A group of quadrature formulae for end-point singular functions is presented generalizing classical end-point corrected trapezoidal quadrature rules. The actual values of the end-point corrections are obtained for each singularity as a solution of a system of linear algebraic equations. The algorithm is applicable to a wide class of monotonic singularities and does not require that an analytical expression for the singularity be known; only the knowledge of its first several moments and the ability to evaluate it on the interval of integration are needed.

End-Point Corrected Trapezoidal Quadrature Rules for Singular Functions

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1. Introduction

When a numerical quadrature rule for a class of singular functions is derived, it is usually a generalization of some technique for numerical integration of non-singular functions. [3, 4, 5] use Richardson-style extrapolation to construct quadrature rules for singularities of the form $x^\gamma, -1 < \gamma < 1$. [7, 8, 9] generalize the Euler-Maclaurin expansion for integrands with certain kinds of singularities. In the present paper, the end-point corrected trapesoidal quadrature rules are generalized. While the standard end-point corrected trapezoidal rules are usually derived by means of the Euler-Maclaurin formula, their generalizations for singular functions are obtained in this paper as solutions of certain systems of linear algebraic equations (see Section 2). The rate of convergence of resulting quadrature rules is investigated analytically for a fairly broad class of monotonic singularities in Sections 3 - 5. However, our numerical experiments indicate that these quadratures can be effectively applied to a considerably broader class of singularities than the ones investigated in Sections 3 - 5 (see Section 6).

The principal advantage of the approach of this paper is its generality (see Sections 3 - 6). Also, since almost all integration weights are equal, it is convenient from the programming point of view (see, for example, [2]). An obvious drawback of the algorithm is the fact that there is no simple analytical expression for the corrections; they have to be evaluated numerically for each type of singularity, and for each subdivision of the interval of integration, unless the singularity is either of the form $log(x)$, or of the form x^γ.

2. End-point corrected trapezoidal rules for singular functions

A right-end point corrected trapezoidal rule T_α^n is defined by the formula

$$T_\alpha^n(f) = h \cdot (\frac{f(x_n)}{2} + \sum_{i=1}^{n-1} f(x_i)) + h \cdot \sum_{j=1}^{m} \alpha_j \cdot f(x_{n-j+1}) \tag{2.1}$$

where $f : (0,1] \to R^1$ is an integrable function, n, m are a pair of natural numbers, $h = \frac{1}{n}, x_i = \frac{i}{n}$, for $i = 1, 2, ..., n$, and $\alpha = (\alpha_1, \alpha_2, ..., \alpha_m)$ is a finite sequence of real numbers. We will say that the rule T_α^n is of right-end order $k \geq 1$ iff for any $f \in c^{k+1}[0,1]$ such that $f(0) = f'(0) = ... = f^{(k)}(0) = 0$, there exists $c > 0$ such that

$$| T_\alpha^n(f) - \int_0^1 f(t)dt |< \frac{c}{n^k}. \tag{2.2}$$

It easily follows from the Euler-Maclaurin formula that for any $k \geq 1$, there exists a vector $\alpha = (\alpha_1, ..., \alpha_k)$ such that the right- end order of the formula T_α^n is equal to k (see, for example, [6]).

Suppose now that the function $f : (0,1] \to R^1$ is of the form

$$f(x) = \phi(x) \cdot s(x) + \psi(x) \tag{2.3}$$

with $\phi, \psi \in c^k[0,1]$, and $s \in c(0,1]$ an integrable function with a singularity at zero. For a finite sequence $\beta = (\beta_1, \beta_2, ..., \beta_m)$, we will define the mapping $T_{\alpha\beta}^n : c(0,1] \to R^1$ by the formulae

$$T_{\alpha\beta}^n(f) = T_\alpha^n(f) + h \cdot \sum_{i=1}^{m} \beta_i f(\chi_i), \tag{2.4}$$

$$\chi_i = i \cdot \frac{h}{m}, i = 1, 2, ..., m. \tag{2.5}$$

We will use expressions $T^n_{\alpha\beta}$ with appropriately chosen α, β as quadrature formulae for for functions of the form (2.3), and the following construction provides a tool for finding β once α is given.

For a pair of natural numbers k, n, we will consider the following system of linear algebraic equations with respect to the unknowns $\beta^n_j, j = 1, 2, ..., 2k$:

$$\sum_{j=1}^{2k} \chi_j^{i-1} \cdot \beta_j^n = \int_0^1 x^{i-1} dx - T^n_\alpha(x^{i-1}) \tag{2.6}$$

for $i = 1, 2, ..., k$, and

$$\sum_{j=1}^{2k} \chi_j^{i-k+1} \cdot s(\chi_j) \cdot \beta_j^n = \int_0^1 s(x) \cdot x^{i-1} dx - T^n_\alpha(s(x) \cdot x^{i-1}) \tag{2.6}$$

for $i = k+1, k+2, ..., 2k$. We will denote the matrix of the system (2.6), (2.7) by A^{nk}_s, its right-hand side by Y^{nk}_s and its solution $(\beta^n_1, \beta^n_2, ..., \beta^n_{2k})$ by β^n_s. When there is no danger of confusion, we will omit some of the indices, and write $(\beta_1, \beta_2, ..., \beta_{2k})$ and β or β^n, instead of $(\beta^n_1, \beta^n_2, ..., \beta^n_{2k})$ and β^n_s respectively. The use ef expressions $T^n_{\alpha\beta}$ as quadrature formulae for functions of the form (2.3) is based on the following theorem.

Theorem 2.1.

Suppose that the systems (2.6), (2.7) have solutions $\beta^n = (\beta^n_1, \beta^n_2, ..., \beta^n_{2k})$ for all sufficiently large n, and that the sums

$$\sum_{j=1}^{2k} (\beta^n_j)^2 \tag{2.8}$$

are bounded uniformly with respect to n. Suppose further that the function $f : (0, 1] \to R^1$ is defined by (2.3). Then there exists such $c > 0$ that

$$| T^n_{\alpha\beta^n}(f) - \int_0^1 f(t) dt | < \frac{c}{n^k}. \tag{2.9}$$

for all sufficiently large n.

Proof.

Applying the Taylor expansion to the functions ϕ, ψ at $x = 0$, we obtain

$$f(x) = P(f)(x) + R_k(\phi)(x) \cdot s(x) + R_k(\psi), \tag{2.10}$$

where

$$P(f)(x) = s(x) \cdot \sum_{i=0}^{k} \frac{\phi^{(i)}(0)}{i!} \cdot x^i + \sum_{i=0}^{k} \frac{\psi^{(i)}(0)}{i!} \cdot x^i, \tag{2.11}$$

and $R_k(\phi), R_k(\psi)$ are such functions $[0, 1] \to R^1$ that

$$R_k(\phi)(0) = (R_k(\phi))'(0) = ... = (R_k(\phi))^{(k)}(0) = 0, \tag{2.12}$$

$$R_k(\psi)(0) = (R_k(\psi))'(0) = ... = (R_k(\psi))^{(k)}(0) = 0. \tag{2.13}$$

Substituting (2.10) into the left-hand side of (2.9), we obtain

$$
\begin{aligned}
&| T^n_{\alpha\beta^n}(f) - \int_0^1 f(t)dt | \leq \\
&| T^n_{\alpha\beta^n}(P(f)) - \int_0^1 P(f)(x)dx | \\
&+ | T^n_{\alpha\beta^n}(R_k(\phi)\cdot s) + R_k(\psi)) \\
&- \int_0^1 (s(x)\cdot R_k(\phi)(x) + R_k(\psi)(x))dx | .
\end{aligned}
\tag{2.14}
$$

Due to (2.6), (2.7),

$$
T^n_{\alpha\beta^n}(P(f)) - \int_0^1 P(f)(x)dx = 0, \tag{2.15}
$$

and we have

$$
\begin{aligned}
&| T^n_{\alpha\beta^n}(f) - \int_0^1 f(t)dt | \leq \\
&| T^n_{\alpha}(s\cdot R_k(\phi)) - \int_0^1 s(x)\cdot R_k(\phi)(x)dx | \\
&+ | T^n_{\alpha}(R_k(\psi)) - \int_0^1 R_k(\psi)(x)dx | \\
&+ | \sum_{j=1}^{2k}(R_k(\phi)(\chi_j)\cdot s(\chi_j) \\
&+ R_k(\psi)(\chi_j))\cdot \beta^n_j | .
\end{aligned}
\tag{2.16}
$$

Now the conclusion of the theorem follows from (2.2) (2.8), (2.12), (2.13), and Lemma A.2.

3. Convergence rates for singularities of the forms x^γ and $log(x)$

For the remainder of this paper, $\phi_1, \phi_2, ..., \phi_{2k}$ will denote functions $(0,1] \to R^1$ defined by the formulae

$$
\phi_i(x) = x^{i-1} \; for \; i = 1, 2, ..., k, \tag{3.1}
$$

$$
\phi_i(x) = x^{i-1}\cdot s(x) \; for \; i = k+1, k+2, ..., 2k. \tag{3.2}
$$

Lemma 3.1.

If $s(x) = x^\gamma$ with γ a real number such that $0 <| \gamma |< 1$ then the functions $\phi_1, \phi_2, ..., \phi_{2k}$ constitute a Chebychev system on the interval $(0,1]$ (i.e. the determinant of the $2k \times 2k$ -matrix B defined by the formula $B_{ij} = \phi_i(t_j)$ is non-zero) for any $2k$ distinct points $t_1, t_2, ..., t_{2k}$ on that interval.

Proof.

For a finite sequence $p_1, p_2, ..., p_{2k}$ of $2k$ real numbers, P will denote a mapping $(0,1] \to R^1$ defined by the formula

$$
P(t) = \sum_{i=1}^{2k} p_i \cdot \phi_i(t). \tag{3.2}
$$

We will prove the lemma by showing that if $t_1, t_2, ..., t_{2k}$ are distinct points on the interval $(0,1]$ and $P(t_i) = 0$ for all $i = 1, 2, ..., 2k$ then all $2k$ coefficients $p_1, p_2, ..., p_{2k}$ are equal to zero. By repeated application of the Rolle theorem, we conclude that there exist k distinct points $y_1, y_2, ..., y_k$ on the interval $(0,1)$ such that $P^{(k)}(y_i) = 0$ for all $i = 1,2,...,k$. Differentiating (3.2) k times, we obtain

$$P^{(k)}(y_j) = y_j^{\gamma-k} \cdot \sum_{i=1}^{k} p_{k+i} \cdot w_i \cdot y_j^{i-1} \tag{3.3}$$

with $w_i = (i-1+\gamma)(i-2+\gamma)...(i-k+\gamma)$, and it is clear that $w_i \neq 0$ for all $i = 1,2,...,k$. Now it follows from Lemma A.3 that

$$p_{k+1} = p_{k+2} = ... = p_{2k} = 0. \tag{3.4}$$

Substituting (3.4) into (3.2) and applying Lemma A.3 again, we see that $p_1 = p_2 = ... = p_k = 0$.

Theorem 3.1.

If $s(x) = x^\gamma$ with $0 <| \gamma |< 1$ then the convergence rate of the quadrature rule $T^n_{\alpha\beta^n}$ is at least k.

Proof.

It immediately follows from Lemma 3.1 that the matrix of the system (2.6), (2.7) is non-singular. We rescale the system (2.6), (2.7) by multiplying its $i-th$ equation by $(n \cdot k)^{i-1}$ for $i = 1,2,...,k$, and by $(n \cdot k)^{i-1-k+\gamma}$ for $i = k+1, k+2, ..., 2k$, obtaining the system of equations

$$\begin{aligned}
1^0 \cdot \beta_1^n + 2^0 \cdot \beta_2^n + ... + (2k)^0 \cdot \beta_{2k}^n &= \frac{(\int_0^1 1dx - T_\alpha^n(1))}{(n\cdot k)^0} \\
1^1 \cdot \beta_1^n + 2^1 \cdot \beta_2^n + ... + (2k)^1 \cdot \beta_{2k}^n &= \frac{(\int_0^1 xdx - T_\alpha^n(x))}{(n\cdot k)^1} \\
&\dots\dots\dots\dots \\
&\dots\dots\dots\dots \\
1^{k-1} \cdot \beta_1^n + 2^{k-1} \cdot \beta_2^n + ... + (2k)^{k-1} \cdot \beta_{2k}^n &= \frac{(\int_0^1 x^{k-1}dx - T_\alpha^n(x^{k-1}))}{(n\cdot k)^{k-1}} \\
1^{\gamma} \cdot \beta_1^n + 2^{\gamma} \cdot \beta_2^n + ... + (2k)^{\gamma} \cdot \beta_{2k}^n &= \frac{(\int_0^1 x^{\gamma}dx - T_\alpha^n(x^{\gamma}))}{(n\cdot k)^{\gamma}} \\
1^{\gamma+1} \cdot \beta_1^n + 2^{\gamma+1} \cdot \beta_2^n + ... + (2k)^{\gamma+1} \cdot \beta_{2k}^n &= \frac{(\int_0^1 x^{\gamma+1}dx - T_\alpha^n(x^{\gamma+1}))}{(n\cdot k)^{\gamma+1}} \\
&\dots\dots\dots\dots \\
&\dots\dots\dots\dots \\
1^{\gamma+k-1} \cdot \beta_1^n + 2^{\gamma+k-1} \cdot \beta_2^n + ... + (2k)^{\gamma+k-1} \cdot \beta_{2k}^n &= \frac{(\int_0^1 x^{\gamma+k-1}dx - T_\alpha^n(x^{\gamma+k-1}))}{(n\cdot k)^{\gamma+k-1}}
\end{aligned} \tag{3.5}$$

with respect to the unknowns $\beta_n^1, \beta_n^2, ..., \beta_{2k}^n$, and we will denote the matrix of the system (3.5) by B_k , and its right-hand side by Z_k^n . Obviously, B_k is independent of n, and $|Z_k^n|$ is bounded uniformly with respect to n due to Lemma A.2. Consequently, the solution of (3.5) is bounded uniformly with respect to n, and due to Theorem 2.1, the convergence rate of $T^n_{\alpha\beta^n}$ is at least k.

The proofs of the Lemma 3.1 and Theorem 3.1 can be repeated almost verbatim with $s(x) = log(x)$ instead of $s(x) = x^\gamma$, resulting in the following theorem.

Theorem 3.2.

If $s(x) = log(x)$ then the convergence rate of the quadrature rule $T^n_{\alpha\beta^n}$ is at least k.

4. Convergence rates for more general singularities

Theorem 4.1.

Suppose that the function $s : (0,1] \rightarrow R^1$ is such that

$$\lim_{x\to 0} \frac{x \cdot s'(x)}{s(x)} = a \tag{4.1}$$

with $0 <| a |< 1$. Then for sufficiently large n, the matrix A^{nk}_s of the system (2.6), (2.7) is non-singular, and the convergence rate of $T^n_{\alpha\beta^n}$ at least k.

Proof.

The proof below effectively consists of approximating $s(x)$ on the interval $[\chi_1, \chi_{2k}]$ by the function $\tilde{s} = \frac{s(\chi_1)}{\chi_1^a} \cdot x^a$ and using the Theorem 3.2.

We rescale the system (2.6), (2.7) by multiplying its $i-th$ equation by $(n \cdot k)^{i-1}$ for $i = 1, 2, ..., k$, and by $(n \cdot k)^{i-k-1}$ for $i = k+1, k+2, ..., 2k$, thus obtaining the system

$$\begin{aligned}
1^0 \cdot \beta_1^n + 2^0 \cdot \beta_2^n + ... + (2k)^0 \cdot \beta_{2k}^n &= \frac{(\int_0^1 1dx - T^n_\alpha(1))}{(n \cdot k)^0} \\
1^1 \cdot \beta_1^n + 2^1 \cdot \beta_2^n + ... + (2k)^1 \cdot \beta_{2k}^n &= \frac{(\int_0^1 xdx - T^n_\alpha(x))}{(n \cdot k)^1} \\
&\dots\dots\dots\dots\dots\dots \\
&\dots\dots\dots\dots\dots\dots \\
1^{k-1} \cdot \beta_1^n + 2^{k-1} \cdot \beta_2^n + ... + (2k)^{k-1} \cdot \beta_{2k}^n &= \frac{(\int_0^1 x^{k-1}dx - T^n_\alpha(x^{k-1}))}{(n \cdot k)^{k-1}} \\
1^0 \cdot \frac{s(\chi_1)}{s(\chi_1)} \cdot \beta_1^n + 2^0 \cdot \frac{s(\chi_2)}{s(\chi_1)} \cdot \beta_2^n + & \\
... + (2k)^0 \cdot \frac{s(\chi_{2k})}{s(\chi_1)} \cdot \beta_{2k}^n &= \frac{(\int_0^1 x^0 \cdot s(x)dx - T^n_\alpha(x^0 \cdot s(x)))}{s(\chi_1) \cdot (n \cdot k)^0} \\
1^1 \cdot \frac{s(\chi_1)}{s(\chi_1)} \cdot \beta_1^n + 2^1 \cdot \frac{s(\chi_2)}{s(\chi_1)} \cdot \beta_2^n + & \\
... + (2k)^1 \cdot \frac{s(\chi_{2k})}{s(\chi_1)} \cdot \beta_{2k}^n &= \frac{(\int_0^1 x^1 \cdot s(x)dx - T^n_\alpha(x^1 \cdot s(x)))}{s(\chi_1) \cdot (n \cdot k)^1} \\
&\dots\dots\dots\dots\dots\dots \\
&\dots\dots\dots\dots\dots\dots \\
1^{k-1} \cdot \frac{s(\chi_1)}{s(\chi_1)} \cdot \beta_1^n + 2^{k-1} \cdot \frac{s(\chi_2)}{s(\chi_1)} \cdot \beta_2^n + & \\
... + (2k)^{k-1} \cdot \frac{s(\chi_{2k})}{s(\chi_1)} \cdot \beta_{2k}^n &= \frac{(\int_0^1 x^{k-1} \cdot s(x)dx - T^n_\alpha(x^{k-1} \cdot s(x)))}{s(\chi_1) \cdot (n \cdot k)^{k-1}},
\end{aligned} \tag{4.2}$$

whose matrix we will denote by $\tilde{B}_k^n$. Due to Lemma A.2, the right-hand side of (4.2) is bounded for sufficiently large n, and by applying Lemma A.5, it is easy to see that

$$\tilde{B}_k^n = B_k + \delta_k^n \tag{4.3}$$

with $(\delta_k^n), k = 1, 2, ...$ a sequence of $2k \times 2k$ matrices such that $\lim_{n\to\infty} \|\delta_k^n\| = 0$. Now it follows from Lemma A.4 that for sufficiently large n, $\|(B_k^n)^{-1}\|$ is uniformly bounded. Thus, the solution of (4.2) is uniformly bounded for sufficiently large n, and due to Theorem 2.1, the convergence rate of $T_{\alpha\beta^n}^n$ is at least k.

Theorem 4.2.

Suppose that $k \geq 1$ and a function $s : (0, 1] \to R^1$ is such that

1.. $s(x)$ is integrable on the interval $(0, 1]$.

2.. $\tilde{s}(x) = \frac{1}{s(x)}$ is integrable on the interval $(0, 1]$.

3.. s is monotonic in some neighborhood of 0.

4.. The system (2.6), (2.7) has a unique solution for all sufficiently large n.

5.. The convergence rate of $T_{\alpha\beta_s^n}^n$ is at least k.

Then the convergence rate of the quadrature rule $T_{\alpha\beta_{\tilde{s}}^n}^n$ is at least $k - 1$.

Proof.

Again, we start with rescaling the equations (2.6), (2.7). We define a diagonal $2k \times 2k$ -matrix D by the formula

$$D_{ii} = \frac{1}{s(\chi_i)} \tag{4.4}$$

for $i = 1, 2, ..., 2k$, and the theorem easily follows from the observation that $A_{\tilde{s}}^{nk} = A_s^{nk} \cdot D$.

Observation 4.1.

The combination of the Theorems 3.1, 3.2, 4.1, 4.2 permits one to apply end-point corrected trapezoidal quadrature rules to a fairly wide variety of singular functions, including linear combinations of powers of x, products of powers of x with $log(x)$, etc. Further genaralizations of the quadrature rules $T_{\alpha\beta^n}^n$ are discussed in Section 7.

5. Asymptotic behaviour of correction coefficients as $n \to \infty$

An obvious drawback of the expressions $T_{\alpha\beta^n}^n$ as practical quadrature rules is the fact that the weights $\beta_1^n, \beta_2^n, ..., \beta_{2k}^n$ have to be determined for each value of n by solving a system of linear algebraic equations (albeit a small-scale one). In this section, we eliminate this problem for the cases $s(x) = x^\gamma$ and $s(x) = log(x)$ by constructing a new set of correction weights $\lambda_1, \lambda_2, ..., \lambda_{2k}$ independent of n, and such that the quadrature rules $T_{\alpha\lambda}^n$ are still of order not less than k.

Lemma 5.1.

Suppose that $\alpha = (\alpha_1, \alpha_2, ..., \alpha_m)$ is such that the right-end order of the quadrature formula T_α^n is m. Then for any $a > 0$ there exists $c > 0$ such that

$$\mid p^{a+1} \cdot (T_\alpha^p(x^a) - \int_0^1 x^a dx) - q^{a+1} \cdot (T_\alpha^q(x^a) - \int_0^1 x^a dx) \mid < \frac{c}{p^m} \tag{5.1}$$

for any integer p, q such that $p < q$.

Proof.

From the formula (2.1), it is easy to see that

$$\begin{aligned} T^q_\alpha(x^a) - \int_0^1 x^a dx &= \frac{1}{2q} + \frac{1}{q}\sum_{i=1}^{q+1}(\frac{i}{q})^a + \frac{1}{q}\sum_{j=1}^{m}\alpha_j(\frac{q-j+1}{q})^a - \int_0^1 x^a dx \\ &= (\frac{p}{q})^{a+1}\cdot\frac{1}{p}\sum_{i=1}^{p-1}(\frac{i}{p})^a + (\frac{1}{q}\sum_{j=1}^{m}\alpha_j(\frac{p-j+1}{q})^a \\ -\frac{1}{q}\sum_{j=1}^{m}\alpha_j(\frac{p-j+1}{q})^a) &+ \frac{1}{2q} + \frac{1}{q}\sum_{j=1}^{m}\alpha_j(\frac{q-j+1}{q})^a - \int_0^1 x^a dx \\ = (\frac{p}{q})^{a+1}\cdot(\frac{1}{p}\sum_{i=1}^{p-1}(\frac{i}{p})^a &+ \frac{1}{q}\sum_{j-1}^{m}\alpha_j(\frac{p-j+1}{a})^a + \frac{1}{2p}) - \int_0^{\frac{p}{q}} x^a dx + R_{pq} \end{aligned} \tag{5.2}$$

with R_{pq} defined by the formula

$$\begin{aligned} R_{pq} &= (\frac{1}{2q}(\frac{p}{q})^a + \frac{1}{q}\sum_{i=p+1}^{q-1}(\frac{1}{p})^a + \frac{1}{2q}) \\ &+ \frac{1}{q}\sum_{j=1}^{m}\alpha_j(\frac{q-j+1}{q})^a - \frac{1}{q}\sum_{j=1}^{m}\alpha_j(\frac{p-j+1}{q})^a - \int_{\frac{p}{q}}^1 x^a dx \end{aligned} \tag{5.3}$$

Due to Euler-Maclaurin formula,

$$R_{pq} = O((\frac{p}{q})^{m-a}\cdot(\frac{1}{q})^{m+1}) = O(\frac{1}{p^m}\cdot\frac{1}{q^{a+1}}) \tag{5.4}$$

and we conclude that

$$T^q_\alpha(x^a) - \int_0^1 x^a dx = (\frac{p}{q})^{a+1}\cdot(T^p_\alpha(x^a) - \int_0^1 x^a dx) + O(\frac{1}{p^m}\cdot\frac{1}{q^{a+1}}) \tag{5.5}$$

which is equivalent to (5.1).

Theorem 5.1.

Suppose that k, m are two natural numbers such that $k \leq m-1$ and that $\alpha = (\alpha_1, \alpha_2, ..., \alpha_m)$ is such that the quadrature rule T^n_α is of right-end order m. Suppose further that $s(x) = x^\gamma$ with $0 <| \gamma |< 1$, and that the coefficients $\beta^n_1, \beta^n_2, ..., \beta^n_{2k}$ are defined as solutions of the system (2.6), (2.7). Then

1.. There exists a limit

$$\lim_{n\to\infty} \beta^n_i = \lambda_i \tag{5.6}$$

for each $i = 1, 2, ..., 2k$.

2.. for all $i = 1, 2, ..., 2k$,

$$| \beta^n_i - \lambda_i |= O(\frac{1}{n^{m-k}}). \tag{5.7}$$

3.. λ_i do not depend on m, as long as $m \geq k+1$.

4.. The quadrature formulae $T^n_{\alpha\lambda}$ are of order at least k.

Proof.

Suppose that p, q are two natural numbers, and $p < q$. Obviously,

$$\begin{aligned} \beta^p &= (B_k)^{-1} \cdot Z_k^p \\ \beta^q &= (B_k)^{-1} \cdot Z_k^q \\ \beta^p - \beta^q &= B_k^{-1}(Z_k^p - Z_k^q). \end{aligned} \tag{5.8}$$

Due to Lemma 5.1, there exists $c > 0$ such that

$$\|Z_k^p - Z_k^q\| < (\frac{c}{p^{m-k}}), \tag{5.9}$$

and by combining (5.8) and (5.9), we see that for some $\tilde{s} > 0$,

$$\|\beta^p - \beta^q\| < \frac{\tilde{c}}{p^{m-k}}. \tag{5.10}$$

Since $\beta^1, \beta^2, ...$ constitute a Cauchy sequence, they converge to some limit $\lambda = (\lambda_1, \lambda_2, ..., \lambda_{2k})$, which proves 1., and 2.,3.,4., easily follow from (5.6),(5.10),(5.1), and (3.5).

The proof of the following theorem is a repetition almost verbatim of the proofs of the Lemma 5.1 and Theorem 5.1.

Theorem 5.2.

If under the conditions of the Theorem 5.1, the singularity $s(x) = x^\gamma$, is replaced with the singularity $s(x) = log(x)$, the conclusions 1. - 4. of the Theorem 5.1 remain correct.

Remark 5.1.

For singularities of the forms $x^\gamma, log(x)$, Theorems 5.1, 5.2 reduce the quadratures $T^n_{\alpha\beta^n}$ to a more "conventional" form

$$\int_0^1 f(x)dx \approx T^n_{\alpha\lambda}(f) = h \cdot (\sum_{i=1}^{n-1} f(x_i) + \frac{f(1)}{2} + h \cdot \sum_{j=1}^{m} \alpha_m f(x_{n-j+1}) + h \cdot \sum_{j=1}^{2k} \lambda_j f(\chi_j) \tag{5.8}$$

where f is defined by (2.3), $h = \frac{1}{n}, x_i = i \cdot h$ with $i = 1, 2, ..., n, \chi_j = j \cdot \frac{h}{2k}$ with $j = 1, 2, ..., 2k$, and the coefficients λ_j are independent of n.

Remark 5.2.

Theorems 3.1, 3.2, 4.1, 4.2, 5.1, 5.2 establish that under certain conditions the order of the quadrature rules $T^n_{\alpha\beta^n}, T^n_{\alpha\lambda}$ is not less than k, where $2k$ is the length of the vectors $\beta^n = (\beta_1^n, \beta_2^n, ..., \beta_{2k}^n), \lambda = (\lambda_1, \lambda_2, ..., \lambda_{2k})$. Somewhat more detailed versions of the proofs of these theorems show that the order of these quadratures always lies between k and $k+1$, and is in some cases equal to $k+1$. In the examples presented in the following section, we note the cases when the latter situation occures.

6. Numerical Results

Algorithms have been implemented for evaluating the quadratures $T^n_{\alpha\beta^n}$ under the conditions of the Theorems 3.1, 4.1, 4.2, and the quadratures $T^n_{\alpha\lambda}$ under the conditions of the Theorems 5.1, 5.2. The implementation of the algorithm for evaluating the quadratures $T^n_{\alpha\beta^n}$ is completely stright-forward. After evaluating the matrix A^{nk}_s and the right-hand side Y^{nk}_s of the system (2.6), (2.7), the system is solved by means of a LINPAK Gaussian elimination subroutine, and the resulting correction weights are used in the quadrature formulae $T^n_{\alpha\beta^n}$ (see formula (2.4)).

In order to evaluate the coefficients $\lambda_1, \lambda_2, ... \lambda_{2k}$ for singularities of the forms $x^\gamma, log(x)$, we start with a right-end corrected trapezoidal rule T^n_α of order 20, obtained by means of the Euler-Maclaurin formula. Under these conditions,

$$| \beta^n_i - \lambda_i | < O(\frac{1}{n^{20-k}}) \qquad (6.1)$$

for all $i = 1, 2, ..., 2k$ (see Theorems 5.1, 5.2), and for reasonable k, the convergence of β^n_i to λ_i is almost instantaneous. We used $n = 64$ and REAL *16 arithmetic to obtain 15 significant digits presented in the examples below.

In the Tables 1 - 6, the coefficients $\lambda_1, \lambda_2, ... \lambda_{2k}$ are listed for singularities of the forms $log(x), x^{\frac{1}{2}}, x^{-\frac{1}{2}}, x^{\frac{1}{3}}, x^{-\frac{1}{3}}, x^{-\frac{9}{10}}$, and $k = 2, 3, 4$. It is clear from these tables that the correction weights $\lambda_1, \lambda_2, ... \lambda_{2k}$ grow rapidly as k increases, causing increased round-off errors and making the use of large k impractical in actial computations.

In many cases, $k = 3$ appears to be a reasonable compromise, resulting in roughly 4-th order convergent rules, and not involving unreasonably large correction weights. Combining such a rule with a standard 4-th order end-point corrections at the right end of the interval (see, for example, [1]) we obtain the following quadrature formula

$$\int_0^1 f(x)dx = h \cdot (\sum_{i=1}^{n} f(x_i) + \sum_{j=1}^{6} \lambda_j \cdot f(x_j) - \frac{f(x_n)}{2} - \frac{1}{24}(f(x_{n-2}) - 4f(x_{n-1}) + 3f(x_n))) \qquad (6.2)$$

with $h = \frac{1}{n}, x_i = i \cdot h$ for $i = 1, 2, ..., n$, and $\chi_j = \frac{h}{6} \cdot j$ for $j = 1, 2, ..., 6$. For the six singularities listed above, the coefficients $\lambda_1, \lambda_2, ... \lambda_6$ can be found in the middle columns of the Tables 1 - 6. In the Table 7, convergence results are presented for some of the rules $T^n_{\alpha\beta}$ and $T^n_{\alpha\lambda}$ with $k = 3$ and T^n_α a standard 4-th order end-point correction. Column 1 of this table contains the numbers of nodes into which the interval $[0, 1]$ was discretized. In all cases, the integrand was of the form

$$f(x) = (sin(23x) + cos(24x)) \cdot s(x) + (sin(21x) + cos(22x)), \qquad (6.3)$$

with columns 2, 3, 4 containing the relative errors for the rule $T^n_{\alpha\lambda}$ with $s(x)$ equal to $log(x), x^{\frac{1}{2}}$, and $x^{-\frac{9}{10}}$ respectively. Columns 5, 6 contain relative errors for the rule $T^n_{\alpha\beta^n}$ with $s(x)$ equal to $x^{-\frac{2}{3}} \cdot log(x) + x^{-\frac{1}{4}}$ and $(log(x))^2$ respectively. Finally, column 7 contains relative errors for the standard 4-th order end-point corrected trapezoidal rule applied to the function $(sin(21x) + cos(22x))$, presented here for comparison.

The following observations can be made from Table 7, and are typical for the quadratures $T^n_{\alpha\lambda}, T^n_{\alpha\beta^n}$.

1.. In all cases, the speed of convergence is roughly the same as for the end-point corrected trapezoidal rule applied to the function $(sin(21x) + cos(22x))$ (column 7).

2.. For the singularities $log(x)$ and $x^{\frac{1}{2}}$, the rules $T^n_{\alpha\lambda}$ display a typical 4-th order convergence.

3.. In columns 3 - 5, the convergence is somewhat erratic, especially for $s(x) = x^{-\frac{9}{10}}$, in which case the rule seems to fail after $n = 320$. In order to clarify the situation, the 4-th column of the Table 7 was extended with $n = 2560, 5120, 10240, 20480$. The extension is shown in Table

8, from which it is clear that the bottom part of the column 4 in Table 7 should be described as erratic convergence, rather than a failure to converge.

4.. It appears from the 5-th column of Table 7 that the rule $T^n_{\alpha\beta^n}$ converges quite well for $s(x) = (log(x))^2$, even though this singularity is not covered by any of the theorems of the present paper. This has been repeatedly observed when the singularity s is monotonic, and in such cases a version of Theorem 4.1 is usually fairly easy to prove.

7. Generalizations and conclusions

The algorithm of the present paper admits several strightforward generalizations.

1.. There are classes of singularities not covered by this paper for which some versions of Theorems 3.1 and/or 5.1 can be fairly easily proven. The convergence of the quadrature rule for one of them ($(log(x))^2$) is demonstrated in the preceeding section.

2.. Correction nodes $\chi_1, \chi_2, ..., \chi_{2k}$ do not have to be equispaced. A different distribution of nodes could possibly reduce absolute values of the correction weights $\lambda_1, \lambda_2, ...\lambda_{2k}$ and $\beta_1, \beta_2, ...\beta_{2k}$, thus improving the convergence. However, such specialized choice of correction nodes would have to be performed separately for each singularity s.

3.. The quadratures can be easily modified to handle functions of the form

$$f(x) = \psi(x) + \sum_{i=1}^{m} \phi_i(x) \cdot s_i(x) \tag{7.1}$$

where $\psi, \phi_1, \phi_2, ..., \phi_m$ are smooth functions, and $s_1, s_2, ..., s_m$ are several different singularities. However, it is easy to see that the absolute values of the weights β^n_i tend to grow very rapidly as m increases, and the author doubts the practical usefulness of such rules with $m > 2$.

4.. Quadrature rules $T^n_{\alpha\lambda}$, $T^n_{\alpha\beta^n}$ have fairly obvious analogues in two and three dimensions. However, the proofs of multi-dimensional versions of Theorems 3.1, 3.2, 4.1, 4.2, 5.1 are somewhat more involved than those of their one-dimensional counterparts. These results will be reported at a later date.

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Table 1

Correction Weights for the Singularity $s = log(x)$

k=2	k=3	k=4
0.160129841535717E+01	0.222876601846009E+01	0.309348340177712E+01
-.338255852191949E+01	-.123121207006261E+02	-.310178837674079E+02
0.362788846443413E+01	0.315796599730867E+02	0.136205915590327E+03
-.134662835787181E+01	-.384039159001043E+02	-.314747480872421E+03
	0.226735045911525E+02	0.421505412761263E+03
	-.526589398196889E+01	-.328785403878733E+03
		0.138801167137067E+03
		-.245552103718723E+02

Table 2

Correction Weights for the Singularity $s = x^{\frac{1}{2}}$

k=2	k=3	k=4
0.107622636973350E+01	0.140373389574362E+01	0.176138469558481E+01
-.147247373014210E+01	-.610626975465971E+01	-.138211834485298E+02
0.138293501775035E+01	0.145821441189467E+02	0.545915011781337E+02
-.486687657341754E+00	-.163961527863182E+02	-.117357484549871E+03
	0.895228275571686E+01	0.150779019932162E+03
	-.193573822942934E+01	-.114778491157932E+03
		0.476230959836121E+02
		-.829784263315958E+01

Table 3

Correction Weights for the Singularity $s = x^{-\frac{1}{2}}$

k=2	k=3	k=4
0.333895462377735E+01	0.515686238420012E+01	0.788957615797699E+01
-.103691855551396E+02	-.371802541857231E+02	-.101483910269331E+03
0.123881739056139E+02	0.105027804788073E+03	0.498205235333950E+03
-.485794297425160E+01	-.138820513091881E+03	-.124177860454341E+04
	0.879943166414350E+02	0.175109399358045E+04
	-.216782165361041E+02	-.141908515209795E+04
		0.617986326801910E+03
		-.112327464963600E+03

Table 4
Correction Weights for the Singularity $s = x^{\frac{1}{3}}$

k=2	k=3	k=4
0.120275440902998E+01	0.159679209113902E+01	0.207566347869413E+01
-.191590588964576E+01	-.749191954692780E+01	-.176817793306071E+02
0.189021521886824E+01	0.182610902534004E+02	0.723376732327415E+02
-.677063738252464E+00	-.210496743900247E+02	-.159272316539246E+03
	0.117997957518642E+02	0.207188787576306E+03
	-.261608415945115E+01	-.158671438914327E+03
		0.660717800591290E+02
		-.115483695626909E+02

Table 5
Correction Weights for the Singularity $s =^{-\frac{1}{3}}$

k=2	k=3	k=4
0.245072941794592E+01	0.363848721531386E+01	0.538493619088162E+01
-.671933111554788E+01	-.239520591801675E+02	-.636859586874130E+02
0.775314064392466E+01	0.653732223792864E+02	0.300979353674521E+03
-.298453894632270E+01	-.840421842099929E+02	-.731168698310276E+03
	0.520805019262272E+02	0.101261655245219E+04
	-.125979681306671E+02	-.809425283937431E+03
		0.348533467508443E+03
		-.627343688909117E+02

Table 6
Correction Weights for the Singularity $s = x^{-\frac{9}{10}}$

k=2	k=3	k=4
0.184790352839992E+02	0.321040181373839E+02	0.535441666101165E+02
-.765330172344763E+02	-.289780736142061E+03	-.846379842042659E+03
0.992955952836217E+02	0.895220650155513E+03	0.456845469197409E+04
-.407416133331446E+02	-.126326771498802E+04	-.121296416031938E+05
	0.841976333390815E+03	0.179000593914225E+05
	-.215752550553635E+03	-.150266053430178E+05
		0.673612868399159E+04
		-.125506014574396E+04

Table 7

Examples of Convergence of Quadrature Rules

n	$log(g)$	$x^{\frac{1}{2}}$	$x^{-\frac{9}{10}}$	$x^{-\frac{2}{3}}$ $\cdot log(x)$ $+x^{-\frac{1}{4}}$	$(log(x))^2$	
10	.503E-01	.326E-01	.157E+00	.870E-01	.105E+00	.246E+00
20	.412E-03	.478E-03	.189E-01	.121E+00	.590E-02	.177E-01
40	.546E-04	.498E-04	.964E-03	.148E-02	.219E-03	.115E-02
80	.102E-04	.506E-05	.422E-04	.584E-04	.651E-05	.722E-04
160	.992E-06	.359E-06	.146E-05	.243E-05	.434E-07	.453E-05
320	.803E-07	.233E-07	.359E-08	.679E-07	.180E-07	.283E-06
640	.600E-08	.147E-08	.958E-08	.159E-08	.241E-08	.177E-07
1280	.425E-09	.911E-10	.157E-08	.616E-09	.234E-09	.109E-08

Table 8

Extended Convergence Results for $s(x) = x^{-\frac{9}{10}}$

n	10	20	40	80	160	320
δ	.157E+00	.189E-01	.964E-03	.422E-04	.146E-05	.359E-08
n	640	1280	2560	5120	10240	20480
δ	.958E-08	.157E-08	.218E-9	.269E-10	.319E-11	.334E-12