$$p_{n+1}(x) = (\gamma_n x - \alpha_n)\, p_n(x) - \beta_n p_{n-1}(x), \quad n = 0, 1, \ldots, \tag{B.6}$$

where we take $p_{-1}(x) = 0$, and

$$\alpha_n = \frac{\gamma_n \langle x p_n, p_n \rangle}{\langle p_n, p_n \rangle}, \quad n = 0, 1, \dots,$$

$$\beta_n = \frac{\gamma_n \langle x p_n, p_{n-1} \rangle}{\langle p_{n-1}, p_{n-1} \rangle} = \frac{\gamma_n}{\gamma_{n-1}} \frac{\langle p_n, p_n \rangle}{\langle p_{n-1}, p_{n-1} \rangle}, \quad n = 1, 2, \dots .$$

The three-term recurrence relation for $p_n(x)$ yields a "backward" recurrence for an efficient computation of a series expansion of the form

$$f(x) = \sum_{k=0}^{N} c_k p_k(x).$$

Simply set

$$B_k = \begin{cases} 0 & \text{for } k > n, \\ c_k + (\gamma_{k+1} x - \alpha_{k+1}) B_{k+1} - \beta_{k+2} B_{k+2} & \text{for } 0 \le k \le n. \end{cases} \tag{B.7}$$

Then

$$f(x) = \gamma_0 B_0. \tag{B.8}$$

EXAMPLE B.1. To compute Chebyshev expansions $f(x) = \sum_{k=0}^{N} c_k T_k(x)$, choose $\alpha_k = 0$, $\beta_k = 1$, $\gamma_0 = \gamma_1 = 1$, and $\gamma_k = 2$ for $k \ge 2$.

Finally, orthogonal polynomials satisfy, among others, the Christoffel–Darboux identity

$$\sum_{k=0}^{n} \frac{p_k(x) p_k(y)}{h_k} = \frac{p_{n+1}(x) p_n(y) - p_n(x) p_{n+1}(y)}{\gamma_n h_n (x - y)}, \tag{B.9}$$

where $h_k = \langle p_k, p_k \rangle$.

B.1. Zeros of Some Orthogonal Polynomials

Zeros of some orthogonal polynomials are used in quadrature rules. We consider some of the most frequently used polynomials. Information on others is available in the references cited ahead.

1. Chebyshev Polynomials of the First Kind $T_n(x)$ over the interval $[-1,1]$, such that $T_n(1)=1$. The mth zero $x_{n,m}$ of $T_n(x)$ is given by

$$x_{n,m} = \cos\frac{(2m-1)\pi}{2n}.$$

Other relevant data are as follows:

Norm: $$\int_{-1}^{1}\left(1-x^2\right)^{-1/2}\left[T_n(x)\right]^2 dx = \begin{cases} \frac{\pi}{2}, & n \neq 0, \\ \pi, & n=0 \end{cases}$$

Series form: $$T_n(x) = \frac{n}{2}\sum_{k=0}^{[n/2]}(-1)^k\frac{(n-k-1)!}{k!(n-2k)!}(2x)^{n-2k} = \cos(n\arccos x)$$

Indefinite and definite integrals: $$\int T_0\,dx = T_1,\quad \int T_1\,dx = \frac{T_2}{4},$$

$$\int T_n\,dx = \frac{1}{2}\left[\frac{T_{n+1}(x)}{n+1} - \frac{T_{n-1}(x)}{n-1}\right],\quad \int_{-1}^{1} T_n\,dx = \begin{cases} \frac{2}{1-n^2}, & n \text{ even}, \\ 0, & n \text{ odd} \end{cases}$$

Inequality: $\left|T_n(x)\right| \le 1, \quad -1 \le x \le 1$

Rodrigues' formula: $$T_n(x) = \frac{(-1)^n\left(1-x^2\right)^{1/2}\sqrt{\pi}}{2^{n+1}\,\Gamma(n+1/2)}\frac{d^n}{dx^n}\left\{(1-x^2)^{n-1/2}\right\}.$$

2. Chebyshev Polynomials of the Second Kind $U_n(x)$ over the interval $[-1,1]$, such that $U_n(1)=n+1$. The mth zero $x_{n,m}$ of $U_n(x)$ is given by

$$x_{n,m} = \cos\frac{m\pi}{n+1}.$$

Other relevant data include:

Norm: $$\int_{-1}^{1}\left(1-x^2\right)^{1/2}\left[U_n(x)\right]^2 dx = \frac{\pi}{2}$$

Series form: $$U_n(x) = \sum_{k=0}^{[n/2]}(-1)^k\frac{(n-k)!}{k!(n-2k)!}(2x)^{n-2k} = \frac{T'_{n+1}(x)}{n+1},$$

$$U_n(\cos\theta) = \frac{\sin(n+1)\theta}{\sin\theta}$$

Definite integral: $$\int_{-1}^{1} U_n\,dx = \begin{cases} \frac{2}{n+1}, & n = 2m, \\ 0, & n = 2m+1 \end{cases}$$

Inequality: $\left|U_n(x)\right| \le n+1, \quad -1 \le x \le 1,$

Rodrigues' formula: $$U_n(x) = \frac{(-1)^n(n+1)\sqrt{\pi}}{(1-x^2)^{1/2}\,2^{n+1}\,\Gamma(n+3/2)}\frac{d^n}{dx^n}\left\{(1-x^2)^{n+1/2}\right\}.$$

3. Gegenbauer (or Ultraspherical) Polynomials $C_n^\mu(x)$ over the interval $[-1,1]$ such that $C_n^\mu(1) = \binom{n+2\mu-1}{n}$. Other relevant data are the following:

$$\text{Norm:} \int_{-1}^{1} (1-x^2)^{\mu-1/2} \left[C_n^\mu(x)\right]^2 dx = \frac{\pi 2^{1-2\mu}\,\Gamma(n+2\mu)}{n!\,(n+\mu)\,[\Gamma(\mu)]^2}$$

$$\text{Series form:}\ C_n^\mu(x) = \frac{1}{\Gamma(\mu)} \sum_{k=0}^{[n/2]} (-1)^k \frac{\Gamma(\mu+n-k)!}{k!(n-2k)!} (2x)^{n-2k}$$

$$\text{Inequality:} \max_{-1\le x\le 1} \left|C_n^\mu(x)\right| = \begin{cases} \binom{n+2\mu-1}{n}, & \text{if } \mu > 0, \\ \left|C_n^\mu(x')\right|, & \text{if } -1/2 < \mu < 0 \end{cases}$$

where $x' = 0$ if $n = 2k$; $x' =$ maximum point nearest zero if $n = 2k+1$.

$$\text{Rodrigues' formula:}\ C_n^\mu(x) = \frac{(-1)^n 2^n n!\,\Gamma(\mu+n+1/2)}{\Gamma(\mu+1/2)\,\Gamma(n+2\mu)\ (1-x^2)^{\mu-1/2}} \times \\ \times \frac{d^n}{dx^n}\left\{(1-x^2)^{n+\mu-1/2}\right\}.$$

4. Hermite Polynomials $H_n^{(\alpha)}(x)$ over the interval $(-\infty,\infty)$, such that

$$\text{Norm:} \int_{-\infty}^{\infty} e^{-x^2} \left[H_n^{(\alpha)}(x)\right]^2 dx = \sqrt{\pi}\, 2^n\, n!,$$

$$\text{Inequality:}\ \left|H_{2n}(x)\right| \le e^{x^2/2}\, 2^{2n}\, n! \left[2 - \frac{1}{2^{2n}}\binom{2n}{n}\right],$$

$$\left|H_{2n+1}(x)\right| \le |x| e^{x^2/2} \frac{(2n+2)!}{(n+1)!}$$

$$\text{Rodrigues' formula:}\ H_n(x) = (-1)^n\, e^{x^2} \frac{d^n}{dx^n} e^{-x^2}.$$

5. Jacobi Polynomials $P_n^{\alpha,\beta}(x)$ over the interval $[-1,1]$, such that $P_n^{\alpha,\beta}(1) = \binom{n+\alpha}{n}$. Other relevant data are:

$$\text{Norm:} \int_{-1}^{1} (1-x)^\alpha (1+x)^\beta \left[P_n^{\alpha,\beta}(x)\right]^2 dx$$

$$= \frac{2^{\alpha+\beta+1}\,\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{(2n+\alpha+\beta)n!\Gamma(n+\alpha+\beta+1)}$$

$$\text{Series form:}\ P_n^{\alpha,\beta}(x) = \frac{1}{2^n} \sum_{k=0}^{[n/2]} \binom{n+\alpha}{k} \binom{n+\beta}{n-k} (x-1)^{n-k}(x+1)^k,$$

$$\text{Inequality:} \quad \max_{-1\le x\le 1} \left|P_n^{\alpha,\beta}(x)\right| = \begin{cases} \binom{n+q}{n} \sim n^q & \text{if } q = \max(\alpha,\beta) \ge -1/2, \\ \left|P_n^{\alpha,\beta}\right|(x') \sim n^{-1/2} & \text{if } q < -1/2 \end{cases}$$

where x' is one of the two maximum points nearest $(\beta-\alpha)/(\alpha+\beta+1)$,,

$$\text{Rodrigues' formula:} \quad P_n^{\alpha,\beta}(x) = \frac{(-1)^n}{2^n n!(1-x)^\alpha(1+x)^\beta} \times \frac{d^n}{dx^n}\left\{(1-x)^{n+\alpha}(1+x)^{n+\beta}\right\}.$$

6. Laguerre Polynomials $L_n(x)$ over the interval $[0,\infty)$, such that $L_n(0) = n!$ and

$$\int_0^\infty e^{-x}\, L_n(x) L_m(x)\, dx = \begin{cases} 0 & \text{if } n \ne m, \\ (n!)^2 & \text{if } n = m. \end{cases}$$

Its mth zero $x_{n,m}$ is given by

$$x_{n,m} = \frac{j_m^2}{4k_n}\left(1 + \frac{j_m^2 - 2}{48k_n^2}\right) + O\left(n^{-5}\right),$$

where $k_n = n + 1/2$ and j_m is the m-th positive zero of the Bessel function $J_n(x)$. Other relevant data are

$$\text{Norm:} \quad \int_0^\infty e^{-x}\left[L_n(x)\right]^2 dx = 1,$$

$$\text{Series form:} \quad L_n(x) = \sum_{k=0}^n (-1)^k \binom{n}{n-k} \frac{1}{k!}\, x^k,$$

$$\text{Inequality:} \quad \left|L_n(x)\right| = \begin{cases} e^{x/2}, & \text{if } x \ge 0, \\ \left[2 - \frac{1}{n!}\right] e^{x/2}, & \text{if } x \ge 0, \end{cases}$$

$$\text{Rodrigues' formula:} \quad L_n(x) = \frac{1}{n! e^{-x}} \frac{d^n}{dx^n}\left\{x^n\, e^{-x}\right\}.$$

7. Generalized Laguerre Polynomials $L_n^{(\alpha)}(x)$ over the interval $[0,\infty)$, such that its mth zero $x_{n,m}$ is given by

$$x_{n,m} = \frac{j_{\alpha,\beta}^2}{4k_n}\left(1 + \frac{2\left(\alpha^2-1\right) + j_{\alpha,m}^2}{48k_n^2}\right) + O\left(n^{-5}\right),$$

where $k_n = n + (\alpha+1)/2$, $\alpha > -1$, and $j_{\alpha,m}$ is the m-th positive zero of the

Bessel function $J_n(x)$. Other relevant data are

$$\text{Norm:} \int_0^\infty x^\alpha e^{-x} \left[L_n^{(\alpha)}(x)\right]^2 dx = \frac{\Gamma(n+\alpha+1)}{n!}$$

$$\text{Series form:} \ L_n^{(\alpha)}(x) = \sum_{k=0}^{n} (-1)^k \binom{n+\alpha}{n-k} \frac{1}{k!} x^k$$

$$\text{Inequality:} \ \left|L_n^{(\alpha)}(x)\right| = \begin{cases} \dfrac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)} e^{x/2}, & \text{if } x \ge 0,\ \alpha \ge 0, \\ \left[2 - \dfrac{\Gamma(n+\alpha+1)}{n!\Gamma(n+1)}\right] e^{x/2}, & \text{if } x \ge 0,\ -1 < \alpha < 0, \end{cases}$$

$$\text{Rodrigues' formula:} \ L_n^{(\alpha)}(x) = \frac{1}{n! x^\alpha e^{-x}} \frac{d^n}{dx^n} \left\{x^{n+\alpha} e^{-x}\right\}.$$

8. Legendre Polynomials $P_n(x)$ over the interval $[-1, 1]$, such that $P_n(1) = 1$. If $x_{n,m}$ denotes the mth zero of $P_n(x)$, where $x_{n,1} > x_{n,2} > \cdots > x_{n,n}$, then

$$x_{n,m} = \left(1 - \frac{1}{8n^2} + \frac{1}{8n^3}\right) \cos \frac{(4m-1)\pi}{4n+2} + O\left(n^{-4}\right).$$

Other relevant data are:

$$\text{Norm:} \int_{-1}^{1} \left[P_n(x)\right]^2 dx = \frac{2}{2n+1},$$

$$\text{Series form:} \ P_n(x) = \frac{1}{2^n} \sum_{k=0}^{[n/2]} (-1)^k \binom{n}{k} \binom{2n-2k}{n} x^{n-2k},$$

$$\text{Indefinite Integral:} \int P_n(x)\, dx = \frac{1}{2n+1} \left[P_{n+1}(x) - P_{n-1}(x)\right],$$

$$\text{Inequality:} \ \left|P_n(x)\right| \le 1, \quad -1 \le x \le 1,$$

$$\text{Rodrigues' formula:} \ P_n(x) = \frac{(-1)^n}{2^n\, n!} \frac{d^n}{dx^n} \left\{(1-x^2)^n\right\}.$$

Zeros of the Legendre polynomial of degree 9 are
$x_1 = -0.96816$, $x_2 = -0.836031$, $x_3 = -0.613372$, $x_4 = -0.324253$, $x_5 = 0$, $x_6 = 0.324253$, $x_7 = 0.613372$, $x_8 = 0.836031$, $x_9 = 0.96816$

Zeros of the shifted Legendre polynomial of degree 9 are
$y_1 = 0.01592$, $y_2 = 0.081984$, $y_3 = 0.193314$, $y_4 = 0.337874$, $y_5 = 0.5$, $y_6 = 0.662127$, $y_7 = 0.806686$, $y_8 = 0.918016$, $y_9 = 0.98408$.

Some of the weights w'_j corresponding to the shifted Legendre polynomials are $w'_1 = w'_9 = 0.040637$, $w'_2 = w'_8 = 0.090325$, $w'_3 = w'_7 = 0.13030$, $w'_4 = w'_6 = 0.15617$, $w'_5 = 0.16512$.

REFERENCES USED: Abramowitz and Stegun (1964), Davis and Rabinowitz (1967).

C

Whittaker's Cardinal Function

C.1. Basic Results

Let $h > 0$ be the step size, and let $\mathcal{B}(h)$ denote the family of functions $f \in L_2(\mathbb{R})$ that are analytic on the entire complex plane $\mathbb{C}$ such that

$$\left|f(z)\right| \le C\, e^{\pi|z|/h}, \tag{C.1.1}$$

where C is a positive constant. Let m denote an integer, and set

$$S(m,h)(z) = \frac{\sin \dfrac{\pi}{h}(z - mh)}{\dfrac{\pi}{h}(z - mh)}. \tag{C.1.2}$$

Then for f defined in $\mathbb{R}$ the Whittaker's cardinal function for f with step size h is defined by

$$C(f,h)(z) \stackrel{\text{def}}{=} \sum_{m=-\infty}^{\infty} f(mh)\, S(m,h)(z). \tag{C.1.3}$$

This function was discovered by E. T. Whittaker (1915), who studied its mathematical properties and used it as an alternate expression for entire functions. He posed the interpolation problem of finding a function that passes through the points $(a + nw, f_n)$, where a, w are complex, and n is an integer. He called the class of all such functions the *cotabular set* associated with $\{f_n\}$ and showed that the sum of the cardinal series, as it is called now, picks out a special member that we call now the "cardinal" function of this cotabular set. Whittaker found that this function is special because it is entire and has no "violent oscillations," i.e., it is "band-limited." The Whittaker series for the cardinal function f, as given in his (1915) article, has the form $\sum f(a_n w)\,\dfrac{\sin\pi(x-a-nw)/w}{\pi(x-a-nw)/w}$. The name "cardinal series" was assigned to it by his second son, J. M. Whittaker, around 1920. The younger Whittaker extended this study in his 1927 and 1935 publications. The function $C(f,h)$ has played an important role in engineering applications for approximating f in the transformation of information (Hartley 1928, Nyquist 1928, and Shannon 1948). Since then engineers have called $C(f,h)$ the "sinc function" or the "band-limited" expansion of f, as mentioned above. An interesting account about the philosophy and historical analysis of this function can be found in Higgins (1985).

We now discuss some properties of the function $C(f,h)$. Let

$$\delta_{jm}^{(n)} = S^{(n)}(j,1)(m) = \left(\frac{d}{dx}\right)^n S(j,1)(x)\Big|_{x=m}. \tag{C.1.4}$$

In particular,

$$\begin{aligned}
\delta_{jm}^{(0)} &= \begin{cases} 1 & \text{if } j=m,\\ 0 & \text{if } j\neq m,\end{cases}\\
\delta_{jm}^{(1)} &= \begin{cases} 0 & \text{if } j=m,\\ \dfrac{(-1)^{m-j}}{m-j} & \text{if } j\neq m,\end{cases}\\
\delta_{jm}^{(2)} &= \begin{cases} -\dfrac{\pi^2}{3} & \text{if } j=m,\\ -\dfrac{2(-1)^{m-j}}{(m-j)^2} & \text{if } j\neq m.\end{cases}
\end{aligned} \tag{C.1.5}$$

The following results present explicit relations between $C(f,h)$ and $S(m,h)$. Let $f\in\mathcal{B}(h)$. Then

$$f(z) = C(f,h)(z) \quad \text{for all } z\in\mathbb{C}; \tag{C.1.6}$$

$$\int_{\mathbb{R}} f(x)\,dx = h\sum_{m=-\infty}^{\infty} f(mh); \tag{C.1.7}$$

$$\int_{\mathbb{R}} |f(x)|^2\,dx = h\sum_{m=-\infty}^{\infty} |f(mh)|^2; \tag{C.1.8}$$

thus, the set $\{h^{-1/2}\,S(m,h)\}_{m=-\infty}^{\infty}$ is a complete orthonormal sequence in $\mathcal{B}(h)$.

There exists a unique function $g \in L_2(-\pi/h, \pi/h)$ such that

$$f(z) = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} e^{-izs} g(s)\, ds, \tag{C.1.9}$$

where $g(x)$ is defined as the complex Fourier transform

$$g(x) = \int_{\mathbb{R}} e^{ixs}\, f(s)\, ds = \begin{cases} h \sum_{m=-\infty}^{\infty} f(mh)\, e^{-imhx} & \text{if } -\dfrac{\pi}{h} < x < \dfrac{\pi}{h}, \\ 0 \quad \text{if } |x| > \dfrac{\pi}{h}. \end{cases} \tag{C.1.10}$$

Thus,

$$f(z) = \frac{1}{h} \int_{\mathbb{R}} f(s)\, \frac{\sin \frac{\pi}{h}(z-s)}{\frac{\pi}{h}(z-s)}\, ds; \tag{C.1.11}$$

$$f' \in \mathcal{B}(h),; \tag{C.1.12}$$

$$f^{(n)}(mh) = h^{-n} \sum_{j=-\infty}^{\infty} \delta_{jm}^{(n)}\, f(jh), \tag{C.1.13}$$

where $\delta_{jm}^{(n)}$ is defined by (C.1.4), and thus, in view of (C.1.12) and (C.1.13), we have

$$f^{(n)}(x) = h^{-n} \sum_{j=-\infty}^{\infty} \left[\sum_{j=-\infty}^{\infty} \delta_{jm}^{(n)}\, f(jh) \right] S(m,h)(x). \tag{C.1.14}$$

If g is defined as in (C.1.9), then

$$\int_0^x f(s)\, ds = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} g(s)\, \frac{1 - e^{-isx}}{is}\, ds, \tag{C.1.15}$$

and, in particular,

$$\int_0^x S(m,h)(s)\, ds = h \left[\sigma_m + \frac{1}{\pi} \int_0^{\pi} \frac{\sin\left(\frac{x}{h} - m\right) s}{s}\, ds \right], \tag{C.1.16}$$

where

$$\sigma_n = \frac{1}{\pi} \int_0^{\pi} \frac{\sin ns}{s}\, ds = \int_0^n \frac{\sin \pi x}{\pi x}\, dx \quad \text{by taking } ns = \pi x. \tag{C.1.17}$$

Moreover, if $\int_{\mathbb{R}} f(s)\,ds = 0$, and if $\int_{-\infty}^{x} f(s)\,ds$ is in $\mathcal{B}(h)$, then

$$\int_{-\infty}^{x} f(s)\,ds = h \sum_{m=-\infty}^{\infty} \left[\sum_{j=-\infty}^{\infty} \sigma_{m-j}\, f(jh) \right] S(m,h)(x). \tag{C.1.18}$$

Note that σ_n in (C.1.16) defines the integral of the sinc function for $n = 0, 1, 2, \dots$; these values are computed in sinc1.nb, and their distribution is presented in Fig.C.1.1.

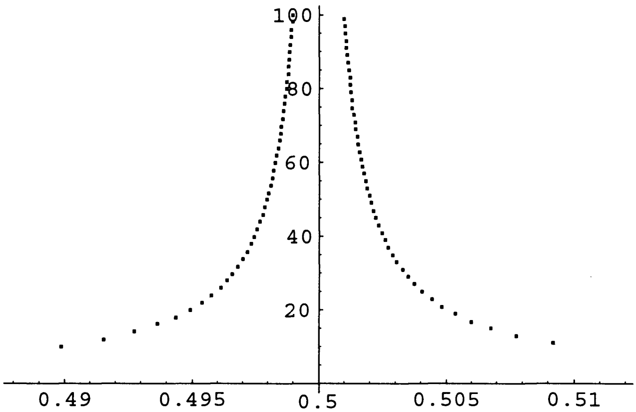

Fig. C.1.1. Distribution of σ_n for $n = 0, 1, \dots, 100$.

Let $0 < \alpha < 1$, and let g be defined as in (C.1.10). Then

$$\int_{\mathbb{R}} |x-s|^{\alpha-1} f(s)\,ds = \frac{\Gamma(\alpha)\,\cos(\pi\alpha/2)}{\pi} \int_{-\pi/h}^{\pi/h} |s|^{-\alpha}\, g(s)\, e^{-ixs}\,ds, \tag{C.1.19}$$

and, in particular,

$$\int_{\mathbb{R}} |x-s|^{\alpha-1}\, S(m,h)(s)\,ds$$

$$= \frac{2h^{\alpha}\Gamma(\alpha)\,\cos(\pi\alpha/2)}{\pi} \int_0^{\pi} s^{-\alpha}\,\cos\left((x-mh)s/h\right)\,ds, \tag{C.1.20}$$

so that

$$\int_{\mathbb{R}} |x-s|^{\alpha-1} f(s)\, ds$$
$$= \frac{2h^{\alpha}\Gamma(\alpha)\cos(\pi\alpha/2)}{\pi} \sum_{m=-\infty}^{\infty} f(mh) \int_0^{\pi} s^{-\alpha} \cos((x-mh)s/h)\, ds. \tag{C.1.21}$$

Finally, let g be defined as in (C.1.10). Then

$$\int_{\mathbb{R}} \log|x-s|\, f(s)\, ds = \frac{1}{4}\int_{-\pi/h}^{\pi/h} \frac{g(0)-e^{-ixs}g(s)}{|s|}\, ds - \frac{1}{2}\left[\gamma + \log\left(\frac{\pi}{h}\right)\right] g(0), \tag{C.1.22}$$

and, in particular,

$$\int_{\mathbb{R}} \log|x-s|\, S(m,h)(s)\, d$$
$$= -\frac{h}{2}\left\{\gamma + \log\left(\frac{\pi}{h}\right) - \int_0^{\pi} \frac{1-\cos((x-mh)s/h)}{s}\, ds\right\}, \tag{C.1.23}$$

so that

$$\int_{\mathbb{R}} \log|x-s|\, f(s)\, ds$$
$$= -\frac{h}{2} \sum_{m=-\infty}^{\infty} f(mh) \left\{\gamma + \log\left(\frac{\pi}{h}\right) - \int_0^{\pi} \frac{1-\cos((x-mh)s/h)}{s}\, ds\right\}. \tag{C.1.24}$$

The cardinal series

$$\sum_{n=1}^{\infty} c_n \frac{\sin\pi(t-n)}{\pi(t-n)} = \frac{\sin\pi t}{\pi} \sum_{n=1}^{\infty} c_n \frac{(-1)^n}{t-n}, \tag{C.1.25}$$

can be obtained by some simple methods, two of which are as follows:

(i) Consider a function $f(z)$ at points $z = -m, \dots, 9, \dots, m$. The Lagrange interpolation formula that interpolates $f(z)$ at these points is given by

$$H_m(z)\left\{\frac{f(0)}{z} + \sum_{n=1}^{\infty} \frac{f(n)}{H_m'(n)(z-n)} + \frac{f(-n)}{H_m'(-m)(z+n)}\right\}, \tag{C.1.26}$$

where

$$H_m(z) = z \prod_{n=1}^{m} \left(1 - \frac{z^2}{n^2}\right),$$

and the cardinal series (C.1.25) is obtained by letting $m \to \infty$. This method is due to Brown (1915–1916) and Ferrar (1925, p.270).

(ii) A formal approach is to regard the cardinal series as a special case of Cauchy's partial-fractions expansion for a suitably restricted meromorphic function $F(z)$ with poles at the points t_n, i.e.,

$$F(z) = \sum \text{Res of } \frac{F(w)}{z-w} \text{ at the points } w = t_n;$$

then apply this to $F(z) = f(z) \csc \pi z$, where f is entire (see Ferrar 1925, p. 281).

C.2. Approximation of an Integral

The approximation of an integral on an interval $\Gamma = [a, x]$ of the type

$$I(x) = \int_a^x g(t)\, dt, \quad x \in \Gamma, \tag{C.2.1}$$

is given by the following result (Stenger 1981).

THEOREM C.2.1. Let $g \in B_1(\Omega_d)$ and let $\left|\frac{g(x)}{F'(x)}\right| \le C\, e^{-\alpha'|F(x)|}$ along Γ, where C and α' are positive constants. Let $0 < \beta < \pi/d$, and let

$$q(x) = \int_a^x g(t)\, dt - \frac{e^{\beta F(x)/2}}{e^{\beta F(x)/2} e^{-\beta F(x)/2}} \int_a^b g(t)\, dt \in B_1(\Omega_d), \tag{C.2.2}$$

where Ω_d is defined in §10.2. If $\alpha = \min(\alpha', \beta)$, then for $h = \sqrt{\pi d/(\alpha N)}$ and all $x \in \Gamma$

$$\left| q(x) - h \sum_{j=-N}^{N} \left\{ \sum_{m=-N}^{N} \sigma_{j-m} \left[\frac{g(z_m)}{F'(z_m)} - \frac{\beta}{\left(e^{\beta m h/2} - e^{-\beta m h/2}\right)^2} \int_\Gamma g(t)\, dt \right] \right\} \right.$$
$$\left. \times\ S(j,h) \circ F(x) \right| \le C_1 N e^{-\sqrt{\pi d \alpha N}}, \tag{C.2.3}$$

where σ_j is defined by (C.1.17), and C_1 depends only on g, d and α.

The formula (C.2.3) is useful in approximating integrals like $\int_0^x t^{-2/3}(1-t)^{-5/4} \log t \, dt$, $x \in [0,1]$. However, in practice, the integral (C.2.1) is generally approximated by the formula

$$\left| \int_\Gamma g(t)\, dt - h \sum_{j=-N}^{N} \frac{g(z_j)}{F'(z_j)} \right| \le C_1 e^{-\sqrt{2\pi d \alpha N}}, \tag{C.2.4}$$

where C_1 depends only on g, d, and α.

REFERENCES USED: Brown (1915–1916), Carslaw (1921), Ferrar (1925), Hartley 1928), Higgins (1985), McNamee, Stenger and Whitney (1971), Nyquist (1928), Shannon (1948), Stenger (1981), Walker (1991), Whittaker (1915), Whittaker and Watson (1973).

D

Singular Integrals

D.1. Cauchy Principal-Value Integrals

Consider the improper integral $\int_a^b \frac{dx}{x-s}$, $a < s < b$, which is evaluated as follows:

$$\begin{aligned}\int_a^b \frac{dx}{x-s} &= \lim_{\substack{\varepsilon_1\to 0\\ \varepsilon_2\to 0}} \left(-\int_a^{s-\varepsilon_1} \frac{dx}{s-x} + \int_{s+\varepsilon_2}^b \frac{dx}{x-s} \right) \\ &= \ln\frac{b-s}{s-a} + \lim_{\substack{\varepsilon_1\to 0\\ \varepsilon_2\to 0}} \ln\frac{\varepsilon_1}{\varepsilon_2}.\end{aligned} \tag{D.1.1}$$

The limit on the right side depends on how ε_1 and ε_2 go to zero. This integral is known as a *singular integral*. But this integral can become meaningful if we assume that a relationship exists between ε_1 and ε_2. For example, if $\varepsilon_1 = \varepsilon_2 = \varepsilon$, i.e., if the deleted interval is symmetric about the point s, then it leads to the concept of the Cauchy principal value (p.v.) of the singular integral, which, denoted by a bar across the integral sign and defined as

$$⨍_a^b \frac{dx}{x-s}, \quad a < s < b, \tag{D.1.2}$$

is the number $\lim_{\varepsilon\to 0} \left(\int_a^{s-\varepsilon} + \int_{s+\varepsilon}^b \right) \frac{dx}{x-s}$ which, in view of (D.1.1), has the value

$$\int_a^b \frac{dx}{x-s} = \ln \frac{b-s}{s-a}. \tag{D.1.3}$$

The notation used for the Cauchy p.v. integrals is, however, not necessary, because if an integral of the type $\displaystyle\int_a^b \frac{\phi(x)}{x-s}\,dx$ exists as a proper or improper integral, then it exists only in the sense of the Cauchy p.v., and their values coincide. But if we regard a singular integral in the sense of the Cauchy p.v. integral, the above notation becomes very useful.

For a generalization, consider a singular integral over the interval $[a, b]$ such that the integrand has a singularity of the type $\dfrac{1}{x-s}$ at an interior point s, $a < s < b$, and the regular part of the integrand is a function $\phi(x) \in C^0[a, b]$ which satisfies the Hölder condition

$$\left|\phi(x) - \phi(s)\right| \leq A\,|x-s|^{\alpha},$$

where $0 < \alpha \leq 1$, and $|A| < \infty$. Then the Cauchy p.v. integral is defined by

$$\int_a^b \frac{\phi(x)}{x-s}\,dx = \lim_{\varepsilon \to 0} \left(\int_a^{s-\varepsilon} + \int_{s+\varepsilon}^b \right) \frac{\phi(x)}{x-s}\,dx, \quad a < s < b, \tag{D.1.4}$$

where

$$\begin{aligned} \int_a^s \frac{\phi(x)}{x-s}\,dx &= \lim_{\varepsilon \to 0} \left\{ \int_a^{s-\varepsilon} \frac{\phi(x)}{x-s}\,dx - \phi(s)\,\ln \varepsilon \right\}, \\ \int_s^b \frac{\phi(x)}{x-s}\,dx &= \lim_{\varepsilon \to 0} \left\{ \int_{s+\varepsilon}^b \frac{\phi(x)}{x-s}\,dx + \phi(s)\,\ln \varepsilon \right\}, \end{aligned} \tag{D.1.5}$$

provided these limiting processes are taken together, since each of them does not exist independently. In fact, using the identity

$$\int_a^b \frac{\phi(x)}{x-s}\,dx = \int_a^b \frac{\phi(x)-\phi(s)}{x-s}\,dx + \phi(s) \int_a^b \frac{dx}{x-s}$$

and (D.1.3), we find that

$$\int_a^b \frac{\phi(x)}{x-s}\,dx = \int_a^b \frac{\phi(x)-\phi(s)}{x-s} + \phi(s)\,\ln \frac{b-s}{s-a}, \tag{D.1.6}$$

since $\phi(x)$ satisfies the Hölder condition on $[a, b]$.

D.2. P.V. of a Singular Integral on a Contour

Consider the singular integral

$$\int_\Gamma \frac{\phi(\zeta)}{\zeta - z}\, d\zeta \quad \text{for } z, \zeta \in \Gamma, \tag{D.2.1}$$

on a contour Γ with endpoints a and b ($a = b$ if Γ is closed). Draw a circle of radius ρ with center at a point $z \in \Gamma$, and let z_1 and z_2 be the points of intersection of this circle with Γ. We take ρ small enough so that the circle has no other points of intersection with Γ. Let γ denote the part of the contour Γ cut out by this circle. Then the integral on the remaining contour $\Gamma - \gamma$ is $\displaystyle\int_{\Gamma-\gamma} \frac{\phi(\zeta)}{\zeta - z}\, d\zeta$, and the principal value of the singular integral (D.2.1) is given by $\displaystyle\lim_{\rho\to 0} \int_{\Gamma-\gamma} \frac{\phi(\zeta)}{\zeta - z}\, d\zeta$. Since

$$\int_\Gamma \frac{\phi(\zeta)}{\zeta - z}\, d\zeta = \int_\Gamma \frac{\phi(\zeta) - \phi(z)}{\zeta - z}\, d\zeta + \phi(z) \int_\Gamma \frac{d\zeta}{\zeta - z},$$

we find in the same way as in §D.1 that the singular integral (D.2.1) exists as a Cauchy p.v. integral for any function $\phi(\zeta)$ that satisfies the Hölder condition, and

$$⨍_\Gamma \frac{\phi(\zeta)}{\zeta - z}\, d\zeta = ⨍_\Gamma \frac{\phi(\zeta) - \phi(z)}{\zeta - z}\, d\zeta + \phi(z)\, \ln \frac{b - z}{z - a}, \tag{D.2.2a}$$

or

$$⨍_\Gamma \frac{\phi(\zeta)}{\zeta - z}\, d\zeta = ⨍_\Gamma \frac{\phi(\zeta) - \phi(z)}{\zeta - z}\, d\zeta + \phi(z) \left(\ln \frac{b - z}{z - a} + i\pi \right). \tag{D.2.2b}$$

Moreover, if the contour Γ is closed, then we let $a = b$ and obtain

$$⨍_\Gamma \frac{\phi(\zeta)}{\zeta - z}\, d\zeta = ⨍_\Gamma \frac{\phi(\zeta) - \phi(z)}{\zeta - z}\, d\zeta + i\pi\, \phi(z). \tag{D.2.3}$$

Now consider the Cauchy-type integral

$$\Phi(z) = \frac{1}{2i\pi} \int_\Gamma \frac{\phi(\zeta)}{\zeta - z}\, d\zeta, \tag{D.2.4}$$

where Γ is a closed or nonclosed contour and $\phi(\zeta)$ satisfies the Hölder condition on Γ. This integral has limit values $\Phi^+(z)$ and $\Phi^-(z)$ at any point $z \in \Gamma$ (z not equal to a or b) as $z \to \zeta$ from the left or from the right, respectively, along any path. These two limit values can be expressed in terms of the function $\phi(\zeta)$, which is known as the *density* of the integral, by the PLEMELJ FORMULAS

$$\begin{aligned}\Phi^+(z) &= \frac{1}{2}\,\phi(z) + \frac{1}{2i\pi} \int_\Gamma \frac{\phi(\zeta)}{\zeta - z}\,d\zeta,\\ \Phi^-(z) &= -\frac{1}{2}\,\phi(z) + \frac{1}{2i\pi} \int_\Gamma \frac{\phi(\zeta)}{\zeta - z}\,d\zeta,\end{aligned} \tag{D.2.5}$$

such that

$$\begin{aligned}\Phi^+(z) + \Phi^-(z) &= \frac{1}{i\pi} \int_\Gamma \frac{\phi(\zeta)}{\zeta - z}\,d\zeta,\\ \Phi^+(z) - \Phi^-(z) &= \phi(z).\end{aligned} \tag{D.2.6}$$

If Γ is the real axis, then the Plemelj formulas become

$$\begin{aligned}\Phi^+(x) &= \frac{1}{2}\,\phi(x) + \frac{1}{2i\pi} \int_{-\infty}^{\infty} \frac{\phi(s)}{s - x}\,ds,\\ \Phi^-(x) &= -\frac{1}{2}\,\phi(x) + \frac{1}{2i\pi} \int_{-\infty}^{\infty} \frac{\phi(s)}{s - x}\,ds,\end{aligned} \tag{D.2.7}$$

and

$$\Phi^+(\infty) = \frac{1}{2}\,\phi(\infty), \quad \Phi^-(\infty) = -\frac{1}{2}\,\phi(\infty). \tag{D.2.8}$$

Hence, from (D.2.7) and (D.2.8) we have

$$\Phi^+(\infty) + \Phi^-(\infty) = 0, \quad \lim_{x\to\infty} \int_{-\infty}^{\infty} \frac{\phi(s)}{s - x}\,ds = 0. \tag{D.2.9}$$

We use the first property in (D.2.9) to represent a piecewise analytic function in the upper and the lower half-plane by an integral over the real axis. Consider a Cauchy-type integral over the real axis:

$$\Phi(z) = \frac{1}{2i\pi} \int_{-\infty}^{\infty} \frac{\phi(x)}{x - z}\,dx, \tag{D.2.10}$$

where z is complex and $\Phi(z)$ is a complex-valued function of a real variable x, which satisfies the Hölder condition on the real axis. If a function $\phi(x)$ is analytic on the upper half-plane D^+, is continuous on the closed upper half-plane, and satisfies the Hölder condition on the real axis, then

$$\frac{1}{2i\pi} \int_{-\infty}^{\infty} \frac{\phi(x)}{x - z}\,dx = \begin{cases} \phi(z) - \frac{1}{2}\,\phi(\infty) & \text{for } \Im\{z\} > 0,\\ -\frac{1}{2}\,\phi(\infty) & \text{for } \Im\{z\} < 0;\end{cases} \tag{D.2.11}$$

also,

$$\frac{1}{2i\pi}\int_{-\infty}^{\infty}\frac{\phi(x)-\phi(\infty)}{x-z}\,dx=\begin{cases}\frac{1}{2}\,\phi(\infty) & \text{for } \Im\{z\}>0,\\ -\phi(z)+\frac{1}{2}\,\phi(\infty) & \text{for } \Im\{z\}<0,\end{cases}\tag{D.2.12}$$

provided $\phi(z)$ is analytic on the lower half-plane D^-, is continuous on the closed lower half-plane, and satisfies the Hölder condition on the real axis.

EXAMPLE D.2.1. If $\Gamma=\{|z|=1\}$, and $\phi(\zeta)=\dfrac{2}{\zeta(\zeta-2)}=\dfrac{1}{\zeta-2}-\dfrac{1}{\zeta}$, and $\phi(\infty)=0$, then

$$\begin{aligned}\Phi(z)&=\frac{1}{2i\pi}\int_\Gamma\frac{1}{\zeta-2}\,\frac{d\zeta}{\zeta-z}-\frac{1}{2i\pi}\int_\Gamma\frac{1}{\zeta}\,\frac{d\zeta}{\zeta-z}\\&=\begin{cases}\dfrac{1}{z-2}-\dfrac{1}{z} & \text{for } \Im\{z\}>0,\\ \dfrac{1}{z} & \text{for } \Im\{z\}<0,\end{cases}\end{aligned}$$

by (D.2.11) and (D.2.12). Hence,

$$\Phi^+(z)=\frac{1}{z-2}\quad\text{and}\quad\Phi^-(z)=\frac{1}{z}.\ \blacksquare$$

Another useful formula is the POINCARÉ–BERTRAND FORMULA:

$$\frac{1}{i\pi}\int_\Gamma\frac{d\zeta}{\zeta-z}\cdot\frac{1}{i\pi}\int_\Gamma\frac{g(\zeta,\zeta_1)}{\zeta-\zeta_1}\,d\zeta_1=g(z,z)+\frac{1}{i\pi}\int_\Gamma d\zeta_1\cdot\frac{1}{i\pi}\int_\Gamma\frac{g(\zeta,\zeta_1)}{(\zeta-z)(\zeta-\zeta_1)}\,d\zeta,\tag{D.2.13}$$

or, alternatively,

$$\int_\Gamma\frac{d\zeta}{\zeta-z}\cdot\int_\Gamma\frac{g(\zeta,\zeta_1)}{\zeta-\zeta_1}\,d\zeta_1=\pi^2\,g(z,z)+\int_\Gamma d\zeta_1\cdot\int_\Gamma\frac{g(\zeta,\zeta_1)}{(\zeta-z)(\zeta-\zeta_1)}\,d\zeta,\tag{D.2.14}$$

where the function $g(\zeta,\zeta_1)$ satisfies the Hölder condition with respect to both variables. This formula is useful when changing the order of integration in singular integrals. Thus, the pair of iterated singular integrals

$$\begin{aligned}F(\zeta)&=\frac{1}{i\pi}\int_\Gamma\frac{d\zeta}{\zeta-z}\cdot\frac{1}{i\pi}\int_\Gamma\frac{g(\zeta,\zeta_1)}{\zeta-\zeta_1}\,d\zeta_1,\\G(\zeta)&=\frac{1}{i\pi}\int_\Gamma d\zeta_1\cdot\frac{1}{i\pi}\int_\Gamma\frac{g(\zeta,\zeta_1)}{(\zeta-z)(\zeta-\zeta_1)}\,d\zeta,\end{aligned}$$

are not equal, although they differ in the order of integration.

D.3. Hadamard's Finite-Part Integrals

If $\phi(x) \in C^1[a,b]$, the Cauchy p.v. integral (D.1) becomes the first-order two-sided Hadamard's (or finite-part) integral, and the integrals (D.2) are then equivalent to first-order one-sided finite-part integrals.

Consider an improper integral on the interval $[a,b]$ such that (i) the integrand has a singularity of the type $\dfrac{1}{(x-s)^2}$ at an interior point s, $a < s < b$, and (ii) the regular part of the integrand is a function $\phi(x)$, $a \le x \le b$, which satisfies a Hölder continuous first-derivative condition

$$\left|\phi(x) - \phi(s) - (x-s)\,\phi'(s)\right| \le A\,|x-s|^{\alpha+1},$$

where $0 < \alpha \le 1$ and $|A| < \infty$, as before. Then a Hadamard's (finite-part) integral is defined by

$$⨎_a^b \frac{\phi(x)}{(x-s)^2}\,dx = \lim_{\varepsilon\to 0}\Big\{\Big(\int_a^{s-\varepsilon} + \int_{s+\varepsilon}^b\Big)\frac{\phi(x)}{(x-s)^2}\,dx - \frac{2\phi(s)}{\varepsilon}\Big\}, \tag{D.3.1}$$

where the neighborhood ε is symmetric about the singular point s. This integral can also be evaluated on both sides of the singular point as first-order one-sided integrals

$$\begin{aligned} ⨎_a^s \frac{\phi(x)}{(x-s)^2}\,dx &= \lim_{\varepsilon\to 0}\Big\{\int_a^{s-\varepsilon} \frac{\phi(x)}{(x-s)^2}\,dx - \frac{\phi(s)}{\varepsilon} - \phi'(s)\,\ln s\Big\}, \\ ⨎_s^b \frac{\phi(x)}{(x-s)^2}\,dx &= \lim_{\varepsilon\to 0}\Big\{\int_{s+\varepsilon}^b \frac{\phi(x)}{x-s}\,dx - \frac{\phi(s)}{\varepsilon} + \phi'(s)\,\ln s\Big\}, \end{aligned} \tag{D.3.2}$$

both of which must be taken together.

Differentiation of the Cauchy p.v. integrals with respect to s is carried out by using the Leibniz rule* which yields

$$\frac{d}{ds} \int_a^b \frac{\phi(x)}{x-s}\,dx = \lim_{\varepsilon\to 0} \frac{d}{ds}\left(\int_a^{s-\varepsilon} + \int_{s+\varepsilon}^b\right) \frac{\phi(x)}{x-s}\,dx$$
$$= \lim_{\varepsilon\to 0}\left\{\left(\int_a^{s-\varepsilon} + \int_{s+\varepsilon}^b\right) \frac{\phi(x)}{(x-s)^2}\,dx - \frac{\phi(s-\varepsilon)+\phi(s+\varepsilon)}{\varepsilon}\right\}. \tag{D.3.3}$$

Since ϕ is continuous on $a \le x \le b$, we have $\phi(s-\varepsilon) = \phi(s+\varepsilon) = \phi(s)$ as $\varepsilon \to 0$. Then formula (D.3.3) becomes

$$\frac{d}{ds} \int_a^b \frac{\phi(x)}{x-s}\,dx = \lim_{\varepsilon\to 0}\left\{\left(\int_a^{s-\varepsilon} + \int_{s+\varepsilon}^b\right) \frac{\phi(x)}{x-s}\,dx - \frac{2\phi(s)}{\varepsilon}\right\}, \tag{D.3.4}$$

which is the same as (D.3.1). Hence, we obtain the formula

$$\frac{d}{ds} \int_a^b \frac{\phi(x)}{x-s}\,dx = \int_a^b \frac{\phi(x)}{(x-s)^2}\,dx, \tag{D.3.5}$$

which is very useful in evaluating Hadamard's finite-part integrals.

D.4. Two-Sided Finite-Part Integrals

If we take $\phi(x) = \phi(x) - \phi(s) + \phi(s)$ in the Cauchy p.v. integral (D.1), then

$$\int_a^b \frac{\phi(x)}{x-s}\,dx = \int_a^b \frac{\phi(x)-\phi(s)}{x-s}\,dx + \phi(s) \int_a^b \frac{dx}{x-s}, \tag{D.4.1}$$

where

$$\int_a^b \frac{dx}{x-s} = \left[\ln|x-s|\right]_a^b = \ln\left|\frac{b-s}{s-a}\right|. \tag{D.4.2}$$

*The Leibniz rule for differentiating an integral with respect to a parameter is

$$\frac{\partial}{\partial y} \int_a^b g(t,y)\,dt = \int_a^b g_y(t,y)\,dt,$$

$$\frac{\partial}{\partial y} \int_{h_1(y)}^{h_2(y)} g(t,y)\,dt = \int_{h_1(y)}^{h_2(y)} g_y(t,y)\,dt + h_2'(y)\,g\left(h_2(y),y\right) - h_1'(y)\,g\left(h_1(y),y\right).$$

For details, see Williamson, Crowell, and Trotter (1962, p.316).

If $\phi \in C^1[a,b]$, the continuity requirement on $\phi'(x)$ is a necessary condition for a Taylor's series expansion of the function $\phi(x)$. But if $\phi(x) \notin C^1$, i.e., it does not have a high degree of continuity so as not to allow a Taylor's series expansion, a sufficient condition for the existence of finite-part integral is that $\phi(x)$ satisfy a Hölder or Lipschitz condition, i.e., $|\phi(x) - \phi(s)| \le A\,|x-s|^\alpha$, $0 < \alpha \le 1$, $|A| < \infty$. This condition also guarantees that the first integral on the right side of (D.4.1) is, at most, weakly singular. Now, integrating (D.1.4) by parts we get

$$\fint_a^b \frac{\phi(x)}{x-s}\,dx = \phi(b)\,\ln|b-s| - \phi(a)\,\ln|a-s| - \int_a^b \phi'(x)\,\ln|x-s|\,dx, \tag{D.4.3}$$

where $\phi(x) \in C^1[a,b]$. Then differentiation of (D.4.3) with respect to s yields

$$\frac{d}{ds}\fint_a^b \frac{\phi(x)}{x-s}\,dx = \frac{\phi(a)}{a-s} - \frac{\phi(b)}{b-s} + \fint_a^b \frac{\phi'(x)}{x-s}\,dx, \tag{D.4.4}$$

where $\phi'(x)$ satisfies the Hölder condition $\left|\phi'(x_1) - \phi'(x_2)\right| \le A\left|x_1 - x_2\right|^\alpha$.

Similarly, the finite-part integral of $\phi(x) \in C^2[a,b]$ is defined by

$$\begin{aligned} \mathop{=\!\!\!\!\!\!\!\int}_a^b \frac{\phi(x)}{(x-s)^2}\,dx = \int_a^b &\frac{\phi(x) - \phi(s) - (x-s)\phi'(s)}{(x-s)^2}\,dx \\ &+ \phi(s)\mathop{=\!\!\!\!\!\!\!\int}_a^b \frac{dx}{(x-s)^2} + \phi'(s)\fint_a^b \frac{dx}{x-s}, \end{aligned} \tag{D.4.5}$$

where on the right side the last integral is evaluated in (D.4.2), while the second integral is given by

$$\mathop{=\!\!\!\!\!\!\!\int}_a^b \frac{dx}{(x-s)^2} = \left[-\frac{1}{x-s}\right]_a^b = \frac{1}{a-s} - \frac{1}{b-s}. \tag{D.4.6}$$

In the case when $\phi(x) \notin C^2$, i.e., it does not have a high degree of continuity to allow a Taylor's series expansion, a sufficient condition for the existence of the finite-part integral in (D.4.5) is that $\phi(x)$ satisfy a Hölder-continuous first derivative condition as in §D.2, which also guarantees that the first integral on the right side of (D.4.5) is, at most, weakly singular.

Integrating a finite-part integral by parts we get

$$\mathop{=\!\!\!\!\!\!\!\int}_a^b \frac{\phi(x)}{(x-s)^2}\,dx = \frac{\phi(a)}{a-s} - \frac{\phi(b)}{b-s} + \fint_a^b \frac{\phi'(x)}{x-s}\,dx, \tag{D.4.7}$$

where $\phi(x) \in C^1[a,b]$ satisfies the Hölder condition. If we compare (D.4.7) and (D.4.4), we obtain

$$\frac{d}{ds} \int_a^b \frac{\phi(x)}{x-s}\,dx = \,\mathrm{f\!\!\!\!=}\!\!\int_a^b \frac{\phi(x)}{(x-s)^2}\,dx, \tag{D.4.8}$$

which shows that differentiation can be carried out under the integral sign.

D.5. One-Sided Finite-Part Integrals

Consider the case when the integrand has a singularity at an endpoint of the interval $[a,b]$, that is, either $a \equiv s$ or $b \equiv s$. Then the finite-part of a first-order function $\phi(x) \in C^1[a,s]$ or $\phi(x) \in C^1[s,b]$ is defined, respectively, by

$$⨍_a^s \frac{\phi(x)}{x-s}\,dx = \int_a^s \frac{\phi(x)-\phi(s)}{x-s}\,dx + \phi(s) ⨍_a^s \frac{dx}{x-s} \tag{D.5.1}$$

or

$$⨍_s^b \frac{\phi(x)}{x-s}\,dx = \int_s^b \frac{\phi(x)-\phi(s)}{x-s}\,dx + \phi(s) ⨍_s^b \frac{dx}{x-s}, \tag{D.5.2}$$

where

$$⨍_a^s \frac{dx}{x-s} = \text{finite part of } \big[\ln|x-s|\big]_a^s = -\ln|a-s| \tag{D.5.3}$$

or

$$⨍_s^b \frac{dx}{x-s} = \text{finite part of } \big[\ln|x-s|\big]_s^b = \ln|b-s|, \tag{D.5.4}$$

If $\phi(x) \notin C^1$, a sufficient condition for the existence of the finite-part integrals in (D.5.1) and (D.5.2) is that $\phi(x) \in C^0$ and satisfies a Hölder condition. If we use (D.5.1) and (D.5.2) to derive (D.4.1), we find that finite-part integrals exist iff the function $\phi(x)$ is continuous at the singular point s.

Similarly, the second-order one-sided finite-part integral of a function $\phi(x) \in C^2$ is given by

$$\begin{aligned} \,\mathrm{f\!\!\!\!=}\!\!\int_a^s \frac{\phi(x)}{(x-s)^2}\,dx &= \int_a^s \frac{\phi(x)-\phi(s)-(x-s)\phi'(s)}{(x-s)^2}\,dx \\ &\quad + \phi(s)\,\mathrm{f\!\!\!\!=}\!\!\int_a^s \frac{dx}{(x-s)^2} + \phi'(s) ⨍_a^s \frac{dx}{x-s}, \end{aligned} \tag{D.5.5}$$

or

$$\begin{aligned}\fint_s^b \frac{\phi(x)}{(x-s)^2}\,dx = \int_s^b \frac{\phi(x)-\phi(s)-(x-s)\phi'(s)}{(x-s)^2}\,dx \\ + \phi(s)\fint_s^b \frac{dx}{(x-s)^2} + \phi'(s)\fint_s^b \frac{dx}{x-s},\end{aligned} \tag{D.5.6}$$

according as the singularity is at the endpoint b or the endpoint a of the interval $[a, b]$. In these cases then

$$\fint_a^s \frac{dx}{(x-s)^2} = \text{finite part of}\left[-\frac{1}{x-s}\right]_a^s = \frac{1}{a-s}, \tag{D.5.7}$$

or

$$\fint_s^b \frac{dx}{(x-s)^2} = \text{finite part of}\left[-\frac{1}{x-s}\right]_s^b = \frac{1}{s-b}, \tag{D.5.8}$$

respectively. If $\phi(x) \notin C^2$, a sufficient condition for the existence of the finite-part integrals in (D.5.5) and (D.5.6) is that $f(x) \in C^1$ and satisfy a Hölder condition. If we use (D.5.1) and (D.5.2) to derive (D.4.1), we find that finite-part integrals exist iff the function $\phi'(x)$ is continuous at the singular point s.

D.6. Examples of Cauchy P.V. Integrals

EXAMPLE D.1. Let a Cauchy p.v. integral, denoted by $C_\nu(s)$, be defined by

$$C_\nu(s) = \fint_0^1 \frac{x^\nu}{x-s}\,dx, \quad 0 < s < 1, \quad \nu > -1. \tag{D.6.1}$$

Then the following results hold for rational ν:

$$\begin{aligned}&\text{(i) } C_{\nu+1}(s) = s\,C_\nu(s) + \frac{1}{\nu+1};\\ &\text{(ii) } C_\nu(s) = -\pi s^\nu \cot \pi\nu - \sum_{n=0}^{\infty} \frac{s^{n-\nu}}{n-\nu} \quad -1 < \nu < 0,\ \nu \text{ not integer};\\ &\text{(iii) } C_n(s) = s^n \ln\left(\frac{1-s}{s}\right) + \sum_{k=1}^{n} \frac{s^{n-k}}{k} \quad \text{for integer } n.\end{aligned} \tag{D.6.2}$$

PROOF. (i) Take $x = x - s + s$; then

$$C_{\nu+1}(s) = \fint_0^1 \frac{x^{\nu+1}}{x-s}\,dx = \int_0^1 x^\nu\,dx + s \fint_0^1 \frac{x^\nu}{x-s}\,dx,$$

which proves the result.

(ii) For $-1 < \nu < 0$, set $x = su$; then

$$\begin{aligned} C_\nu(s) &= \fint_0^1 \frac{x^\nu}{x-s}\,dx = s^\nu \fint_0^1 \frac{x^\nu}{x-1}\,dx \\ &= s^\nu \left[\int_0^\infty \frac{x^\nu}{x-1}\,dx - \int_{1/s}^\infty \frac{x^\nu}{x-1}\,dx\right] \\ &= -\pi s^\nu \cot \pi\nu - s^\nu \int_0^s \frac{z^{-\nu-1}}{n-\nu}\,dz, \quad \text{where } x = 1/z, \\ &= -\pi s^\nu \cot \pi\nu - \sum_{n=0}^\infty \frac{s^n}{n-\nu}, \quad -1 < \nu < 0,\ \nu \neq n, \end{aligned}$$

where we have used $\dfrac{1}{1-s} = \displaystyle\sum_{n=0}^\infty s^n$.

(iii) For $\nu = n$ (integer) we use recursion and get

$$\begin{aligned} C_0(s) &= \fint_0^1 \frac{1}{x-s}\,dx = \ln\left(\frac{1-s}{s}\right), \\ C_1(s) &= \fint_0^1 \frac{x}{x-s}\,dx = 1 - s\,\ln\left(\frac{1-s}{s}\right), \\ C_2(s) &= \fint_0^1 \frac{x^2}{x-s}\,dx = \frac{1}{2} + s + s^2\,\ln\left(\frac{1-s}{s}\right), \\ C_3(s) &= \fint_0^1 \frac{x^3}{x-s}\,dx = \frac{1}{3} + \frac{s}{2} + s^2 + s^3\,\ln\left(\frac{1-s}{s}\right), \end{aligned}$$

and so on. Thus, by induction we have

$$\begin{aligned} C_n(s) &= s^n\,\ln\left(\frac{1-s}{s}\right) + s^{n-1} + \frac{s^{n-2}}{2} + \cdots + \frac{1}{n} \\ &= s^n\,\ln\left(\frac{1-s}{s}\right) + \sum_{k=1}^n \frac{s^{n-k}}{k}. \blacksquare \end{aligned}$$

EXAMPLE D.2. If we denote the Cauchy p.v. integral by

$$I_{1,\nu} \equiv C_\nu(s) = \fint_0^1 \frac{x^\nu}{x-s}\,dx, \quad 0 < s < 1,$$

then by repeated differentiation we obtain the integral $I_{\alpha,\nu}$ for positive integer α as

$$I_{\alpha,\nu} = \fint_0^1 \frac{x^\nu}{(x-s)^\alpha}\,dx, \quad 0 < s < 1. \tag{D.6.3}$$

PROOF. We use formula (D.4.8), which, in view of (D.6.2(ii)), for non-integral ν yields

$$\begin{aligned}
I_{1,\nu} &= \fint_0^1 \frac{x^\nu}{x-s)}\,dx = -\pi s^\nu \cot \pi\nu - \sum_{n=0}^\infty \frac{s^{n-\nu}}{n-\nu}, \\
I_{2,\nu} &= \frac{d}{ds}\,(I_{1,\nu}) = -\pi \cot \pi\nu \cdot \nu s^{\nu-1} - \sum_{n=1}^\infty \frac{n\, s^{n-1}}{n-\nu}, \\
I_{3,\nu} &= \frac{d}{ds}\,(I_{2,\nu}) = -\pi \cot \pi\nu \cdot \nu(\nu-1) s^{\nu-1} - \sum_{n=2}^\infty \frac{n(n-1)\, s^{n-2}}{n-\nu},
\end{aligned}$$

and so on. Thus, by induction

$$I_{\alpha,\nu} = -\frac{\pi\Gamma(\nu+1)\, s^{\nu-\alpha+1} \cot \pi\nu}{\Gamma(\nu-\alpha+2)\,(\alpha-1)!} - \sum_{n=\alpha-1}^\infty \frac{n!\; s^{n-\alpha+1}}{(n-\alpha+1)!\,(\alpha-1)!\,(n-\nu)}. \tag{D.6.4}$$

For integer $\nu = n$ we have

$$\begin{aligned}
I_{\alpha,n} = &\sum_{j=0}^{\alpha-2} \binom{n}{j} \frac{s^{n-j}\left[(1-s)^{j-\alpha+1} - (-s)^{j-\alpha+1}\right]}{j-\alpha+1} \\
&+ i\,n \binom{n}{\alpha-1} s^{n-\alpha+1} \ln\left(\frac{1-s}{s}\right) \\
&+ \sum_{j=\alpha}^{n} \binom{n}{j} \frac{s^{n-j}\left[(1-s)^{j-\alpha+1} - (-s)^{j-\alpha+1}\right]}{j-\alpha+1}.
\end{aligned} \tag{D.6.5}$$

For details, see Bertram and Ruehr (1992). ∎

D.7. Examples of Hadamard's Finite-Part Integrals

First, we define the Hadamard transform $H_2[\phi]$ for a function $\phi(x)$ as

$$H_2[\phi] = \oint_0^1 \frac{\phi(x)}{(x-s)^2}\,dx, \quad 0 < s < 1. \tag{D.7.1}$$

Notice that this transform is the integral $I_{2,\nu}$. The results, given in Table D.1, hold for various choices of the function ϕ.

Table D.1.

$\phi(s)$	$H_2[\phi]$
s^ν (ν rational)	$-\pi\nu s^{\nu-1}\cot\pi\nu - \dfrac{1}{1-s} - \nu\sum_{n=0}^{\infty}\dfrac{s^n}{n-\nu+1}$
s^m (m integer)	$\dfrac{s^{m-1}}{1-s} + m s^{m-1}\ln\dfrac{1-s}{s} + \sum_{j=2}^{m}\dfrac{\binom{m}{j} s^{m-j}\left[(1-s)^{j-1} - (-s)^{j-1}\right]}{j-1}$
$\left[s(1-s)\right]^{3/2}$	$\dfrac{\pi}{2}\left[\dfrac{3}{4} - 6s(1-s)\right]$
$\dfrac{1}{2} + \dfrac{s-c}{2\lvert s-c\rvert}$	$\dfrac{1}{s-1} + \dfrac{1}{c-s}$
$\dfrac{1}{2}\left[c + (1-2c)s + \lvert s-c\rvert\right]$	$(c-1)\ln\lvert s\rvert - c\ln\lvert 1-s\rvert + \ln\lvert s-c\rvert$
$\dfrac{1}{2} + \dfrac{1}{4\varepsilon}\left[\lvert s-c+\varepsilon\rvert + \lvert s-c-\varepsilon\rvert\right]$	$\dfrac{1}{s-1} + \dfrac{1}{2\varepsilon}\ln\left\lvert\dfrac{s-c-\varepsilon}{s-c+\varepsilon}\right\rvert$
$\dfrac{3}{4}(s-c)^2 - \dfrac{1}{4}(s-c)\lvert s-c\rvert + \dfrac{1}{2}(s-c)\left(c^2+2c-1\right) + \dfrac{1}{2}c\left(c^2-1\right)$	$c+1+\left(s+\dfrac{c^2}{2}-\dfrac{1}{2}\right)\ln\lvert 1-s\rvert + (s-c)\ln\lvert s-c\rvert - \left(2s+\dfrac{c^2}{2}-c-\dfrac{1}{2}\right)\ln\lvert s\rvert$
$\sin\pi s$	$-\pi\sin\pi s\left[\mathrm{Si}\left(\pi(1-s)\right) + \mathrm{Si}(\pi s)\right] + \pi\cos\pi s\left[\mathrm{Ci}(\pi s) - \mathrm{Ci}\left(\pi(1-s)\right)\right]$

Note that if the function $\phi(x) \in C^2[a,b]$ satisfies a Hölder-continuous second-derivative condition, then Hadamard's second-order two-sided finite-part integrals contain the singular part $\dfrac{1}{(x-s)^3}$ and can be defined as above (see Ioakimidas 1988, for details). This concept can be generalized further, but we shall not go into this generalization.

NOTES: Kutt (1975) contains weights w_i to $30S$ for the equally spaced rule

$$\neq\!\!\!\!\!\!\int_0^1 \frac{f(x)}{x^4}\, dx \approx \sum_{i=1}^{n} w_i\, f\left(\frac{i}{n}\right), \quad n = 3(1)20,$$

and the nodes x_i and weights w_i to $30S$ for the Gauss-type quadrature rule

$$\neq\!\!\!\!\!\!\int_0^1 \frac{f(x)}{x^4}\, dx \approx \sum_{i=1}^{n} w_i\, f\left(x_i\right), \quad n = 2(1)20,$$

for $\lambda = 1, 4/3, 3/2, 5/3, 2, 3, 4, 5$. This work also contains weights for computation of the finite-part integrals of the form

$$\neq\!\!\!\!\!\!\int_0^1 \frac{f(x)}{(x-s)^4}\, dx, \quad \lambda = 2, 3, 4, 5$$

for the equally spaced case.

REFERENCES USED: Bertram and Ruehr (1992), Davis and Rabinowitz (1967), Hadamard (1923), Haji-Sheikh et al. (1991), Ioakimidas (1988), Ivanov (1968), Kutt (1975), Linz (1985), Lu (1984), Paget (1981), Polyanin and Manzhirov (1998), Pukhteev (1980), Williamson, Crowell, and Trotter (1962).

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