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A formula for optimal integration in H^2

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Abstract

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The weights $\hat{a}_j$ of the optimal integration formula $\hat{Q} = \Sigma_j \hat{a}_j f(z_j)$ in H^2 for given integration points z_j are the exact integrals of the cardinal functions in the corresponding formula for optimal evaluation. By writing these cardinal functions as sums of their principal values, we very easily obtain a closed formula for the weights. In the case of real z_j's, this formula makes explicit a series formula of Wilf. We compare numerically the accuracy of the optimal formula with that of some well-known integration formulae. For points equidistant on a circle of radius r, the formula allows an alternate derivation of a formula obtained by Golomb. We give also the barycentric formula for optimal evaluation with these points, as well as an experimentally stable sequence of radii r for integrating with an increasing number of points.

Keywords: Numerical quadrature; optimal quadrature; optimal approximation.

1. Introduction

Most numerical rules for approximating the integral $If := \int_\Gamma f(z)\,dz$ of a function f along a path $\Gamma \subset \mathbb{C}$ can be written as

$$Q = \sum_{j=0}^{n} a_j f_j, \quad f_j := f(z_j), \tag{1.1}$$

where the z_j's are distinct points on — or outside — Γ and $a_j \in \mathbb{C}$ are the weights associated with the points z_j. Choosing such an integration rule therefore consists of choosing the z_j's and the corresponding a_j's. In some methods (Newton–Cotes, SINC integration, etc.), one chooses the points and defines a process for determining the a_j's as functions of the z_j's. In others (Gauss quadrature, Wilf's quadrature, etc.), one chooses a criterion for determining simultaneously the z_j's and a_j's. Here we will take the first approach, and assume that the points have

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been chosen by the user or are imposed upon him; the goal is then to provide him with the "best" a_j's, i.e., those a_j's for which the error functional

$$E: f \mapsto Ef := If - \sum_{j=0}^{n} a_j f_j$$

has minimal norm on some normed linear space. (The corresponding rule (1.1) is then said to be *optimal with respect to the weights*.)

Among various spaces, the problem has been solved for H^2, the Hilbert space of those functions which are analytic within the unit disk and square integrable in the Lebesgue sense around the unit circle ∂D, with the scalar product

$$(f, g) := \frac{1}{2\pi} \int_{\partial D} f(z)\overline{g(z)}|\mathrm{d}z|$$

(see also the more general setting in [17] and the literature cited there). For example, the functions of the form

$$f(z) = (1+z)^{\alpha}(1-z)^{\beta} \log^{\gamma}(1-z) \log^{\delta}(1+z) g(z), \quad \alpha, \beta > -\tfrac{1}{2}, \tag{1.2}$$

where g is analytical in a domain containing D, belong to H^2.

Sard [19] has proved that for an optimal approximation of bounded linear functionals L, the a_j's in (1.1) must be chosen in such a way that for every f the linear combination in (1.1) equals the result of applying L to the orthogonal projection $f^{\perp}$ of f onto the linear manifold spanned by the values

$$k_j(z) := \frac{1}{1-\bar{z}_j z}, \quad j = 0, \ldots, n, \tag{1.3}$$

of the reproducing kernels at the points z_j. (H^2 is the direct sum of this manifold and the space of the H^2-functions vanishing at all z_j's.) Larkin [14] noticed that $f^{\perp}$ is independent of L and, by choosing L successively as the ordinate evaluation functional at z_j (i.e., $Lf := f(z_j)$), that

$$f^{\perp}(z_j) = f(z_j), \quad j = 0, \ldots, n. \tag{1.4}$$

It follows that solving the optimal linear approximation problem for the a_j's is equivalent to solving the interpolation problem of finding that linear combination $f^{\perp}(z) = \sum_{j=0}^{n} c_j k_j(z)$, $c_j \in \mathbb{C}$, of the k_j's for which the interpolation condition (1.4) holds. In the words of Larkin, "all *optimal linear approximation problems* are made to depend only on this single *interpolation problem*". (This result was already known to Richter-Dyn [17, p.589] and is mentioned also in [10].) $f^{\perp}$ is the minimal norm interpolant [15, p.115] — see the remark after the theorem below.

The functional we want to approximate here is the integration between two points of $\overline{D} := D \cup \partial D$. To use the above theory, we must first check that this functional is bounded.

Theorem 1.1. *Let $f \in H^2$, and let z_S and z_E be two points of $\overline{D}$. Then the linear functional $I: f \mapsto \int_{z_S}^{z_E} f(z)\,\mathrm{d}z$ is bounded.*

Proof. Let Γ denote the segment from z_S to z_E, δ the circle with center at the origin and passing through z_S and z_E, and γ one of the two circular arcs of δ that together with Γ make a closed curve. Then by Cauchy's integral theorem $If = \int_\Gamma f(z)\,dz = \pm\int_\gamma f(z)\,dz$; moreover,

$$\left|\int_\gamma f(z)\,dz\right| \leqslant \int_\gamma |f(z)|\,|dz| \leqslant \int_\delta |f(z)|\,|dz|,$$

and thus ([18, p.338] and Schwarz's inequality)

$$|If| \leqslant \int_{\partial D} |f(z)|\,|dz| \leqslant 2\pi \|f\|_2.$$

Thus $\|I\| \leqslant 2\pi$. Notice that if z_S and z_E are on a diameter through the origin, then $\|I\| \leqslant \pi$ by the Fejér–Riesz inequality [6, p.46]. □

Larkin and Golomb have also given the "Lagrange form" of $f^\perp(z)$,

$$f^\perp(z) = \sum_{j=0}^{n} l_j(z) m_j(z) f_j, \tag{1.5}$$

in which the l_j's are the Lagrange cardinal functions

$$l_j(z) = \frac{\prod_{k=0,k\neq j}^{n}(z - z_k)}{\prod_{k=0,k\neq j}^{n}(z_j - z_k)} \quad \text{and} \quad m_j(z) := \frac{\prod_{k=0}^{n}(1 - \bar{z}_k z_j)}{\prod_{k=0}^{n}(1 - \bar{z}_k z)}.$$

As noticed by Brachmond [5], who derived formulae for optimal differentiation, $l_j(z)m_j(z) = l_j^\perp(z)$ and $f^\perp(z) = \Sigma f_j l_j^\perp(z)$. We remark that for the optimal evaluation of $f(z^*)$, $z^* \in D$, the barycentric formula [3, Theorem 2.1] should be used instead of (1.5) to save computing time and guarantee stability in the vicinity of the z_j's.

2. The weights of optimal integration

The optimal rule $\hat{Q} := \Sigma_{j=0}^{n} \hat{a}_j f_j$ must be such that

$$\hat{Q} = \sum_{j=0}^{n} \hat{a}_j f_j = If^\perp = \sum_{j=0}^{n} I\left(l_j^\perp\right) f_j, \tag{2.1}$$

for all $f \in H^2$. Putting $f := l_k$, $k = 0, \ldots, n$, into (2.1), we see that the optimal weights are given by

$$\hat{a}_j = Il_j^\perp = \int_\Gamma l_j(z) m_j(z)\,dz. \tag{2.2}$$

We shall call $f^\perp$ the *optimal interpolant* and (2.1) with the weights in (2.2) the *optimal integration formula*. Notice that, as integrals of the cardinal functions $l_j(z)m_j(z)$ of optimal interpolation, the $\hat{a}_j$'s do not depend on f; thus, for example, the optimal formula integrates functions such as those in (1.2) without using α, β, γ or δ.

The $l_j(z)$ are entire, whereas the $m_j(z)$ have (simple) poles at $1/\bar{z}_k$, $z_k \neq 0$, which all lie outside D. The integrands in (2.2) are therefore rational functions with numerator degree n;

the degree of their denominators is n if one of the z_j's equals 0, $n+1$ otherwise. We will denote by z_n (one of) the z_j with minimal modulus; then evidently $z_n = 0$ iff one of the z_j's is 0.

Let us now factorize out the constant factors in l_j and m_j as in [3]:

$$l_j(z) = w_j \prod_{\substack{k=0 \\ k\neq j}}^{n} (z - z_k), \quad \text{with } w_j = \frac{1}{\prod_{k=0,k\neq j}^{n}(z_j - z_k)},$$

$$m_j(z) = \frac{v_j}{m(z)}, \quad \text{with } m(z) := \prod_{k=0}^{n} (1 - \bar{z}_k z)$$

$$\text{and } v_j := \prod_{k=0}^{n} (1 - \bar{z}_k z_j) = m(z_j).$$

To integrate $l_j(z)m_j(z)$, we will first compute its partial fraction decomposition. In view of the degrees mentioned above, the division of the numerator by the denominator is the constant $\lim_{z\to\infty} l_j(z)m_j(z)$. Moreover, as any rational function, $l_j(z)m_j(z)$ equals the sum of its principal values [12, p.218] and, since its poles are simple, it can be written as

$$l_j(z)m_j(z) = \sum_{l=0}^{n} \frac{d_{jl}}{1 - \bar{z}_l z}, \tag{2.3}$$

where the d_{jl} are given by

$$d_{jl} = \lim_{z\to 1/\bar{z}_l} l_j(z)m_j(z)(1 - \bar{z}_l z).$$

(Notice that if $z_n = 0$, the above expression for $l = n$ gives the constant term of the integrand: $\lim_{z\to\infty} l_j(z)m_j(z) \neq 0$.) Then

$$\begin{aligned} d_{jl} &= \lim_{z\to 1/\bar{z}_l} w_j v_j \prod_{\substack{k=0 \\ k\neq j}}^{n} (z - z_k) \frac{1}{\prod_{k=0,k\neq l}^{n}(1 - \bar{z}_k z)} \\ &= v_j w_j \lim_{z\to 1/\bar{z}_l} \prod_{\substack{k=0 \\ k\neq j}}^{n} (z\bar{z}_l - z_k \bar{z}_l) \frac{1}{\prod_{k=0,k\neq l}^{n}(\bar{z}_l - \bar{z}_k z\bar{z}_l)} \\ &= v_j w_j \frac{\bar{v}_l}{1 - z_j \bar{z}_l} \bar{w}_l = \frac{b_j \bar{b}_l}{1 - \bar{z}_l z_j}, \end{aligned} \tag{2.4}$$

where $b_j := v_j w_j$ is the weight corresponding to z_j in the barycentric formula for $f^{\perp}$ [3].

Inserted into (2.3), this yields

$$l_j(z)m_j(z) = b_j \sum_{l=0}^{n} \frac{\bar{b}_l}{1 - \bar{z}_l z_j} \frac{1}{1 - \bar{z}_l z}.$$

Recalling (2.2), we see that the optimal weights are given by

$$\hat{a}_j = b_j \sum_{l=0}^{n} \frac{\bar{b}_l}{1 - \bar{z}_l z_j} \int_{\Gamma} \frac{1}{1 - \bar{z}_l z} \mathrm{d}z,$$

and with z_S and z_E denoting respectively the starting and end points of Γ, we get the following formula for the optimal weights:

$$\hat{a}_j = \begin{cases} b_j \sum_{l=0}^{n} \dfrac{\bar{b}_l}{\bar{z}_l(1-\bar{z}_l z_j)} \operatorname{Log} \dfrac{1-\bar{z}_l z_S}{1-\bar{z}_l z_E}, & z_n \neq 0, \\ b_j \left(\sum_{l=0}^{n-1} \dfrac{\bar{b}_l}{\bar{z}_l(1-\bar{z}_l z_j)} \operatorname{Log} \dfrac{1-\bar{z}_l z_S}{1-\bar{z}_l z_E} + \bar{b}_n(z_E - z_S) \right), & z_n = 0, \end{cases} \quad j = 0, \ldots, n. \tag{2.5}$$

Since $1-\bar{z}_l z$ is in the right half-plane $\forall z_l$, $z \in D$, we have taken the principal value of the logarithm, written with capital L following the usual convention [12, p.114]. For such z_l and z, we have $-\frac{1}{2}\pi < \arg \operatorname{Log}(1-\bar{z}_l z) < \frac{1}{2}\pi$, and therefore $\operatorname{Log}(1-\bar{z}_l z_S) - \operatorname{Log}(1-\bar{z}_l z_E) = \operatorname{Log}\{(1-\bar{z}_l z_S)/(1-\bar{z}_l z_E)\}$.

In view of the degrees of the l_j's and m_j's and (2.4) with $\bar{z}_l = 0$ we have the following theorem.

Theorem 2.1. *Let $\{z_j\colon j = 0, \ldots, n\}$ be distinct points in the open unit disk D. Then the weights of the optimal integration formula for $If := \int_{z_S}^{z_E} f(z)\,dz$, z_S, $z_E \in \bar{D}$, are given by* (2.5) *and the optimal formula is*

$$\hat{Q} = \sum_{j=0}^{n} \hat{a}_j f_j = f^{\perp}(\infty)(z_E - z_S) + \sum_{j=0}^{n} \left(\sum_{l=0}^{n^*} \frac{\bar{b}_l}{\bar{z}_l(1-\bar{z}_l z_j)} \operatorname{Log} \frac{1-\bar{z}_l z_S}{1-\bar{z}_l z_E} \right) b_j f_j, \tag{2.6}$$

where

$$n^* = \begin{cases} n, & z_n \neq 0, \\ n-1, & z_n = 0, \end{cases} \qquad b_i = v_i w_i = \frac{\prod_{k=0}^{n}(1-\bar{z}_k z_i)}{\prod_{k=0, k\neq j}^{n}(z_i - z_k)},$$

and

$$f^{\perp}(\infty) := \lim_{z\to\infty} \sum_{j=0}^{n} l_j(z) m_j(z) f_j = \begin{cases} 0, & z_n \neq 0, \\ \bar{b}_n \sum_{j=0}^{n} b_j f_j, & z_n = 0. \end{cases} \tag{2.7}$$

Computing the b_j's requires $\mathcal{O}(n^2)$ operations (notice that when the z_j's are the Chebyshev points of the first kind, a closed formula permits the calculation in $\mathcal{O}(n)$ operations [4]); computing the $\hat{a}_j$'s also involves $\mathcal{O}(n^2)$ operations and, therefore, the total complexity of the formula is $\mathcal{O}(n^2)$.

Remarks 2.2. (1) Notice that $c_l := \sum_j d_{jl} f_j = \bar{b}_l \sum_j \{b_j/(1-\bar{z}_l z_j)\} f_j$ is the coefficient of $k_l(z)$ (see (1.3)) in the orthogonal projection $f^{\perp}$ of f onto $\operatorname{span}\{k_l(z)\colon l = 0, \ldots, n\}$; it is therefore the solution of the system of minimal norm interpolation [15, p.114]

$$\sum_{l=0}^{n} \frac{c_l}{1-\bar{z}_l z_j} = f_j.$$

(2) If the v_j's are independent of j, i.e., $v_j = v$, $\forall j$, the j-sum in (2.6) can be replaced by a value of the interpolating polynomial. Indeed, in that case

$$\sum_{j=0}^{n}\left(\sum_{l=0}^{n^*}\frac{\bar{b}_l}{\bar{z}_l(1-\bar{z}_l z_j)}\operatorname{Log}\frac{1-\bar{z}_l z_S}{1-\bar{z}_l z_E}\right)b_j f_j$$

$$= v\sum_{l=0}^{n^*}\frac{\bar{b}_l}{(\bar{z}_l)^2}\left(\sum_{j=0}^{n}\frac{w_j}{1/\bar{z}_l - z_j}f_j\right)\operatorname{Log}\frac{1-\bar{z}_l z_S}{1-\bar{z}_l z_E},$$

and, since the polynomial interpolating f between the z_j's reads [13, p.237]

$$p_n(z) = \ell(z)\sum_{j=0}^{n}\frac{w_j}{z-z_j}f_j, \tag{2.8}$$

where

$$\ell(z) := (z-z_0)(z-z_1)\cdots(z-z_n), \tag{2.9}$$

(2.6) becomes

$$\sum_{j=0}^{n}\hat{a}_j f_j = f^{\perp}(\infty)(z_E - z_S) + v\sum_{l=0}^{n^*}\frac{\bar{b}_l}{(\bar{z}_l)^2}\frac{1}{\ell(1/\bar{z}_l)}p_n\left(\frac{1}{\bar{z}_l}\right)\operatorname{Log}\frac{1-\bar{z}_l z_S}{1-\bar{z}_l z_E}. \tag{2.10}$$

(3) The problem of optimally choosing the *integration points* has been solved for the most important special cases.

– For a radius, e.g. $z_S = 0$, $z_E = 1$ (i.e., $If = \int_0^1 f(x)\,dx$) and all z_j's in (0, 1) (thus real), Wilf [24] (see also [7]) has given the nonlinear system of $2n+2$ equations

$$\sum_{l=0}^{n}\frac{\hat{a}_l}{1-z_l z_j} = \frac{1}{z_j}\operatorname{Log}\frac{1}{1-z_j}, \qquad j = 0,\ldots,n, \tag{2.11a}$$

$$\sum_{l=0}^{n}\frac{\hat{a}_l z_l}{(1-z_l z_j)^2} = \frac{1}{z_j(1-z_j)} - \frac{1}{z_j^2}\operatorname{Log}\frac{1}{1-z_j}, \qquad j = 0,\ldots,n, \tag{2.11b}$$

for the set of z_j's and $\hat{a}_j$'s minimizing $\|E\|$.

For given points, each of (2.11a) and (2.11b) is a system of $n+1$ *linear* equations that can be solved for the corresponding $\hat{a}_j$'s.

– The symmetric case of the diameter, $z_S = -1$, $z_E = 1$, all z_j's real, has been treated similarly by Engels and Eckardt (references in [9, p.168]); this yields a system similar to (2.11) [9, p.136], and for given points a linear system with same matrix as (2.11a).

Wilf [25, p.141] gave the inverse of the matrix by means of the cofactor formula; this led him to (2.5) in series form for the above cases. However, writing v_j as $z_j^n \ell(1/z_j)$, as Wilf does, is not necessarily a good idea for the practical application of the formula: at such values $1/z_j$ outside D, the evaluation of ℓ is often ill-conditioned and not even defined if $z_j = 0$.

Later Engels [8] also presented a recurrence method for solving (2.11a) for given real z_j's. He also made use of the determinant of the matrix but his method appears to be much more complicated than Wilf's solution.

3. An example: equidistant points on concentric circles

Let the points z_j be equally distributed on the circle of radius $0 < r < 1$, i.e., $z_j = re^{j2\pi/N}$, $j = 0, \ldots, N-1$, $z_j^N = r^N$. For finding the b_j's, note that $w_j = 1/\ell'(z_j)$ [13, p.243]. Here $\ell(z) = z^N - r^N$ and therefore $w_j = 1/(Nz_j^{N-1}) = z_j/(Nr^N)$. Moreover,

$$m(z) = z^N \overline{\ell\left(\frac{1}{\bar{z}}\right)} = 1 - r^N z^N$$

and $v_j = m(z_j) = 1 - r^{2N} = \text{const}$. Thus

$$b_j = v_j w_j = (1 - r^{2N}) \frac{z_j}{Nr^N}. \tag{3.1}$$

Inserting all this into (2.10) and taking into account that here $z_n \neq 0$ and thus (by (2.7)) $f^{\perp}(\infty) = 0$, we get

$$\sum_{j=0}^{N-1} \hat{a}_j f_j = (1 - r^{2N}) \sum_{l=0}^{N-1} \frac{1 - r^{2N}}{Nr^N} \frac{1}{\bar{z}_l} \frac{1}{(1/\bar{z}_l)^N - r^N} p_{N-1}\left(\frac{1}{\bar{z}_l}\right) \operatorname{Log} \frac{1 - \bar{z}_l z_S}{1 - \bar{z}_l z_E}$$

$$= \frac{1 - r^{2N}}{N} \sum_{l=0}^{N-1} \frac{1}{\bar{z}_l} p_{N-1}\left(\frac{1}{\bar{z}_l}\right) \operatorname{Log} \frac{1 - \bar{z}_l z_S}{1 - \bar{z}_l z_E}. \tag{3.2}$$

For the special case $z_S = 0$, (3.2) agrees with [10, formula (5.20)], up to a minus sign that appears to be missing there.

Remarks 3.1. (1) Instead of the classical Lagrange representation for $p_{N-1}(z)$,

$$p_{N-1}(z) = \frac{z^N - r^N}{Nr^N} \sum_{j=0}^{N-1} \frac{z_j}{z - z_j} f_j, \tag{3.3}$$

one should in general use the corresponding barycentric formula [13, p.245], [11, p.51]

$$p_{N-1}(z) = \sum_{j=0}^{N-1} \frac{z_j}{z - z_j} f_j \Big/ \sum_{j=0}^{N-1} \frac{z_j}{z - z_j}. \tag{3.4}$$

Indeed, as z comes very close to one of the z_j's, say z_k, the cancellation effects in $z^N - r^N$ and $z - z_k$ will be different, rendering (3.3) unstable.

(2) In view of (3.1), and since here the conjugate of any node point is also a node point, the barycentric formula for optimal *evaluation* of functions in H^2 [3] is given by

$$f^{\perp}(z) = \frac{1}{1 - z_i z} \sum_{j=0}^{N-1} \frac{z_j}{z - z_j} f_j \Big/ \sum_{j=0}^{N-1} \frac{z_j}{z - z_j} \frac{1}{1 - z_i z_j}, \tag{3.5}$$

where z_i can be anyone of the z_j's, say $z_i = 1$.

Like every barycentric formula, (3.4) and (3.5) are extremely stable in the vicinity of the interpolation points. Moreover, since all weights z_j have the same modulus, these formulae are also very stable with respect to large N [1,2] (as long as the problem is well-conditioned, which is not the case if one interpolates far outside the circle of radius r).

Computing every value of $p_{N-1}(z)$ requires $\mathcal{O}(N)$ operations, so that computing an integral as in (3.2) costs $\mathcal{O}(N^2)$ operations. If several integrals must be evaluated, it is therefore preferable from a complexity point of view to compute the $\hat{a}_j$'s as in (2.5),

$$\hat{a}_j = \frac{(1-r^{2N})^2}{N^2 r^{2N}} \sum_{l=0}^{N-1} \frac{1}{1/z_j - \bar{z}_l} \operatorname{Log} \frac{1-\bar{z}_l z_S}{1-\bar{z}_l z_E}, \tag{3.6}$$

and then $\Sigma_{j=0}^{N-1} \hat{a}_j f_j$ for every integral to be approximated.

4. Numerical examples

We have performed two kinds of tests for our formulae.

First, we have computed the real integral

$$\int_{-1}^{1} f(x)\,\mathrm{d}x$$

for functions $f(x)$ similar to those optimally evaluated in [3], that is,

(1) The two entire functions $\cos x$ (exact integral $2 \sin 1$) and e^{-3x^2} (exact integral $\sqrt{\frac{1}{3}\pi}\,\operatorname{erf}(x)$, where erf is the error function computed here with IMSL [26]).

(2) The function $1/(1+ax^2)$, which belongs to H^2 iff $|a|<1$, and whose exact integral is

$$\begin{cases} \dfrac{2}{\sqrt{a}} \arctan \sqrt{a}\,, & \text{if } a>0,\ a\neq 1, \\ \dfrac{1}{\sqrt{a}} \ln \left| \dfrac{1+\sqrt{a}}{1-\sqrt{a}} \right|, & \text{if } a<0. \end{cases}$$

(3) The functions $f_{\alpha\beta\gamma}(x) := (1+x)^{\alpha}(1-x)^{\beta} \log^{\gamma}(1-x)$, which belong to H^2 iff α and $\beta > -\frac{1}{2}$; $f_{\alpha\beta\gamma}$ is denoted by (α, β, γ) in the tables. Here the exact value has been computed with the subroutine DQDAWS of IMSL, an efficient method when α, β and γ are known.

As node points, we chose here

(1) Legendre points computed with the IMSL library in double precision;

(2) Chebyshev points of the first kind, which all lie inside $(-1, 1)$;

(3) Stenger's SINC points [22, p.226 with $p=2$],

$$x_j = \tanh jh, \quad h = \frac{\pi}{2\sqrt{N}}, \quad j = -N, \ldots, N, \quad n = 2N.$$

For this h, a rational approximant of Stenger's which converges exponentially toward $f(x)/(1-x^2)$ [22] is optimal (in Sard's sense) [3]; however, considerable numerical evidence in the latter work demonstrates that the optimal interpolant is better in practice.

As weights, we tried the optimal ones of (2.5) for the three sets of points, as well as the Gauss–Legendre weights for the Legendre points and the SINC weights $a_j = h/\cosh^2 jh$ (see [20] with $q = \mathrm{e}^h$, [23]) for the SINC points. Exponential convergence of the SINC quadrature is shown in [20,21].

Table 1
Errors with the optimal formula and 21 points

Points	Legendre		Chebyshev	SINC	
Weights	Polynomial $V=10^2, W=10^1$	Optimal $V=10^7, W=10^6$	Optimal $V=W=10^7$	SINC $V=W=10^4$	Optimal $V=10^4, W=10^5$
$\cos x$	0.0	$1.8\cdot10^{-7}$	$8.2\cdot10^{-8}$	$5.3\cdot10^{-5}$	$1.0\cdot10^{-5}$
$\exp\{-3x^2\}$	0.0	$3.0\cdot10^{-3}$	$1.1\cdot10^{-3}$	$1.4\cdot10^{-3}$	$1.5\cdot10^{-3}$
$(1+0.5\,x^2)^{-1}$	0.0	$5.3\cdot10^{-5}$	$2.0\cdot10^{-5}$	$2.5\cdot10^{-5}$	$5.7\cdot10^{-5}$
$(1-0.5\,x^2)^{-1}$	0.0	$6.2\cdot10^{-8}$	$2.1\cdot10^{-8}$	$2.3\cdot10^{-4}$	$6.8\cdot10^{-7}$
$(1-0.99\,x^2)^{-1}$	$7.4\cdot10^{-2}$	$1.5\cdot10^{-2}$	$7.8\cdot10^{-3}$	$1.1\cdot10^{-2}$	$6.0\cdot10^{-6}$
$(1+x^2)^{-1}$	0.0	$1.2\cdot10^{-3}$	$4.1\cdot10^{-4}$	$2.5\cdot10^{-4}$	$3.3\cdot10^{-4}$
$(1+2x^2)^{-1}$	$2.2\cdot10^{-12}$	$2.3\cdot10^{-2}$	$7.6\cdot10^{-3}$	$1.8\cdot10^{-3}$	$1.9\cdot10^{-3}$
$(1+25x^2)^{-1}$	$2.4\cdot10^{-4}$	$2.3\cdot10^{1}$	6.4	$1.1\cdot10^{-1}$	$1.1\cdot10^{-1}$
(3, 3, 0)	0.0	$5.0\cdot10^{-5}$	$2.1\cdot10^{-5}$	$4.2\cdot10^{-4}$	$5.0\cdot10^{-4}$
$(\frac{1}{2}, \frac{1}{2}, 0)$	$8.3\cdot10^{-5}$	$3.6\cdot10^{-5}$	$1.1\cdot10^{-5}$	$1.6\cdot10^{-6}$	$2.0\cdot10^{-6}$
$(\frac{1}{4}, \frac{1}{4}, 0)$	$2.5\cdot10^{-4}$	$1.4\cdot10^{-4}$	$5.2\cdot10^{-5}$	$8.2\cdot10^{-6}$	$1.2\cdot10^{-6}$
$(\frac{1}{4}, 0, 0)$	$1.1\cdot10^{-4}$	$6.0\cdot10^{-5}$	$2.2\cdot10^{-5}$	$7.1\cdot10^{-5}$	$4.6\cdot10^{-7}$
$(\frac{1}{4}, \frac{1}{4}, 1)$	$3.7\cdot10^{-4}$	$2.7\cdot10^{-4}$	$1.2\cdot10^{-4}$	$4.8\cdot10^{-5}$	$1.4\cdot10^{-6}$
$(\frac{1}{4}, 0, 1)$	$3.3\cdot10^{-3}$	$2.3\cdot10^{-3}$	$1.0\cdot10^{-3}$	$7.3\cdot10^{-4}$	$3.5\cdot10^{-5}$
$(-\frac{1}{4}, -\frac{1}{4}, 0)$	$7.2\cdot10^{-3}$	$5.7\cdot10^{-3}$	$3.1\cdot10^{-3}$	$1.5\cdot10^{-3}$	$2.4\cdot10^{-4}$
$(-\frac{1}{2}, -\frac{1}{2}, 0)$	$8.1\cdot10^{-2}$	$7.1\cdot10^{-2}$	$4.7\cdot10^{-2}$	$2.2\cdot10^{-2}$	$8.5\cdot10^{-3}$
$(-\frac{3}{4}, 0, 0)$	$7.3\cdot10^{-1}$	$6.9\cdot10^{-1}$	$5.6\cdot10^{-1}$	$3.5\cdot10^{-1}$	$2.4\cdot10^{-1}$

As noticed in [3], the difficulty with this optimal approximation of bounded functionals lies in the extreme difference in the orders of magnitude of the involved quantities. For optimal *evaluation*, the b_j's were the only problem. The difficulty is even accentuated here: in (2.5), the extremely different b_j's are multiplied by sums which, containing the b_j's, are themselves very different and, moreover, suffer large relative errors due to smearing [13]. As in [3], we have largely avoided the problem by computing the $\hat{a}_j$'s as well as the optimal approximation $\Sigma\hat{a}_j f_j$ with fourfold precision (REAL*16) on our VAX/VMS system. Nevertheless, since parts of the computations were done in double precision (unit round-off $\approx 10^{-16}$), errors smaller than $5\cdot10^{-14}$ are diplayed as 0.0 in the tables.

To measure the relative errors that have to be expected, we have recalled $V := \max|b_j|/\min|b_j|$ from [3], and displayed also $W := \max|\hat{a}_j|/\min|\hat{a}_j|$. As V was decisive for the instability due to smearing of the barycentric formula for evaluating $f^{\perp}$, W is decisive for the instability of the optimal integration formula.

Another way of avoiding the problem seems obvious: compute the weights $\hat{a}_j$ as in (2.2) numerically, which must be done only once for all functions to be integrated. For real z_j's, we have done it with the IMSL routines DQDAGS and DQDAG, which are respectively implementations of the routines QAGS and QAG of QUADPACK [16]. The latter are globally adaptive integrators which use a 21-point Gauss–Kronrod rule for estimating the integral over each subinterval. The results were disappointing: those integrators require a very large computing time to give $\hat{a}_j$'s that are no better in practice than those computed with our formula.

Table 2
Same errors as in Table 1, but with 101 points

Points	Legendre	SINC	
Weights	Polynomial $V=10^3$, $W=10^2$	SINC $V=10^{11}$, $W=10^{10}$	Optimal $V=W=10^{11}$
$\cos x$	0.0	$3.9\cdot10^{-10}$	$1.5\cdot10^{-13}$
$\exp\{-3x^2\}$	0.0	$9.2\cdot10^{-10}$	$1.3\cdot10^{-9}$
$(1+0.5\,x^2)^{-1}$	0.0	$4.6\cdot10^{-10}$	$2.3\cdot10^{-11}$
$(1-0.5\,x^2)^{-1}$	0.0	$1.4\cdot10^{-9}$	0.0
$(1-0.99\,x^2)^{-1}$	$8.8\cdot10^{-9}$	$7.2\cdot10^{-8}$	$4.7\cdot10^{-13}$
$(1+x^2)^{-1}$	0.0	$1.1\cdot10^{-9}$	$1.5\cdot10^{-9}$
$(1+2x^2)^{-1}$	0.0	$1.2\cdot10^{-7}$	$1.2\cdot10^{-7}$
$(1+25x^2)^{-1}$	0.0	$4.7\cdot10^{-3}$	$4.7\cdot10^{-3}$
(3, 3, 0)	0.0	$2.0\cdot10^{-12}$	$2.6\cdot10^{-11}$
$(\frac{1}{2}, \frac{1}{2}, 0)$	$7.9\cdot10^{-7}$	0.0	0.0
$(\frac{1}{4}, \frac{1}{4}, 0)$	$5.2\cdot10^{-6}$	$3.0\cdot10^{-12}$	$9.2\cdot10^{-14}$
$(\frac{1}{4}, 0, 0)$	$2.2\cdot10^{-6}$	$4.3\cdot10^{-10}$	0.0
$(\frac{1}{4}, \frac{1}{4}, 1)$	$1.6\cdot10^{-5}$	$3.2\cdot10^{-11}$	$9.4\cdot10^{-13}$
$(\frac{1}{4}, 0, 1)$	$1.5\cdot10^{-4}$	$9.7\cdot10^{-9}$	$9.5\cdot10^{-11}$
$(-\frac{1}{4}, -\frac{1}{4}, 0)$	$7.0\cdot10^{-4}$	$1.8\cdot10^{-7}$	$1.6\cdot10^{-8}$
$(-\frac{1}{2}, -\frac{1}{2}, 0)$	$1.7\cdot10^{-2}$	$5.4\cdot10^{-5}$	$1.4\cdot10^{-5}$
$(-\frac{3}{4}, 0, 0)$	$3.4\cdot10^{-1}$	$1.7\cdot10^{-2}$	$9.8\cdot10^{-3}$

Table 3
Errors of integration with formula (3.2) or (3.6) for (4.1)

N	Error	D
10	$1.7\cdot10^{-2}$	
20	$1.4\cdot10^{-2}$	0.816
40	$5.5\cdot10^{-3}$	0.384
80	$2.2\cdot10^{-3}$	0.397
160	$8.8\cdot10^{-4}$	0.407
320	$3.7\cdot10^{-4}$	0.413
640	$1.5\cdot10^{-4}$	0.417
1280	$6.4\cdot10^{-5}$	0.419
2560	$2.7\cdot10^{-5}$	0.419
5120	$1.1\cdot10^{-5}$	0.420
10240	$4.7\cdot10^{-6}$	0.420

Now to the numbers: for the functions which do not show singularities at the endpoints, and with 21 integration points (see Table 1), Gauss–Legendre integration is clearly superior to the optimal formula. The latter suffers much more when a pole comes close to the interval along the imaginary axis and $f \notin H^2$, but less when it approaches the interval along the real axis. On the other hand, the optimal formula is (slightly) better for all functions that are not differentiable at the endpoints of the interval of integration. The performance of the SINC formula lies somewhere in-between.

Both the optimal and SINC formulae display their full power only for larger numbers of points. With $n = 100$ (101 points, see Table 2) and for $f_{\alpha,\beta,\gamma}$ with $\alpha, \beta < 1$, the optimal formula has at least twice as many correct digits as Legendre's formula; and note, in addition, that (like the SINC formula) it does not require any knowledge of the singularities at the endpoints. For the singular functions in H^2 we have integrated, it is even better than the SINC formula. The latter is itself slightly better for meromorphic functions with poles approaching the interval $[-1, 1]$ along the imaginary axis (see $f = 1/(1+ax^2)$, $a > 0$), but much worse when poles come close on the real axis ($a < 0$).

For $n = 100$ and Chebyshev or Legendre points, W is too big (10^{29} for Legendre points) for a practical use of the coefficients (and nothing much can be done, from the computational point of view, about this problem).

In a second series of experiments, we have applied formulae (3.6) and (3.2) to the computation of integrals from values at equidistant points on circles of radius $r < 1$. Although the $\hat{a}_j$'s are of similar sizes (and, indeed, double precision (COMPLEX*16 on VAXes) is

sufficient here), the results were somewhat disappointing. The reason lies in the ill-conditioning of the continuation processes: to be interesting as a practical alternative to formulae based on polynomial interpolation, the formula must be able to integrate up to the boundary where the singularities can lie. Using $f^{\perp}$ on the path of integration Γ corresponds to continuation from the circle of radius r onto Γ, and such a continuation process may be ill-conditioned in the exterior of the circle [10, p.131]. In order to get good results close to the extremities of the interval, one must therefore choose r close enough to 1. Another reason for this is the fact that for fixed r not close to 1, (3.6) and (3.2) are unstable with respect to increasing N: in (3.6), r^{2N} becomes very small, even smaller than machine precision, and so does the sum, which gets therefore very unprecise due to smearing; in (3.2), $1/\bar{z}_l$ is far from the circle of radius r on which the interpolation points lie, and so $p_{N-1}(1/\bar{z}_l)$ is an even more distant continuation than before, which makes the formula unstable.

This is not to say that (3.6) and (3.2) are always inadequate formulae: for $f = \cos x$, $r = 0.8$ and $n = 51$, $\int_{-1}^{1} f(x)\,dx$ is approximated with an error of 10^{-8}. This, however, is not of much interest, since integrals of such entire functions are better computed by integrating $p_{N-1}(z)$ (as in Gauss–Legendre integration). For functions like $f_{\alpha\beta\gamma}$, $\alpha < 1$, $\beta < 1$, a direct application of the formulae with z_S and z_E on ∂D never resulted in a *fast* converging approximation. We have, however, obtained *stable* results when choosing r such that the unstable denominator of the factor of $\hat{a}_j$ in (3.6) is 1, i.e., $r = N^{-1/N}$. For this r, there does not seem to be a significant difference between (3.2) and (3.6). Table 3 displays the results of the approximation of

$$\int_{i}^{1} 2.5\, z(1-z^2)^{1/4}\,dz = 2^{5/4}, \tag{4.1}$$

for different values of N, as well as the quotient

$$D := \frac{|\hat{Q}_N - If|}{|\hat{Q}_{N/2} - If|}.$$

The latter indicates linear convergence. The efficiency of the method can therefore certainly be improved by applying a convergence acceleration algorithm such as Aitken's extrapolation to the sequence $\{\hat{Q}_N\}$, $N = 2^l$, $l = 1, 2, \ldots$.

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