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A QUADRATURE FORMULA OF RATIONAL TYPE FOR INTEGRANDS WITH ONE ENDPOINT SINGULARITY*

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Abstract. The paper deals with the construction of an efficient quadrature formula of rational type to evaluate the integral of functions which are analytic in the interval of integration, except at the endpoints. Basically our approach consists in introducing a change of variable u_q into the integral $I(f,h,r)$

$$I(f,h,r) = \int_{-(1-h)}^{(1-h)r} f(x)dx = \int_{\mu_q}^{\rho_q} F(u_q(x))u_q'(x)dx = I(f,q,h,r),$$

where $f \in H^p$ and $u_q(x) = w_a^q(x) = w_a(w_a^{q-1}(x))$, $w_a(z) = (z-a)/(1-az)$, $0 < a < 1$.

We evaluate the new form $I(f,q,h,r)$ by a quadrature approximant $Q_n(f) = Q(f,n,q,h,r,a)$ which is based on Hermite interpolation by means of rational functions. The nodes of $Q_n(f)$ are derived from a fundamental result proved by Ganelius [Anal. Math., 5 (1979), pp. 19-33] in connection with the problem of approximating the function $f_\alpha(x) = x^\alpha$, $0 \leq x \leq 1$, by means of rational functions.

We find (a_n) such that $Q_n(f) \to I(f,r) = I(f,0,r)$ as $h_n = \epsilon(1-a_n) \to 0$, for all $f \in H^p$. For functions in H^p, $1 < p < \infty$, which satisfy an integral Lipschitz condition of order β, the following estimate is deduced

$$E_n(f) = |I(f,r) - Q_n(f)| \leq M\sqrt{n}\,\exp\left(-\pi\sqrt{n\beta(2q-1-1/p)}\right).$$

If $\beta = q = 1$ then the upper bound for $E_n(f)$ is that which is exact for the optimal quadrature error in H^p, $p > 1$.

We report some numerical examples to illustrate the behavior of the method for several values of the parameters.

Key words. interpolatory quadrature formulas, rational approximation, order of convergence, boundary singularities.

AMS subject classifications. 41A25, 41A55, 65D30, 65D32.

1. Introduction. In applications the solution of a problem often involves the numerical integration of functions with singularities. The traditional approach in this subject has been based on the use of Gauss quadrature formulas of polynomial type, though more recently some rational versions have also been considered. The latter concerns classes of Gauss quadrature formulas which require the largest degree of exactness for simple rational functions $1/(x-p_i)$. These rational rules are connected with multipoint Padé approximation of Stieltjes functions [12, 13, 14, 15, 16, 17, 28], and with the evaluation of integrals whose integrand has poles close to the integration interval [7, 8, 9, 10].

Another relevant area is that concerned with the use of functions $u(x)$ which transform the integration interval, and increase the efficiency of the numerical procedures. These transformations modify the distribution of the quadrature nodes $\{x_k\}$ in such a way that the new ones, namely $\{u(x_k)\}$, exhibit a higher concentration near those endpoints where the singularities should be located. As far as we know the strategy of fitting a change of variable into an integration rule to increase the efficiency of a numerical procedure, have only been investigated in the polynomial context [1, 20, 21, 22, 23, 24, 25].

When compared to polynomials, rational functions are now considered a nicer class to approximate functions with a variety of singularities. This conclusion has a starting point in 1964 when Newman [26] proved that the function $|x|$, $-1 \leq x \leq 1$, can be uniformly approximated by rational functions much faster than by polynomials. At present, there are additional reasons to assert that the following formulation

$$I(f) = \int_a^b f(x)dx \approx Q_n(f) = \int_a^b R(x)dx, \tag{1.1}$$

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where R is a convenient rational function, is expedient when f is an analytic function with a finite number of singularities on $[a,b]$, or with some poles close to $[a,b]$. A basic argument in favour of the latter is that the term fq in the error $|f-p/q| = |fq-p|/q$, can be better approximated than f by polynomials p, if q annihilates the poles of f closer to $[a,b]$.

The class of functions to be integrated are those defined on the interval $(-1,r]$, $0<r<1$, which admit analytic continuation to the space H^p. Rational approximation of functions in a Hardy space was earlier investigated by Gonchar in [11] as a continuation to Newman's research [26].

In this paper we deal with a method of numerical integration which works, theoretically speaking, on the Hardy space H^p and is based on interpolation by means of rational functions. For each $n \in \mathbb{N}$ this formula has the form given below

$$I_r(f) = \int_{-1}^{r} f(x)dx = \sum_{k=1}^{n-b} A_{n,k} f(z_{n,k}) + \sum_{k=1}^{b} B_{n,k} f^{(k)}(r) + E_{n,r}(f), \tag{1.2}$$

where $0<r<1$, $f \in H^p$, $b=b_n \in \mathbb{N}$, $-1<z_{n,k}<r$, $A_{n,k}, B_{n,j} \in R$, $k=1,...,n-b$, $j=1,...,b$; $f^{(m)}$ is the m-th derivative of f, and $E_{n,r}(f)$ is the quadrature error.

Formula (1.2) is a special case of those studied by Bojanov [4], Newman [27], Andersson [2], Andersson & Bojanov [3]. To understand why rational functions play a role in this theory it is sufficient to consider the general formulation given below

$$\int_t^s f(x)d\mu(x) \approx Q_n(f) = \int_{|z|=1} R_n(z)f(z)dz = \sum_{i=1}^{s}\sum_{j=0}^{m(i)} a_{i,j} f^{(j)}(z_i), \tag{1.3}$$

where $-1 \le t < s \le 1$, μ is a finite and positive measure on $(-1,1)$, R_n is some rational function of order n with poles z_i, $\sum_{i=1}^{s} m(i) = n$, $|z_i|<1$, and $R_n(\infty)=0$. It is well-known that Q_n is a continuous linear functional on H^p, and that Cauchy's integral formula can be applied to yield the finite sum on the right term of (1.3). The exact bound $\exp(-\pi\sqrt{n/p'})$, $1/p+1/p'=1$, for the optimal error $\inf_{Q_n} \|I_1 - Q_n\|$ in H^p, $p>1$, is found in [2, 3].

The main purpose of this paper is to present a new approach to construct an efficient rational quadrature formula to integrate analytic functions with a singularity at only one endpoint of the interval of integration. More precisely, we consider the problem of defining a transformation $u_q(x)$, $q \in \mathbb{N}$, to be introduced into the integral $I_r(f)$. To evaluate the new form of the integral we select the points $z_{n,k}$ in formula (1.2) from a result by Ganelius (Lemma 2.1), and the coefficients $A_{n,k}$, $B_{n,k}$ according to an exactness condition based on interpolation by means of rational functions. Then we prove that the quadrature error is asymptotically of the order $\exp(-c\sqrt{n})$, for functions in H^p which satisfy an integral Lipschitz condition. Besides, we expect that the numerical behavior of such a procedure compares favorably with some other remarkable quadrature rules (cf. [20, 23]).

The paper is organized as follows. Section 2 is devoted to define nodes and coefficients for integration formulas of the form (1.2). Section 3 deals with the construction of a change of variable which we fit into the integral $\int_{-(1-h)}^{(1-h)r} f(x)dx$, to reach an order of convergence which is optimal in n according to the theoretical results obtained by Andersson [2]. Finally, Section 4 contains some remarks and numerical examples to show the power of the method.

2. Construction of the quadrature formula.

The next result can be derived from [6] and is basic for our approach.

LEMMA 2.1. *For $\theta > 0$, n positive integer there exists a constant C_θ which only depends on θ, such that*

$$\max_{x\in[0,1]} x^\theta \prod_{k=1}^{n} \left| \frac{x - y_{\theta,n,k}}{x + y_{\theta,n,k}} \right| \le C_\theta \exp(-\pi\sqrt{n\theta}), \tag{2.1}$$

where $y_{\theta,n,k} = \phi(k)/\phi(n - b_{n,\theta})$, $b_{n,\theta} = [48\pi\sqrt{3\theta n/2}] + 1$ ($[X]$ denotes the integer part of X), $n > 34110\theta$, $k = 0, 1, ..., n - b_{n,\theta}$, $\phi(u) = \exp(\pi\sqrt{u/\theta})$; and $y_{\theta,n,k} = 1$ for $k = n - b_{n,\theta} + 1, ..., n$.

Lemma 2.1 is based on the strong connection between rational approximation and some equilibrium problems. This result was used by Ganelius to obtain the exact order of convergence for the best uniform approximation of x^α, $0 \le x \le 1$, by means of rational functions of orden n. Next we describe some of the most relevant aspects of Ganelius' technique to obtain estimate (2.1).

Given the Green function of the right half plane Ω, namely

$$g(z, \omega) = \log \left| \frac{z + \omega}{z - \omega} \right|,$$

singular at ω, $\Re\omega < 0$, consider the problem of estimating from below the potential of the positive measure ν on $[0, 1]$ defined by $d\nu(y) = a\log^+(\omega y)dy/y + b\delta(y - 1)$, where $\omega > 1$, $a = 2\theta/\pi^2$, δ is the Dirac measure concentrated in $x = 0$, $||\nu|| = n$ and b is some positive number.

By direct calculations it is deduced in [6] that the condition $\log\omega = \pi\sqrt{(n - b)/\theta}$ must be assumed, and for all $n \ge b$

$$\int_0^1 g(x, y)d\nu(y) + \theta\log\frac{1}{x} \ge$$

$$\pi\sqrt{\theta(n - b)} + \frac{b}{4}x(1 + 2(1 - x))^{-2} - 3\theta - 12\pi x\sqrt{\theta n/2}(1 + 2(1 - x))^{-1}.$$

The following step is to take $b = b_{n,\theta}$ as that given in Lemma 2.1, to find

$$\int_0^1 g(x, y)d\nu(y) + \theta\log\frac{1}{x} \ge \pi\sqrt{\theta n} - 192\pi^2\theta. \tag{2.2}$$

Notice that $n > 34110\theta$ implies $n \ge b_{n,\theta}$.

At this point the nature of the number $b = b_{n,\theta}$ and the role played by it in this theory should be clear enough to the reader. Of course, much more details can be seen in the paper of Ganelius.

After obtaining (2.2) the proof of lemma 2.1 is practically concluded. To derive the inequality (2.1) from (2.2), it only remains to replace the distribution ν by a discrete measure ν_n. Despite all the technical difficulties of this proof, the suitable location of the mass-points $y_{\theta,n,k}$, where the discrete distribution ν_n is supported, doesn't seem very hard to obtain. The importance of the points $y_{\theta,n,k}$ for our work, comes from the fact that the nodes $z_{n,k}$ in (1.2) will be expressed in terms of the former.

Andersson [2] applied Lemma 2.1 to find the exact rate of convergence of the optimal quadrature error in Hardy spaces. We also applied this result in Section 3 to obtain an upper

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bound for the quadrature error $E_{n,r}(f)$ generated by formula (1.2) after introducing a change of variable (see also [18]). The notation in Lemma 2.1 will be kept in the rest of the article.

The proof of the following result is straightforward.

LEMMA 2.2. *Let h, δ, γ, ρ and μ be real numbers such that*

$$0 < h < 1, \quad -1 < \delta < \mu < \rho < \gamma < 1.$$

Let $\alpha = (\gamma-\rho)/(\rho-\delta)$ and Γ be the circle with center at $C = (\gamma+\delta)/2$ and radius $K = (\gamma-\delta)/2$. In addition, let consider the following rational functions

$$\xi(z) = \alpha\frac{z-\delta}{\gamma-z}, \quad \Phi_n(x) = \frac{P_n(x)}{P_n(-x)}, \tag{2.3}$$

where P_n is given by

$$P_n(x) = \prod_{k=1}^{n}(t_{n,k}-x),$$

with $0 < t_{n,k} \leq 1$, $k = 1, \ldots, n$, $n \in \mathbb{N}$.
Then, Φ_n and ξ satisfy the following properties

1. $\Gamma = \{z/\ \Re\xi(z) = 0\}$.
2. $\xi(\rho) = 1$.
3. $z \to \xi(z)$ *is an increasing function on* $R\backslash\{\gamma\}$.
4. $0 < \xi(z) \leq 1$, $z \in [\mu,\rho]$.
5. *If* $s \in \Gamma$ *then* $|\Phi_n(\xi(z))| = 1$.

LEMMA 2.3. *Let Φ_n and ξ be the rational functions defined in Lemma 2.2. Let R_n be the rational function given by the following equation*

$$R_n(z) = \frac{1}{2\pi i}\int_{\Gamma}\frac{\Phi_n(\xi(s)) - \Phi_n(\xi(z))}{(s-z)\Phi_n(\xi(s))}F(s)ds, \quad z \in [\mu,\rho], \tag{2.4}$$

where F is an analytic function in the unit disk $|z| < 1$.

If $W(x)$ is a non-negative and continuous function on $[\delta,\gamma]$ then the rational function R_n interpolates to F at the zeros of $\Phi_n(\xi(z))$, and the quadrature formula

$$I_{\rho,\mu}(F) = \int_{\mu}^{\rho} F(x)W(x)dx \approx Q_{\rho,\mu,n}(F) = \int_{\mu}^{\rho} R_n(x)W(x)dx, \tag{2.5}$$

is of the form (1.3) and it integrates exactly any rational function $g_n(z)$,

$$g_n(z) = \frac{p_{n-1}(z)}{P_n(-\xi(z))},$$

where p_{n-1} is a polynomial of degree at most $n-1$.

Proof. We use Fubini's theorem to obtain

$$\int_{\mu}^{\rho} R_n(x)W(x)dx = \frac{1}{2\pi i}\int_{\Gamma} F(z)\frac{q_n(z)}{P_n(\xi(z))}dz, \tag{2.6}$$

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where $q_n(z)$ is the following polynomial of degree at most $n-1$

$$q_n(z) = \int_\mu^\rho \frac{P_n(\xi(x))P_n(-\xi(z)) - P_n(\xi(z))P_n(-\xi(x))}{P_n(-\xi(x))(x-z)} W(x)dx.$$

To deduce the expression of the approximant in (1.3), we consider the expansion of $q_n(z)/P_n(\xi(z))$ in a sum of simple rational functions to which we apply Cauchy's integral theorem.

The nodes $z_{n,k}$ of formula (2.5) are the zeros of $P_n(\xi(z))$, and they can be easily calculated as follows

$$z_{n,k} = \frac{\gamma\, t_{n,k} + \alpha\, \delta}{t_{n,k} + \alpha}, \quad k = 1, ..., n. \tag{2.7}$$

Likewise, the zeros $p_{n,k}$ of $P_n(-\xi(z))$ are the poles of $\Phi_n(\xi(z))$. They appear in the statement of the exactness condition for formula (2.5), and their formulation can be deduced from the following representation of $\Phi_n(\xi(z))$

$$\Phi_n(\xi(z)) = \prod_{k=1}^{n} \left(\frac{t_{n,k} + \alpha}{\gamma\, t_{n,k} - \alpha\, \gamma} \right) \prod_{k=1}^{n} \left(\frac{z_{n,k} - z}{\dfrac{z(\alpha - t_{n,k})}{\gamma t_{n,k} - \alpha\delta} + 1} \right). \tag{2.8}$$

The expression of the quadrature error of formula (2.5) is the following

$$E_n(F) = \int_\mu^\rho \Phi_n(\xi(x)) \left(\frac{1}{2\pi i} \int_\Gamma \frac{P_n(-\xi(s))F(s)}{(s-x)P_n(\xi(s))} ds \right) W(x)dx. \tag{2.9}$$

The exactness condition given in the lemma follows from (2.9). In effect, if we put $F(z) = p_{n-1}(z)/P_n(-\xi(z))$ in (2.9), where p_{n-1} is a polynomial of degree at most $n-1$, the integrand of the integral between parenthesis can be written as a sum of terms of the form

$$\frac{\lambda_k}{(s-z)(s-z_{n,k})^m}, \quad m = 1, ..., n,$$

whose corresponding integrals can be evaluated by means of residues to obtain that all of them are zero. $\square$

The inequality $\alpha > 0$ makes possible that $\alpha = t_{n,k}$ for some values of n and k. It is the reason for which formula (2.8) can be considered as a suitable manner of representing the poles of $\Phi_n(\xi(z))$. In case of $p_{n,k} = \infty$ it means that quadrature formula (2.5) is exact for some polynomials as well.

We observe that quadrature formula (2.5) depends on the parameters n, δ, γ, μ and ρ. Moreover, if we put $t_{n,k} = y_{\theta,n,k}$ for some suitable $\theta > 0$, then we obtain a quadrature approximant of the same form as that in (1.2) with $b = b_{n,\theta}$.

3. An upper bound for the quadrature error. In this section we construct a special analytic change of variable u_q, $q \in \mathbb{N}$, to be introduced into the integral

$$I_{r,h}(f) = \frac{1}{(1-h)} \int_{-(1-h)}^{(1-h)r} f(x)dx,$$

where $0 < h < 1$, $0 < r < 1-h$, $f \in H^p$, $p \ge 1$.

Next we evaluate $I_{r,h}(f) = I_{\rho_q,\mu_q}(F_{q,h})$, with $F_{q,h}(x) = f(u_q(x))$, $W(x) = u_q'(x)$, and $u_q([\rho_q,\mu_q]) = [-(1-h),(1-h)r]$, using the corresponding quadrature approximant (2.5) to approximate $I_{r,h}$ with an error of order $\exp(-c\sqrt{\theta n})$ (Lemma 3.7). The last step of the procedure consists in evaluating $I_{r,0}$ by using the same approximant with $h \to 0$.

Let us consider the rational functions

$$w_a(z) = \frac{z-a}{1-az}.$$

For $a \in (-1,1)$ the function w_a is a conformal mapping from the unit disk onto itself which satisfies $w_a(-1) = -1$ and $w_a(1) = 1$. Here we will only consider the case $0 \leq a < 1$.

To construct u_q we need the following sequences.

DEFINITION 3.1. *For every a and t, $0 \leq a < 1$, $-1 < t < 1$, we define the sequence*

$$A_{q+1}(t) = \frac{a + A_q(t)}{1 + aA_q(t)}, \quad q = 0, 1, \ldots \quad A_0(t) = t. \tag{3.1}$$

In particular $A_q = A_q(0)$, $q \in \mathbb{N}$.

Let E be a non empty set and $g : E \to E$ be a function on E. As usual we define $g^q(x) = g(g^{q-1}(x))$, $q \geq 1$, and $g^0(x) = x$, $x \in E$.

LEMMA 3.2. *For every $a > 0$, $q \geq 0$ and $0 < h < 1$, we have the following relations*

$$w_{A_q}(x) = w_a^q(x), \tag{3.2}$$

$$t = w_{A_q}(A_q(t)). \tag{3.3}$$

Proof. Relation (3.2) is trivially true for $q = 1$. It remains to show that the assertion relative to the integer q implies the assertion relative to the integer $q+1$. It means that we are assuming that $w_a(w_{A_q}(x)) = w_a^{q+1}(x)$.

Therefore, we obtain

$$w_a(w_{A_q}(x)) = \left(\frac{x(1+aA_q) - (a+A_q)}{(1+aA_q) - x(a+A_q)}\right) = \left(\frac{x - A_{q+1}}{1 - xA_{q+1}}\right) = w_{A_{q+1}}(x).$$

Equation (3.3) is directly obtained from the definition of $A_q(t)$. $\square$

LEMMA 3.3. *Let t be a fixed number in $(-1,1)$. The following properties take place.*

1. $A_q(t_2) > A_q(t_1)$ *provided that* $1 > t_2 > t_1 > -1$, $q = 0, 1, 2, \ldots$
2. $1 > A_{q+1}(t) \geq A_q(t) \geq t, \quad q \in \mathbb{N}$,

3. $\lim_{q\to\infty} A_q(t) = 1$, $0 < a < 1$,
4. $\lim_{a\to 1} A_q(t) = 1, \;\; q \geq 1$.
5. $1 - A_q(t) = \dfrac{(1-a)^q(1-t)}{(1+aA_{q-1}(t))\cdots(1+aA_1(t))(1+at)}$, $q \geq 1$.
6. $A_q(t_2) - A_q(t_1) = \dfrac{(1-a^2)^q(t_2-t_1)}{(1+aA_{q-1}(t_2))(1+aA_{q-1}(t_1))\cdots(1+at_2)(1+at_1)}$, *where* $t_1, t_2 \in (-1,1)$ *and* $q \geq 1$.

Proof. It is trivial that property 1 is true for $q = 0$. For $q+1$ we use that $t \to (a+t)/(1+at)$ is a non decreasing function with respect to t as well as the induction hypothesis on q. The existence of the limit in property 3 is guaranteed by property 2, and its value is obtained by taking limits on both sides of equation (3.1). After assuming that property 5 is true for q we multiply both sides by the factor $(1-a)/(1+aA_q(t))$ to obtain the relation for $q+1$.

Property 6 follows from the following equality (see (3.1))

$$A_{q+1}(t_2) - A_{q+1}(t_1) = \frac{(1-a^2)(A_q(t_2)-A_q(t_1))}{(1+aA_q(t_1))(1+aA_q(t_2))}. \tag{3.4}$$

Both properties 2 and 4 can also be easily proven by induction on q. The proof of Lemma 3.3 is complete. ☐

From now on we will assume that $h = \epsilon(1-a)$ with $0 < \epsilon \leq 1$, $a \in (0,1)$.

LEMMA 3.4. *Let* r, h *and* a *be real numbers such that* $0 < r < 1-h$, $0 < a < 1$. *Put* $\delta_q = A_q(-1+h/2)$, $\gamma_q = A_q((1-h)(r+1)/2)$, $\mu_q = A_q(-1+h)$ *and* $\rho_q = A_q(r(1-h))$, $q \in \mathbb{N}$. *Then*

$$-1 < \delta_q < \mu_q < \rho_q < \gamma_q < 1, \tag{3.5}$$

$$\gamma_q - \mu_q \asymp \frac{(1-a)^{q-1}}{2^{q-2}\epsilon}, \;\; q \geq 1, \;\; a \to 1, \tag{3.6}$$

$$\gamma_q - \rho_q \asymp \frac{(1-a)^q(1-r)}{2^{q-2}(r+1)(r+3)}, \;\; q \geq 1, \;\; a \to 1, \tag{3.7}$$

$$\rho_q - \delta_q \asymp \frac{(1-a)^{q-1}}{2^{q-1}\epsilon}, \;\; q \geq 1, \;\; a \to 1, \tag{3.8}$$

$$\mu_q - \delta_q \asymp \frac{(1-a)^{q-1}}{2^{q-2}\epsilon}, \;\; q \geq 1, \;\; a \to 1. \tag{3.9}$$

Proof. We use property 1 and 2 of Lemma 3.3 to obtain (3.5).

Let $p \geq 1$. From the definition of $A_q(t)$ we get the expression

$$1 + aA_0(-1+h) = (1-a)(1+\epsilon),$$

from which we obtain the following formula

$$1 + aA_q(-1+h) = \frac{(1-a)^q + \epsilon(\nu(a) + a\sigma(a))}{(1-a)^{q-1} + \epsilon\,\nu(a)}, \tag{3.10}$$

where $\lim_{a\to 1}\sigma(a) = \lim_{a\to 1}\nu(a) = 2^{q-1}$, $\sigma(a)+\nu(a) = (a+1)^q$ and $\sigma(a)-\nu(a) = (1-a)^q$, $q \geq 1$. From relation (3.10) we deduce that $1 + aA_q(-1+h) \to 2$, $a \to 1$, for $q \geq 1$.

A similar deduction is made to obtain that $1 + aA_q(-1+h/2) \to 2$, $a \to 1$, $q \geq 1$.

On the other hand, $1 + aA_0(1-h)(r+1)/2) = 1 + a(1-h)(r+1)/2$, and for $p \geq 1$ we have $1 + aA_q((1-h)(r+1)/2) \to 2$, as $a \to 1$. Similarly, we easily obtain that $1 + A_0((1-h)r) = 1 + a(1-h)r$, and $1 + aA_q((1-h)r) \to 2$ as $a \to 1$, $q \geq 1$.

Now we apply property 6 of Lemma 3.3 to all of the differences $\gamma_q - \rho_q$, $\gamma_q - \mu_q$, $\rho_q - \delta_q$ and $\mu_q - \delta_q$ to finish the proof of Lemma 3.4. □

Below we construct a suitable interval transformation to be coupled with the quadrature formula (2.5). We start considering the substitution $w_a(x)$

$$\int_{-1+h}^{(1-h)r} f(x)dx = \int_{\mu_1}^{\rho_1} f(w_a(x))[w_a(x)]'dx. \tag{3.11}$$

Next, we give an extension of formula (3.11) in order to put the parameter q into the integral.

LEMMA 3.5. *The following equality takes place for* $q \in \mathbb{N}$*,* $a, h \in (0,1)$

$$\int_{-1+h}^{(1-h)r} f(x)dx = (1 - A_q^2)\int_{\mu_q}^{\rho_q} f(w_{A_q}(x))\frac{dx}{(1-xA_q)^2}. \tag{3.12}$$

Proof. Equation (3.12) is proved by induction on q using Lemma 3.2 and the definition of both sequences (ρ_q) and (μ_q). □

Equality (3.12) can be seen as a consequence of applying q times the change of variable (3.11) to the integral in the left hand side of (3.12).

The approximation formula which is given in (3.13) is the result of coupling the approximant $Q_{r,h,n}(f)$ in (2.5) by putting $\rho = \rho_q$, $\mu = \mu_q$, $\delta = \delta_q$ and $\gamma = \gamma_q$ with the change of variable in (3.12). The final version of our quadrature formula is

$$\int_{-1}^{r} f(x)dx \approx \int_{\mu_q}^{\rho_q} F_{h,q,a}(x)W_{h,q,a}(x)dx = Q_{r,h,n,q,a}(f) + E_{r,h,n,q,a}(f), \tag{3.13}$$

where

$$F_{h,q,a}(x) = f(w_{A_q}(x)), \tag{3.14}$$

$$Q_{r,h,n,q,a}(f) = \frac{1}{(1-h)}Q_{\rho_q,\mu_q,n}(F_{h,q,a}), \tag{3.15}$$

$$E_{r,h,n,q,a}(f) = E_n(F_{h,q,a}), \tag{3.16}$$

where $E_n(\cdot)$ is the quadrature error whose expression is given in (2.9), and

$$W_{h,q,a}(x) = \frac{(1-A_q^2)}{(1-h)(1-xA_q)^2}. \tag{3.17}$$

Equations (3.11–3.13) comprise the process of constructing the substitution $u_q(x) = w_{A_q}(x)$ which we will introduce into the integral $I_{r,h}(f)$. The factor $(1-h)^{-1}$ in (3.15) and (3.17) is given in connection with the integral modulus of continuity which is used below in the analysis of error (see Definition 3.8).

Property 3 of Lemma 3.3 and (3.12) suggest that the effect which the parameter a produces in formula (3.13) as $a \to 1$, should be the same as that produced by q, as $q \to \infty$.

The following lemma can be deduced from the theory in Newman [26].

LEMMA 3.6. *For $0 < \rho < 1$ we have the estimate*

$$\frac{\rho}{\pi}\int_{-\pi}^{\pi}\frac{dt}{|\rho+e^{i\,t}|} \le \log\left(\frac{1+\rho}{1-\rho}\right).$$

Let $R_n = R_{r,h,n,q,a}$ be the rational function which produces the quadrature approximation in (3.13). It means that R_n is the rational function associated with $F_{h,q,a}$ according to the procedure given by (2.5). The weight function given by (3.17) corresponds to the statement of Lemma 2.3, and will play a relevant role in applying Lemma 2.1 to our approach.

Though we are mainly interested in evaluating the integral $\int_{-1}^{r} f(x)dx$, $f \in H^p$, $1 \le p < \infty$, we need the following result.

LEMMA 3.7. *Let q be a positive integer. Let $f \in H^p$, $p \ge 1$ and $r \in (0,1)$. Let $Q_n(f) = Q_{r,h,n,q,a}(f)$ be the quadrature approximant of formula (3.13) with nodes (2.7) for which the points $t_{n,k}$ are selected as those given by Lemma 2.1. For n sufficiently large, $0 < a < 1$, $\theta > 0$, $\eta \ge 0$, $q \in N$ and $r < 1-h$ the following estimate holds.*

$$|I_{r,h}(f) - Q_n(f)| \le \frac{M_0}{(1-a)^{\eta}}\log\left(\frac{1}{1-a}\right)\,\exp(-\pi\sqrt{n\theta}), \tag{3.18}$$

where the positive constant M_0 depends neither on n nor a, $h = \epsilon(1-a)$ and $\theta = \eta + 2q - 1 - 1/p$.

Proof. Let $F_{q,a}$ be the function given by (3.14). We also assume that $W_{q,a}$ is the weight function defined in (3.17) and that R_n is the rational function given by (2.4) with respect to the points $y_{q,n,k}$, $\rho = \rho_q$, $\mu = \mu_q$, $\delta = \delta_q$ and $\gamma = \gamma_q$ (see Lemma 2.3 and 3.4).

From (2.9) we easily deduce the following expression for the error of the modified quadrature formula (3.13).

$$E_{r,n,q,a}(f) = \int_{\mu_q}^{\rho_q}\frac{P_n(\xi(x))}{P_n(-\xi(x))}\left(\frac{1}{2\pi i}\int_{\Gamma(q)}\frac{P_n(-\xi(s))F_{q,a}(s)}{(s-x)P_n(\xi(s))}ds\right)\,W_{q,a}(x)dx, \tag{3.19}$$

where $\Gamma(q)$ is the circle with center at $C_q = (\gamma_q + \delta_q)/2$ and radius $K_q = (\gamma_q - \delta_q)/2$.

From property 5 of Lemma 2.2, and (3.19) we obtain the following inequality .

$$|E_{r,n,q,a}(f)| \le \frac{1}{2\pi}\int_{\mu_q}^{\rho_q}\xi(x)^{\theta}\left|\frac{P_n(\xi(x))}{P_n(-\xi(x))}\right|\left(\int_{\Gamma(q)}\left|\frac{F_{q,a}(z)}{(z-x)}\right||dz|\right)\frac{W_{q,a}(x)}{\xi(x)^{\theta}}dx. \tag{3.20}$$

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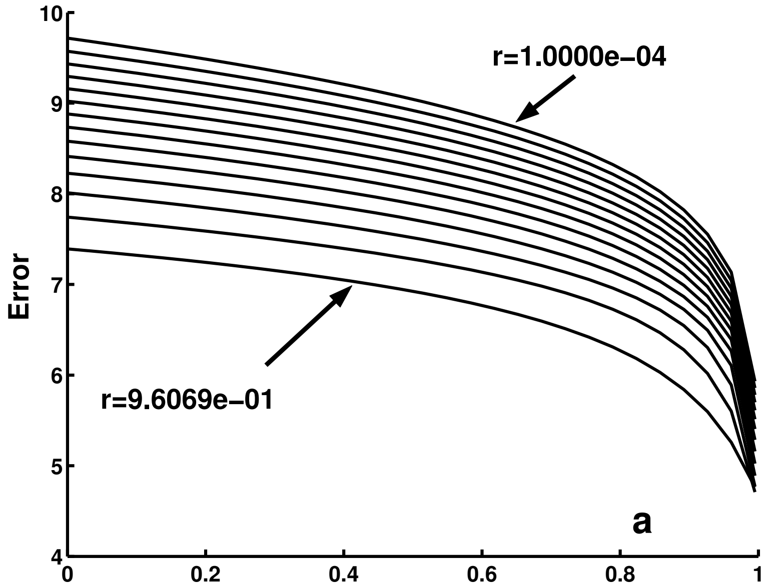

FIG. 3.1. *Error curves when* $f(x) = x^{-0.91}$, $n = 16$, $b = 2$, $q = 1$, $\epsilon = e^{-1}$.

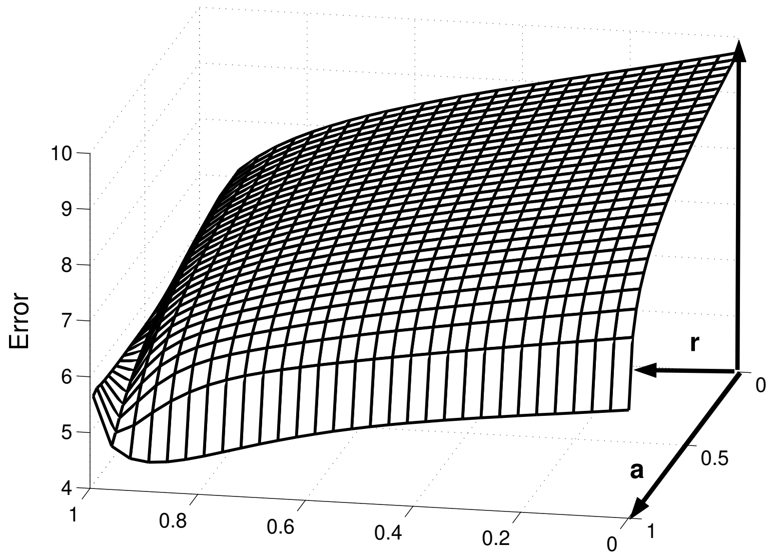

FIG. 3.2. *Error surface when* $f(x) = x^{-0.91}$, $n = 16$, $b = 0$, $q = 1$, $\epsilon = e^{-1}$.

In (3.20) we can consider the distribution

$$d\mu_{h,q,\theta,a}(x) = \frac{W_{q,a}(x)}{\xi(x)^{\theta}}dx,$$

thanks to property 4 of Lemma 2.2 which assures that $\xi(x) > 0$, for $z \in [\mu_q, \rho_q]$.

From Lemma (3.2) the distance from the circle $\Gamma(0) = w_{A_q}(\Gamma(q))$ to $[|z| = 1]$ is $h/2$. We apply to f the principle of maximum to obtain (see [5], pp. 29,36)

$$\max_{z\in\Gamma(q)} |F_{q,a}(z)| = \max_{z\in\Gamma(0)} |f(z)| \leq \max_{|z|=1-h/2} |f(z)| \leq \frac{2^{2/p}\|f\|_p}{\epsilon^{1/p}(1-a)^{1/p}}. \tag{3.21}$$

where $\|\cdot\|_p$ is the norm of the space H^p.

From Lemma 3.6 and the inequality

$$|s-z| \geq |s+1-h|,$$

for all $z \in [\mu_q, \rho_q]$, $s \in \Gamma$, we have that

$$\int_\Gamma \frac{|dz|}{|s-z|} \leq \pi \log\left(\frac{r+3-2h}{h}\right) = O\left(\log\left(\frac{1}{h}\right)\right). \tag{3.22}$$

Let $n > 34110\theta$. Using lemmas 2.1 and 3.3, and equations (3.20), (3.21) and (3.22) we derive the following estimate.

$$|E_{r,n,q,a}(f)| \leq M \log\left(\frac{1}{1-a}\right) \frac{\exp(-\pi\sqrt{n\theta})}{(1-a)^{1/p}} \int_{\mu_q}^{\rho_q} \frac{W_{q,a}(z)}{\xi(z)^\theta} dz, \tag{3.23}$$

where $M > 0$ does not depend[1] on the parameters n and a.

Let $\eta \geq 0$ and $\theta = m(q) - 1/p + \eta$ where $m = m(q) \in N$ will be selected conveniently. From property 4 of Lemma 2.2 and Lemma 3.4 we obtain

$$1 \leq \frac{1}{\xi(z)^{\theta-m}} \leq \frac{(\gamma_q-\mu_q)^{\theta-m}(\rho_q-\delta_q)^{\theta-m}}{(\gamma_q-\rho_q)^{\theta-m}(\mu_q-\delta_q)^{\theta-m}} = O\left(\frac{1}{(1-a)^{\theta-m}}\right),$$

where $z \in [\mu_q, \rho_q]$, $q \geq 1$.

If $\alpha_q = (\gamma_q - \rho_q)/(\rho_q - \delta_q)$ then using Lemma 3.4 we find that $\alpha_q \asymp k_0(1-a)$ as $a \to 1$ for some $k_0 > 0$. On the other hand we obtain by means of integration that

$$\int_{\mu_q}^{\rho_q} \frac{1}{(x-\delta_q)^m(1-xA_q)^2} dx = \sum_{j=2}^{m} \frac{\lambda_j(\rho_q-\mu_q)\psi_q^{j-2}}{(\mu_q-\delta_q)^{j-1}(\rho_q-\delta_q)^{j-1}} + \tag{3.24}$$

$$\lambda_1 \log\left|\frac{\rho_q-\delta_q}{\mu_q-\delta_q}\right| + \zeta_1 \log\left|\frac{1-\rho_qA_q}{1-\mu_qA_q}\right| + \zeta_2 \frac{A_q(\mu_q-\rho_q)}{(1-\mu_qA_q)(1-\rho_qA_q)},$$

where $\psi_q \asymp (1-a)^{q-1}$.

The terms in the right side of (3.24) have the following asymptotical behaviour as $a \to 1$, respectively.

$$O\left(\frac{1}{(1-a)^{(j-1)(q-1)}}\right), \quad O(1), \quad O\left(\log\left(\frac{1}{1-a}\right)\right), \quad O\left(\frac{1}{(1-a)^q}\right),$$

where $(1-a)^{-(m-1)(q-1)}$, $q > 1$, $m > 1$, is the fastest term of those which converge to infinity as $a \to 1$.

[1] But it does depend on θ as can be deduced from [6].

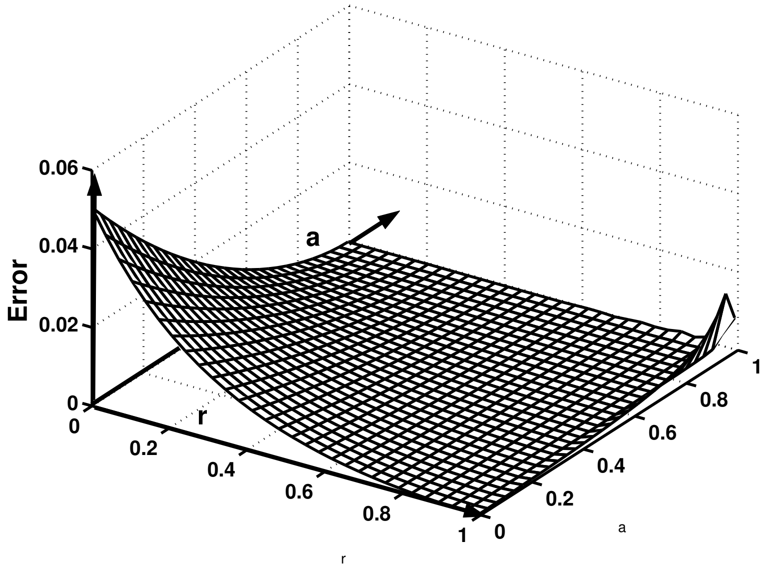

FIG. 3.3. *Error surface when* $f(x) = x\log(x)$, $n = 16$, $b = 0$, $q = 1$, $\epsilon = e^{-1}$.

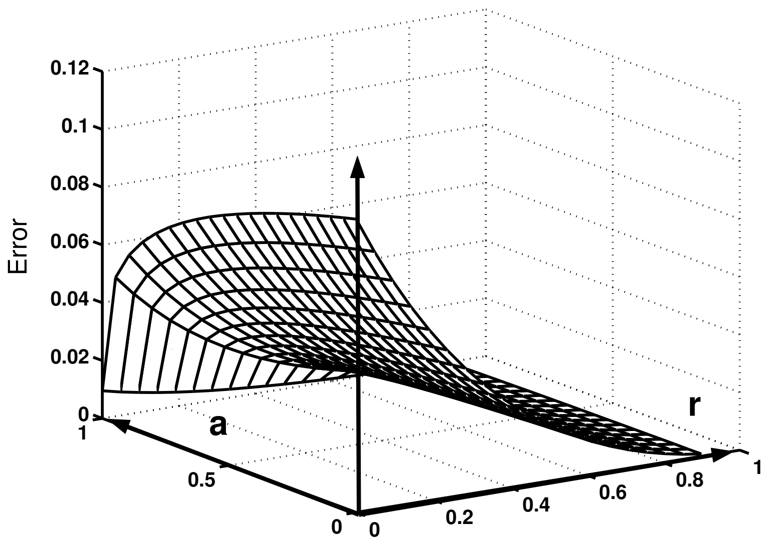

FIG. 3.4. *Error surface when* $f(x) = x\log(x)$, $n = 16$, $b = 0$, $q = 3$, $\epsilon = e^{-1}$.

The contribution of the factors $1 - A_q$, $(\gamma_q - \mu_q)^m$ and $(1-a)^{-m}$ leads us to select $m = 2q - 1$, $q \geq 1$, in order to cancel all those terms which tend to infinity as $a \to 1$, with the exception of $(1-a)^{-1/p}$ which is grouped together with $1/(1-a)^{\eta - 1/p}$. $\square$

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TABLE 3.1
Absolute errors when $f(x) = x^{-1/5}$, $n = 2, 4, 8$, $b = 0$, $q = 1$.

$r = 0.5$, $\epsilon = e^{-1}$		$r = 0.5$, $\epsilon = e^{-1}$		$r = 0.3$, $\epsilon = e^{-5}$	
a	$n = 2$	a	$n = 4$	a	$n = 8$
0.0000000e+00	2.0e–01	0.0000000e+00	1.4e–01	0.0000000000e+00	9.8e–03
1.0000000e–01	2.0e–01	1.0000000e–01	1.3e–01	2.0000000000e–01	8.4e–03
3.0000000e–01	1.8e–01	2.0000000e–01	1.2e–01	5.0000000000e–01	6.1e–03
5.0000000e–01	1.6e–01	3.0000000e–01	1.0e–01	7.0000000000e–01	4.2e–03
7.0000000e–01	1.2e–01	5.0000000e–01	7.1e–02	8.0000000000e–01	3.0e–03
7.5000000e–01	1.1e–01	6.0000000e–01	5.4e–02	9.0000000000e–01	1.5e–03
8.0000000e–01	8.2e–02	8.0000000e–01	1.4e–02	9.5000000000e–01	3.4e–04
8.9000000e–01	9.5e–03	8.6000000e–01	5.7e–04	9.5910000000e–01	2.5e–06
8.9700000e–01	4.4e–04	8.6260000e–01	5.2e–07	9.5915000000e–01	4.1e–07
8.9730000e–01	3.5e–05	8.6260200e–01	8.1e–08	9.5915900000e–01	3.8e–08
8.9732485e–01	1.7e–06	8.6260235e–01	3.8e–09	9.5915970654e–01	2.3e–10

TABLE 3.2
Absolute errors when $f(x) = x^{-1/5}$, $n = 16, 32$, $b = 0$, $q = 1$, $r = 0.5$.

$\epsilon = e^{-1}$		$\epsilon = e^{-5}$	
a	$n = 16$	a	$n = 32$
0.000000000000000e+00	1.4e–01	0.000000000000000e+00	6.4e–07
2.000000000000000e–01	1.2e–01	5.000000000000000e–01	6.4e–07
6.000000000000000e–01	6.6e–02	9.999000000000000e–01	5.9e–07
9.900000000000000e–01	3.4e–03	9.999100000000000e–01	5.8e–07
9.997000000000000e–01	2.1e–05	9.999300000000000e–01	5.6e–07
9.997260000000000e–01	4.6e–07	9.999500000000000e–01	5.3e–07
9.997265600000000e–01	2.8e–09	9.999600000000000e–01	5.1e–07
9.997265635000000e–01	1.2e–10	9.999946849310000e–01	3.8e–07
9.997265635029350e–01	7.4e–11	9.999942747252746e–01	1.2e–11
9.997265635029354e–01	3.5e–12	9.999942747252747e–01	7.8e–12

DEFINITION 3.8. *The integral modulus of continuity of $f \in H^1$ is given by*

$$\omega(f, r, \delta) = \sup_{0<h<\delta} \int_{-1}^{r} |f(x) - f((1-h)x)|dx, \quad 0 < \delta < 1. \tag{3.25}$$

The analysis of error in terms of the modulus (3.25) is the following

$$\left| \int_{-1}^{r} f(x)dx - Q_{r,h,n}(f) \right| \le \omega(f, r, \delta) + |I_{r,h}(f) - Q_{r,h,n}(f)| \,. \tag{3.26}$$

It is well-known that $\lim_{\delta\to 0} \omega(f, r, \delta) = 0$, for all $f \in H^1$, and $0 < r \le 1$ (cf. [5, 18]). Besides, the behaviour of $\omega(f, r, \delta)$ as $\delta \to 0$ does not depend essentially on r, $0 < r < 1$, but on the nature of f in a neighbourhood of the endpoint $x = -1$.

THEOREM 3.9. *Let $q \in N$, $f \in H^p$, $1 < p < \infty$, $0 < r < 1-h$ and $\theta = \eta + 2q - 1 - 1/p$, $\eta \ge 0$. Let (a_n) be a sequence such that*

1. $0 < a_n < 1$,
2. $\lim_n a_n = 1$,
3. $\lim_n \log(1/(1 - a_n)) \exp(-\pi\sqrt{n\theta} + \eta \log(1/(1 - a_n))) = 0$.

Then the quadrature rule $Q_{r,n,q}(f)$ given by (3.13) with $a = a_n$, converges to $\int_{-1}^{r} f(x)\,dx$ for all $f \in H^p$.

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TABLE 3.3
Absolute errors when $f(x) = x^{-1/5}$, $n = 64, 128$, $b = 0$, $q = 1$, $\epsilon = e^{-20}$.

$r = 0.4$		$r = 0.5$	
a	$n = 64$	a	$n = 128$
0.0000000000000000e+00	2.1e–09	0.0000000000000000e+00	1.1e–09
1.0000000000000000e–01	2.0e–09	2.5000000000000000e–01	8.5e–10
3.0000000000000000e–01	1.9e–09	5.0000000000000000e–01	6.2e–10
5.0000000000000000e–01	1.8e–09	7.5000000000000000e–01	3.5e–10
7.0000000000000000e–01	1.6e–09	9.0000000000000000e–01	1.7e–10
9.0000000000000000e–01	1.5e–09	9.5000000000000000e–01	9.8e–11
9.9000000000000000e–01	1.4e–09	9.9000000000000000e–01	2.7e–11
9.9995711428570000e–01	9.0e–10	9.9600000000000000e–01	5.5e–12
9.9995711428571400e–01	7.5e–12	9.9899816849816800e–01	4.4e–13
9.9995711428571430e–01	8.6e–12	9.9899816849816860e–01	2.0e–15

Proof. From Lemma 3.7 and inequality (3.26) with $h \le \delta = (1-a)$, we have the following estimate.

$$\left| \int_{-1}^{r} f(x)dx - Q_{r,n,q,a}(f) \right| \le M\left(\omega(f,r,(1-a)) + U(a,r,q,n)\right), \tag{3.27}$$

where

$$U(a,r,q,n) = \log\left(\frac{1}{1-a}\right)\, \exp\left(-\pi\sqrt{n\theta} + \eta \log\left(\frac{1}{1-a}\right)\right),$$

$Q_{r,n,q,a}(f)$ is the approximant given by (3.13), and the positive constant M depends neither on n nor a.

Convergence follows from estimate (3.27). □

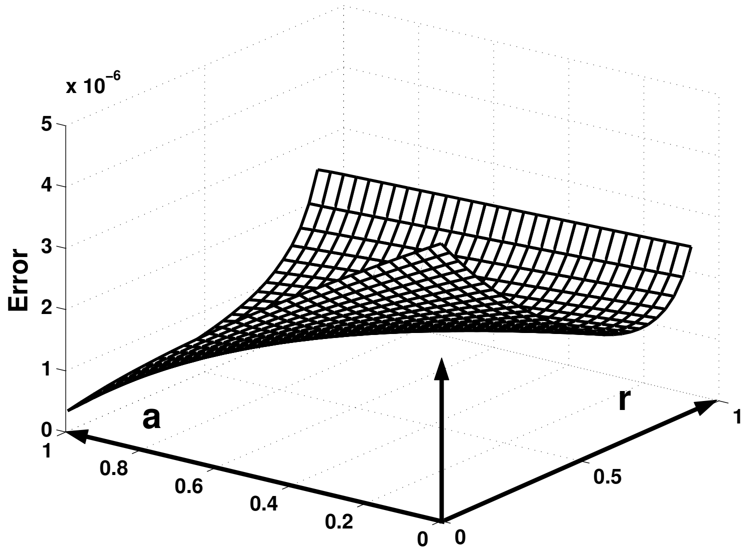

FIG. 3.5. *Error surface when* $f(x) = x^{-1/5}$, $n = 32$, $b = 0$, $q = 1$, $\epsilon = e^{-15}$

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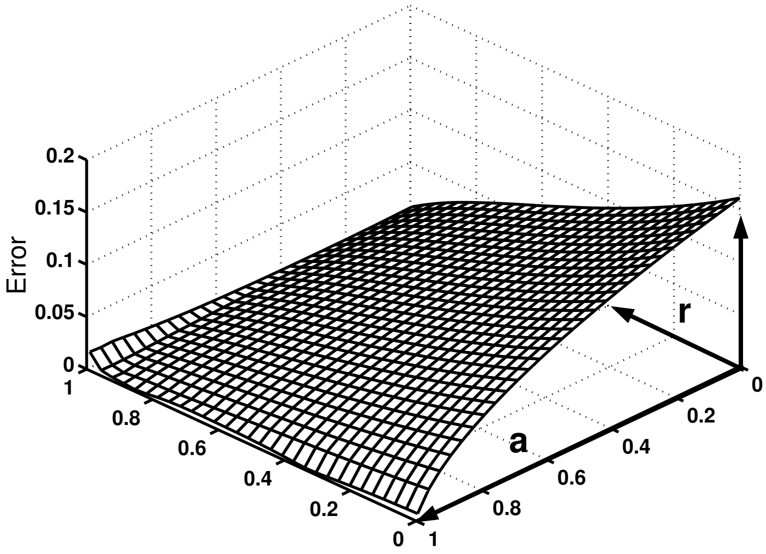

FIG. 3.6. *Error surface when* $f(x) = x^{-1/5}$, $n = 16$, $b = 4$, $q = 1$, $\epsilon = e^{-1}$.

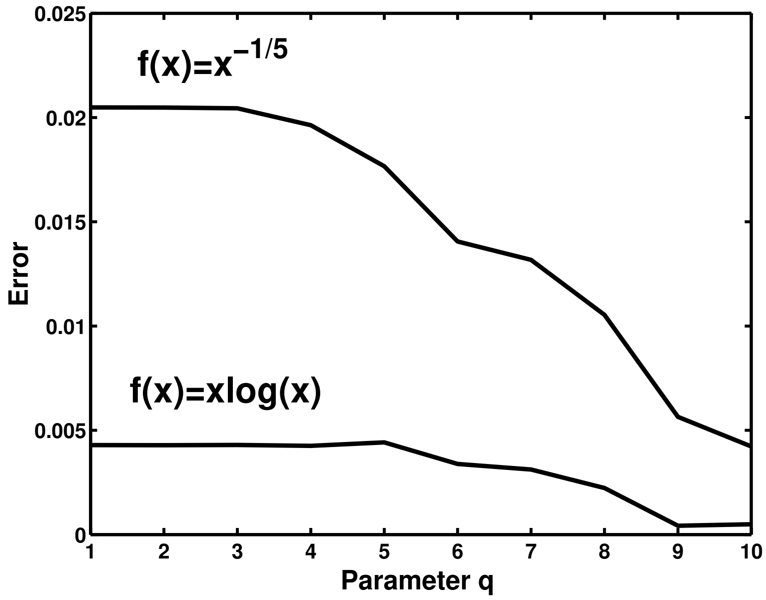

FIG. 3.7. *Error for* $q = 1, \ldots, 10$, $n = 16$, $b = 0$, $\epsilon = e^{-1}$, $r = 0.5$, $a = 0.9$, $\theta = 2q - 1$.

If $\eta > 0$ then every sequence of the form $a_n = 1 - e^{-t\sqrt{n}}$ with $t < \pi\sqrt{\theta}/\eta$, satisfies the conditions of Theorem 3.9. Besides, the rate of convergence of the quadrature error with respect to $\int_{-1}^{r} f(x)dx$ depends on the behavior of the sequence

$$\{\omega(f, r, (1 - a_n))\}_{n=1}^{\infty}.$$

The following result states a class of functions for which we should expect a good behavior

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TABLE 3.4
Absolute errors when $f(x) = x^{1/5}$, $n = 2, 4, 8$, $b = 0$, $q = 1$, $\epsilon = e^{-10}$.

$r = 0.6$		$r = 0.5$		$r = 0.3$	
a	$n = 2$	a	$n = 4$	a	$n = 8$
0.000000000000e+00	3.2e–02	0.00000000e+00	1.1e–02	0.0000000e+00	5.8e–05
5.000000000000e–01	3.0e–02	1.00000000e–01	1.2e–02	2.0000000e+00	4.9e–05
7.000000000000e–01	1.4e–02	5.00000000e–01	1.9e–02	5.0000000e–01	2.1e–05
7.500000000000e–01	5.7e–03	9.50000000e–01	2.0e–02	6.0000000e–01	2.8e–06
7.710000000000e–01	1.4e–03	9.75000000e–01	2.9e–03	6.1000000e–01	5.1e–07
7.750000000000e–01	5.4e–04	9.77000000e–01	1.1e–04	6.1210000e–01	1.3e–08
7.760000000000e–01	3.1e–04	9.77050000e–01	3.3e–05	6.1213000e–01	6.3e–09
7.773000000000e–01	1.1e–05	9.77070000e–01	2.6e–06	6.1213307e–01	5.6e–09
7.773300000000e–01	4.0e–06	9.77072000e–01	3.7e–07	7.0000000e–01	2.7e–05
7.773385518591e–01	2.0e–06	9.77072402e–01	9.7e–07	9.0000000e–01	2.5e–04

of the corresponding numerical procedure. It also shows the effect which the parameter a produces in the quadrature error.

THEOREM 3.10. *Let f be a function in H^p, $1 < p < \infty$, such that $\omega(f, r, \delta) = O(\delta^\beta)$, $0 < \beta \le 1$, $r \in (0, 1)$. Let $Q_{r,n,q} = Q_{r,n,q,a}$ be the approximant given by (3.13). There exists $\theta = \theta(p, q, \beta) > 0$ such that for n sufficiently large the following estimate holds.*

$$\left| \int_{-1}^{r} f(x)dx - Q_{r,n,q}(f) \right| \le M\sqrt{n} \exp\left(-\pi\sqrt{n\beta\theta}\right), \tag{3.28}$$

where $M > 0$ depends neither on n nor a.

Proof. Let us take $\eta = \sqrt{\beta} - \beta$ in the proof of Lemma 3.7. We observe that we must consider $q > 1$ for $p = \beta = 1$, and $q \ge 1$ otherwise. Now the term $U(a, r, q, n)$ in estimate (3.27) becomes

$$U(a, r, q, n, \beta) = \log\left(\frac{1}{1-a}\right) \exp\left(-\pi\sqrt{n\theta} + (\sqrt{\beta} - \beta)\log\left(\frac{1}{1-a}\right)\right).$$

Let f be a function in H^p such that it satisfies a Lipschitz condition of order β. If $a = 1 - \exp(-t\sqrt{n})$ with $t = \pi\sqrt{\theta/\beta}$ and $h = \epsilon(1 - a)$, $0 < \epsilon < 1$, then we have $\omega(f, r, h) \le M \exp(-\pi\sqrt{n\theta\beta})$.

Using estimate (3.27) with $U(a, r, q, n, \beta)$ instead of $U(a, r, q, n)$ we find (3.28). ☐

Choosing θ as that in Theorem 3.10 we see that $\theta \ge 2(q - 1)$, so the upper bound in (3.28) can be transformed into $\sqrt{n}\exp\left(-\pi\sqrt{n\kappa}\right)$, with $\kappa = 2\beta(q - 1)$, which only works for $q > 1$. If $p > 1$ then we may consider $\kappa = 2q - 1 - 1/p$, $q \ge 1$. If we take $q = \beta = 1$ then the latter corresponds to the exact order of convergence for the optimal quadrature error in H^p, $p > 1$ (cf. [2, 3]).

The order of the upper estimate (3.18) can be improved up to $\exp(-cn))$, $c > 0$, if we select the quadrature nodes as those given by Gonchar's technique [11]. However, even in that case the order of convergence given by the corresponding new version of Theorem 3.10 could not be faster than that in (3.28). Besides, the numerical procedure when Gonchar's nodes are considered, is not so efficient as that produced by Ganelius'.

4. Numerical examples. In this section we consider the problem of the numerical evaluation of the integral $I(f)$ given in formula (1.1), where f is analytic on $(c, d]$. For simplicity

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TABLE 3.5
Absolute errors when $f(x) = x^{1/5}$, $n = 16, 32$, $b = 0$, $q = 1$, $r = 0.5$, $\epsilon = e^{-8}$.

a	$n = 16$	a	$n = 32$
0.00000000e+00	2.4e–05	0.000000000000e+00	6.6e–06
1.00000000e–01	2.2e–05	2.000000000000e–01	5.0e–06
2.00000000e–01	1.9e–05	5.000000000000e–01	2.9e–06
4.00000000e–01	1.3e–05	7.000000000000e–01	1.6e–06
6.00000000e–01	7.8e–06	9.000000000000e–01	4.1e–07
8.00000000e–01	2.9e–06	9.900000000000e–01	2.4e–08
9.00000000e–01	4.0e–07	9.950000000000e–01	7.4e–09
9.15200000e–01	1.8e–08	9.970000000000e–01	3.4e–10
9.15500000e–01	9.6e–09	9.970800000000e–01	2.9e–11
9.15823525e–01	2.8e–10	9.970862745095e–01	1.6e–12

TABLE 3.6
Absolute errors when $f(x) = x^{1/5}$, $n = 64, 128$, $b = 0$, $q = 1$, $\epsilon = e^{-8}$.

$r = 0.4$		$r = 0.5$	
a	$n = 64$	a	$n = 128$
0.000000000000000e+00	6.6e–06	0.00000000000000e+00	6.6e–06
6.000000000000000e–01	2.2e–06	2.00000000000000e–01	5.0e–06
9.500000000000000e–01	1.8e–07	5.00000000000000e–01	2.9e–06
9.950000000000000e–01	1.1e–08	9.00000000000000e–01	4.1e–07
9.995000000000000e–01	1.7e–09	9.99000000000000e–01	1.7e–09
9.999787058000000e–01	2.5e–11	9.99967920000000e–01	1.3e–10
9.999787058820000e–01	6.1e–12	9.99967921568600e–01	2.9e–11
9.999787058823529e–01	5.5e–14	9.99967921568627e–01	2.1e–13

TABLE 3.7
Absolute errors when $f(x) = x^{-0.91}$, $n = 2, 4, 8$, $b = 0$, $q = 1$, $\epsilon = e^{-1}$.

$r = 0.6$		$r = 0.5$		$r = 0.3$	
a	$n = 2$	a	$n = 4$	a	$n = 8$
0.00000000e+00	8.7e+00	0.000000000e+00	8.4e+00	0.0000000000e+00	8.7e+00
1.00000000e–01	8.7e+00	1.000000000e–01	8.3e+00	2.0000000000e–01	8.5e+00
3.00000000e–01	8.7e+00	3.000000000e–01	8.1e+00	4.0000000000e–01	8.3e+00
6.00000000e–01	8.6e+00	5.000000000e–01	7.8e+00	6.0000000000e–01	8.0e+00
8.00000000e–01	8.3e+00	7.000000000e–01	7.5e+00	9.0000000000e–01	6.9e+00
9.90000000e–01	5.8e+00	9.000000000e–01	7.1e+00	9.9990000000e–01	4.5e+00
9.99920000e–01	1.4e–01	9.999990000e–01	2.3e+00	9.9999999000e–01	3.8e–01
9.99928000e–01	1.6e–02	9.999999500e–01	8.3e–01	9.9999999500e–01	6.3e–02
9.99928940e–01	1.0e–04	9.999999900e–01	2.6e–02	9.9999999560e–01	4.4e–03
9.99928943e–01	4.8e–05	9.999999905e–01	4.8e–04	9.9999999564e–01	2.4e–04

TABLE 3.8
Absolute errors when $f(x) = x^{-0.91}$, $n = 16, 32$, $b = 0$, $q = 1$, $r = 0.5$, $\epsilon = e^{-1}$.

a	$n = 16$	a	$n = 32$
0.00000000000e+00	8.7e+00	0.00000000000000e+00	8.7e+00
1.00000000000e–01	8.6e+00	1.00000000000000e–01	8.6e+00
2.00000000000e–01	8.5e+00	2.00000000000000e–01	8.5e+00
4.00000000000e–01	8.3e+00	4.00000000000000e–01	8.3e+00
6.00000000000e–01	8.0e+00	6.00000000000000e–01	8.0e+00
8.00000000000e–01	7.5e+00	9.00000000000000e–01	7.0e+00
9.00000000000e–01	7.0e+00	9.99000000000000e–01	4.6e+00
9.99999999000e–01	8.0e–01	9.99999000000000e–01	2.5e+00
9.99999999900e–01	6.8e–02	9.99999999970000e–01	8.3e–01
9.99999999919e–01	6.9e–03	9.99999999972647e–01	2.7e–03

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TABLE 3.9
Absolute errors when $f(x) = x^{-0.91}$, $n = 64, 128$, $b = 0$, $q = 1$, $\epsilon = e^{-1}$.

$r = 0.4$		$r = 0.5$	
a	$n = 64$	a	$n = 128$
0.00000000000000e+00	8.7e+00	0.0000000000000e+00	8.7e+00
3.00000000000000e–01	8.4e+00	1.0000000000000e–01	8.4e+00
5.00000000000000e–01	8.1e+00	3.0000000000000e–01	8.4e+00
7.00000000000000e–01	7.8e+00	5.0000000000000e–01	8.1e+00
9.00000000000000e–01	7.0e+00	7.0000000000000e–01	7.8e+00
9.99000000000000e–01	4.6e+00	9.0000000000000e–01	7.0e+00
9.99999000000000e–01	2.5e+00	9.9999000000000e–01	3.1e+00
9.99999999950000e–01	1.1e+00	9.9999999000000e–01	1.6e+00
9.99999999958000e–01	9.2e–01	9.9999999990000e–01	5.6e–01
9.99999999958809e–01	5.5e–02	9.9999999994258e–01	1.6e–01

TABLE 3.10
Absolute errors when $f(x) = \log(x)$, $n = 2, 4, 8$, $b = 0$, $q = 1$, .

$r = 0.5$	$\epsilon = e^{-5}$	$r = 0.5$	$\epsilon = e^{-1}$	$r = 0.3$	$\epsilon = e^{-1}$
a	$n = 2$	a	$n = 4$	a	$n = 8$
0.00000000e+00	3.2e–02	0.000000e+00	2.7e–01	0.000000e+00	2.4e–01
1.00000000e–01	4.4e–02	1.000000e–01	2.5e–01	1.000000e–01	2.2e–01
3.00000000e–01	5.9e–02	2.000000e–01	2.2e–01	2.000000e–01	2.0e–01
4.00000000e–01	6.0e–02	3.000000e–01	2.0e–01	3.000000e–01	1.8e–01
5.00000000e–01	5.4e–02	4.000000e–01	1.7e–01	5.000000e–01	1.4e–01
6.00000000e–01	3.8e–02	6.000000e–01	9.6e–02	7.000000e–01	9.3e–02
7.00000000e–01	3.0e–03	8.000000e–01	2.1e–03	9.000000e–01	3.9e–02
7.05000000e–01	4.4e–04	8.039000e–01	4.1e–05	9.990000e–01	2.4e–03
7.05851000e–01	4.9e–07	8.039760e–01	3.3e–07	9.992000e–01	8.1e–04
7.05851896e–01	2.9e–08	8.039765e–01	6.6e–08	9.992805e–01	2.6e–07

TABLE 3.11
Absolute errors when $f(x) = \log(x)$, $n = 16, 32$, $b = 0$, $q = 1$, $r = 0.5$, $\epsilon = e^{-1}$.

a	$n = 16$	a	$n = 32$
0.0000000e+00	2.4e–01	0.00000e+00	2.4e–01
1.0000000e–01	2.2e–01	1.00000e–01	2.2e–01
3.0000000e–01	1.8e–01	2.00000e–01	2.0e–01
6.0000000e–01	1.2e–01	4.00000e–01	1.6e–01
9.0000000e–01	3.8e–02	6.00000e–01	1.2e–01
9.9000000e–01	5.1e–03	9.00000e–01	3.8e–02
9.9990000e–01	7.5e–04	9.90000e–01	5.2e–03
9.9998100e–01	2.4e–05	9.99000e–01	6.6e–04
9.9998150e–01	3.2e–06	9.99990e–01	1.0e–05
9.9998158e–01	2.6e–07	9.99999e–01	8.6e–07

TABLE 3.12
Absolute errors when $f(x) = \log(x)$, $n = 64, 128$, $b = 0$, $q = 1$, $r = 0.5$, $\epsilon = e^{-25}$.

a	$n = 64$	a	$n = 128$
0.0e+00	1.4e–10	0.000000000000e+00	6.4e–11
1.0e–01	1.4e–10	1.000000000000e–01	5.8e–11
2.0e–01	1.3e–10	2.000000000000e–01	4.8e–11
3.0e–01	1.3e–10	4.000000000000e–01	3.9e–11
4.0e–01	1.2e–10	6.000000000000e–01	2.7e–11
5.0e–01	1.2e–10	7.000000000000e–01	2.0e–11
6.0e–01	1.1e–10	8.000000000000e–01	1.7e–11
7.0e–01	1.0e–10	9.000000000000e–01	6.9e–12
8.0e–01	9.8e–11	9.780000000000e–01	1.1e–12
9.0e–01	9.2e–11	9.788181818181e–01	9.2e–13

TABLE 3.13
Absolute errors when $f(x) = x\log(x)$, $n = 2, 4, 8$, $b = 0$, $\epsilon = e^{-1}$.

$r = 0.3, q = 1$		$r = 0.99, q = 2$		$r = 0.1, q = 1$	
a	$n = 2$	a	$n = 4$	a	$n = 8$
0.00000000e+00	1.4e–01	0.000000e+00	1.5e–02	0.0000e+00	3.5e–02
1.00000000e–01	1.4e–01	1.000000e–01	1.8e–02	1.0000e–01	2.9e–02
3.00000000e–01	1.3e–01	2.000000e–01	2.1e–02	2.0000e–01	2.3e–02
4.00000000e–01	6.0e–02	3.000000e–01	2.5e–02	3.0000e–01	1.8e–02
5.00000000e–01	1.3e–01	4.000000e–01	2.9e–02	5.0000e–01	9.9e–03
9.00000000e–01	7.8e–02	6.000000e–01	3.8e–02	7.0000e–01	3.8e–03
9.72000000e–01	1.8e–03	9.000000e–01	5.6e–02	9.0000e–01	1.2e–03
9.72700000e–01	6.0e–06	9.880000e–01	1.3e–03	9.3000e–01	5.0e–04
9.72702200e–01	2.3e–07	9.882700e–01	4.1e–05	9.3950e–01	2.6e–05
9.72702285e–01	2.0e–09	9.882787e–01	1.5e–07	9.3991e–01	5.2e–08

TABLE 3.14
Absolute errors when $f(x) = x\log(x)$, $n = 16, 32$, $b = 0$, $q = 1$, $r = 0.5$.

$\epsilon = e^{-1}$		$\epsilon = e^{-10}$	
a	$n = 16$	a	$n = 32$
0.000000e+00	3.5e–02	0.000000000e+00	1.9e–09
1.000000e–01	2.9e–02	1.000000000e–01	1.5e–09
3.000000e–01	1.8e–02	2.000000000e–01	1.2e–09
5.000000e–01	1.0e–02	4.000000000e–01	6.1e–10
7.000000e–01	4.0e–03	5.000000000e–01	3.8e–10
9.000000e–01	5.5e–04	6.000000000e–01	1.9e–10
9.900000e–01	9.5e–06	7.000000000e–01	3.7e–11
9.952700e–01	7.6e–09	7.310000000e–01	1.6e–12
9.952724e–01	3.1e–10	7.318000000e–01	4.8e–14
9.952725e–01	9.8e–14	7.318980068e–01	8.9e–15

we only refer to the case $[c, d] = [0, 1]$. By means of the affine transformation $F_r(x) = (x+1)/(r+1)$, $0 < r < 1$, we apply our method to estimate $I(f) = I_r(f \circ F_r)/(r+1)$, for several values of a and r. If $a = 0$ then it means that no change of variable is made.

The values of the parameter q which we have used to test our approach are $q = 1, ..., 10$. In spite of the theoretical results in the previous section we have obtained very good results for $q = 1$, though instability shows up for $q > 1$ in case of $\epsilon < \exp(-1)$. In this article we report Fig. 3.4 for $q = 3$, Fig. 3.7 to validate the role of q in the procedure and Table 3.13 for the case $q = 2$.

We use the exactness condition for the rational functions $1/(p_{n,k}^{-1}x - 1)$ to implement a numerical procedure for the quadrature rule (3.13). It means that the coefficients $C = (A_{n,1}, ..., A_{n,n-b}, B_{n,1}, ..., B_{n,b})$ of the approximant are calculated as the solution of a linear system of equations which we trasform in $T(a, r, n)C = Y$, where $T(a, r, n)$ is an upper triangular matrix obtained via **QR** factorization. Table 3.17 shows that after scaling the condition number of $T(a, r, n)$ should vary a little as r ranges from 0.01 to 0.99.

Many numerical experiments have shown that the equation $h = \epsilon(1 - a)$ works good enough in the computer. In our opinion this procedure needs a parameter ϵ which ranges from $\exp(-1)$ to $\exp(-25)$. If we make h small it means that either the value of a is very forced to be near the point $a = 1$, which yields a very high concentration of nodes and poles near the point $x = -1$, or $\epsilon \leq \exp(-10)$. Instability is associated with small values of ϵ though it can be observed higher accuracy as well (see Fig. 3.5-3.6). Theorem 3.10 shows that if a is close enough to one then the quadrature error should be small. This effect is certainly produced by the change of variable $w_{A_q}(x)$, though one can detect that the decreasing behaviour of the

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TABLE 3.15
Absolute errors when $f(x) = x\log(x)$*,* $n = 64, 128$*,* $b = 0$*,* $q = 1$*,* $r = 0.5$*.*

$\epsilon = e^{-25}$		$\epsilon = e^{-5}$	
a	$n = 64$	a	$n = 128$
0.00000000000000e+00	1.6e–08	0.00e+00	4.6e–06
1.00000000000000e–01	1.3e–08	1.00e–01	3.8e–06
2.00000000000000e–01	1.1e–08	2.00e–01	3.0e–06
3.00000000000000e–01	8.2e–09	4.00e–01	1.8e–06
4.00000000000000e–01	6.1e–09	6.00e–01	8.3e–07
5.00000000000000e–01	4.3e–09	7.00e–01	4.8e–07
7.00000000000000e–01	1.6e–09	8.00e–01	2.2e–07
9.00000000000000e–01	2.0e–10	9.00e–01	6.1e–08
9.90000000000000e–01	2.2e–12	9.90e–01	7.5e–10
9.90782991202346e–01	—*	9.99e–01	1.3e–13

*The symbol — means that the corresponding numerical result is smaller than 1.00e–15.

TABLE 3.16
Absolute errors when $f(x) = x^{-1/5}$*,* $n = 16, 32$*,* $b = 4$*,* $q = 1$*,* $r = 0.5$*.*

$\epsilon = e^{-1}$		$\epsilon = e^{-5}$	
a	$n = 16$	a	$n = 32$
0.0000000e+00	8.0e–02	0.0000e+00	6.4e–03
1.0000000e–01	7.5e–02	1.0000e–01	6.0e–03
3.0000000e–01	6.6e–02	2.0000e–01	5.5e–03
5.0000000e–01	5.5e–02	3.0000e–01	5.0e–03
7.0000000e–01	4.1e–02	5.0000e–01	3.9e–03
8.0000000e–01	3.2e–02	6.0000e–01	3.3e–03
9.0000000e–01	2.1e–02	8.0000e–01	2.0e–03
9.9000000e–01	2.0e–03	9.9000e–01	2.1e–04
9.9230000e–01	5.1e–05	9.9700e–01	3.8e–05
9.9234833e–01	2.3e–06	9.9763e–01	1.4e–06

error with respect to a is magnified a lot by the condition $h = \epsilon(1 - a)$. When ϵ is too small the slope of the error curve with respect to a is also small except for values of a very close to one. Such a behaviour can be seen in Table 3.1–3.16 for several values of the parameters n, a, r and ϵ.

The variable r plays the role of counterpart of a, in the sense that values of r close to $x = 1$ produce a concentration of nodes on the right side. We display figures 3.1–3.6 to illustrate the behavior of the error as function of the parameters a and r, particularly when they are close to one simultaneously. The error surfaces $z = E(i, j)$ have been defined over the rectangular grid $(r(j), a(i))$, $i, j = 1, ..., K$, $K = 20, 30$, for which $1.0 - 03 \le r(j) \le 9.95e - 01$, $0 \le a(i) \le 9.95e - 01$.

Before making any conclusion on whether the selection $b_{n,q} > 0$ is a reasonable decision for the numerical procedure one has to take into account that condition $b_{n,q} > 0$ implies that some derivatives of the integrand are participating in the calculations. Despite the fact of having used simbolic tools to simulate all the derivatives, it is not surprising that a loss of accuracy is observed in Table 3.16 with respect to Table 3.2. Naturally, this comparison clearly indicates that unless we were able to improve the algorithm, the case $b_{n,q} = 0$ seems to be preferable. As for the use of an integral representation formula to calculate all the coefficients of the quadrature rule (3.13), for the moment we have not been able to reach precision enough in the experiments. For all cases a feature of the integration method (3.13) is that the error strongly depends on the behavior of f near $x = -1$. A class of functions with singularities located at interior points to which can be applied this integration rule, is one as that defined in [19], namely, piecewise H^p functions.

TABLE 3.17
Condition number of matrices $T(a,r,n)$, $a = 0.5$.

b	r	$n=2$	$n=4$	$n=8$	$n=16$	$n=32$	$n=64$	$n=128$
0	0.01	1.2e+00	4.1e+00	4.9e+01	2.6e+03	1.9e+06	7.7e+10	1.4e+13
	0.1	1.3e+00	4.2e+00	4.1e+01	2.7e+03	2.3e+06	8.7e+10	1.7e+13
	0.5	1.6e+00	7.0e+00	8.4e+01	5.2e+03	4.3e+06	2.0e+11	7.7e+13
	0.9	6.9e+00	1.8e+01	3.1e+02	3.1e+04	3.4e+07	2.1e+12	2.1e+15
	0.99	1.7e+01	9.1e+01	8.8e+02	1.9e+05	4.6e+08	5.0e+13	1.3e+17
$[\sqrt{n}]$	0.01	1.3e+00	1.8e+00	4.4e+01	7.1e+03	6.9e+06	1.0e+13	1.8e+20
	0.1	1.2e+00	1.8e+00	4.5e+01	6.9e+03	4.2e+07	6.3e+12	6.6e+19
	0.5	1.4e+00	4.6e+00	5.6e+02	1.2e+06	5.4e+09	8.2e+16	2.7e+20
	0.9	2.0e+00	4.2e+03	3.8e+04	9.0e+10	7.7e+12	1.7e+19	3.7e+23
	0.99	2.5e+00	1.1e+06	3.4e+07	1.0e+12	4.8e+17	2.7e+19	7.0e+19

The reader should consult [23] where the n-point Gauss-Legendre rule and several smoothing transformations are applied together to evaluate the integral of functions with one and two endpoint singularities. To illustrate the efficiency of the method in [23], the authors compare the corresponding numerical results with those generated by the trapezoidal rule when the latter has been modified by a change of variable.

Our approach is based on interpolation of rational functions and it is different from that presented by Monegato and Scuderi in [23]. The latter deals with Gaussian quadrature formulas of polynomial type and smoothing transformations for which some derivatives vanish at the endpoints of the integration interval. Instead, we consider the change of variable $u_q(x) = w_{A_q}(x)$ which simply modifies the distribution of nodes to diminish the adverse effect of the endpoint singularity. However, for the purposes of comparison, we mainly refer to the numerical results in [23] because here we have practically tested the same functions as those reported in that paper.

In spite of the ill conditioned matrices which arise in our implementation, a conclusion is that the accuracy which we can obtain with the rational quadrature rule (3.13) is competent, particularly for those functions f for which estimate (3.28) holds.

All the computations in this work have been performed on a PC using MatLab$^{(R)}$.

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