On generalized Gaussian quadrature rules for singular and nearly singular integrals

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Abstract

We construct and analyze generalized Gaussian quadrature rules for integrands with endpoint singularities or near endpoint singularities. The rules have quadrature points inside the interval of integration and the weights are all strictly positive. Such rules date back to the study of Chebyshev sets, but their use in applications has only recently been appreciated. We provide error estimates and we show that the convergence rate is unaffected by the singularity of the integrand. We characterize the quadrature rules in terms of two families of functions that share many properties with orthogonal polynomials, but that are orthogonal with respect to a discrete scalar product that in most cases is not known a priori.

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Abstract

We construct and analyze generalized Gaussian quadrature rules for integrands with endpoint singularities or near endpoint singularities. The rules have quadrature points inside the interval of integration and the weights are all strictly positive. Such rules date back to the study of Chebyshev sets, but their use in applications has only recently been appreciated. We provide error estimates and we show that the convergence rate is unaffected by the singularity of the integrand. We characterize the quadrature rules in terms of two families of functions that share many properties with orthogonal polynomials, but that are orthogonal with respect to a discrete scalar product that in most cases is not known a priori.

1 Introduction

Gaussian quadrature has many advantages in the numerical integration of

$$\int_a^b w(x)f(x)\,\mathrm{d}x \approx \sum_{j=1}^n w_j f(x_j),$$

with a positive weight function $w(x) > 0$, $\forall x \in [a,b]$. First, all quadrature points w_j lie inside the interval $[a,b]$ of integration and the weights are all positive [8, 27]. As a result, applying such quadrature rules is numerically stable. Second, it is well known that among all interpolatory quadrature rules Gauss-type rules achieve the highest polynomial order. In particular, a Gaussian rule with n points is exact for polynomials at least up to degree $2n-1$. Convergence is therefore quite fast if the integrand is sufficiently smooth. It follows from the Weierstrass theorem and from the positivity of the weights that convergence is guaranteed for all continuous functions f on $[a,b]$. Finally, Gaussian quadrature rules can be computed efficiently owing to their connection to orthogonal polynomials [9, 19], with a computational cost that scales as $O(n^2)$ [10]. A disadvantage of Gaussian rules is their inherent lack of adaptivity: different values of n lead to entirely different sets of quadrature points and weights. This is not the case, for example, for Clenshaw-Curtis rules, that otherwise share many of

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the advantages of Gaussian rules [29]. Several ways have been suggested to remedy the situation, most notably Gauss-Kronrod and Gauss-Kronrod-Patterson extensions [18, 22]. For modest values of n, the issue of adaptivity is less severe. In this paper, we consider the generalization of Gaussian quadrature rules in a different direction, focusing on achieving high accuracy for small n.

The main subject of this paper concerns quadrature rules of Gaussian type for non-smooth functions f. Though convergence of classical Gauss-type quadrature for such functions is possible, the convergence rate is low and the use of large n in quadrature is not recommended. Instead, research has focused on composite quadrature, singularity-removing transformations [28], graded meshes [25] and, in general, adaptive methods [4]. An efficient alternative was suggested however in [20]. Assume the integrand has the general form

$$f(x) = u(x) + v(x)\psi(x),$$

where both u and v are smooth functions, and $\psi(x)$ has an integrable singularity of some kind, such as $\psi(x) = \log(x-a)$ or $\psi(x) = (x-a)^\alpha$ with $\alpha > -1$. It was proved in [20] that for many singular choices of ψ a *generalized Gaussian quadrature* formula exists, of the form $\sum_{j=1}^n w_j f(x_j)$ and with the following properties:

1. $x_j \in (a,b)$ and $w_j > 0, \quad j = 1,\ldots,n,$
2. $\sum_{j=1}^n w_j [x_j^k + x_j^l \psi(x_j)] = \int_a^b w(x)[x^k + x^l\psi(x)]\,\mathrm{d}x, \quad k,l = 0,\ldots,n-1.$

The first property indicates that, like classical Gauss-type rules, the quadrature points lie inside the interval $[a,b]$ and the weights are all positive. The second property states that the singularity is integrated exactly if u and v are polynomials up to degree $n-1$. This rule is said to be Gaussian because $2n$ functions are integrated exactly using only n function evaluations. Note the important property that the rule only evaluates f, and not u or v. It is sufficient that u and v exist – they need not be known explicitly. Thus, the quadrature rule is a numerically stable approach for integrating non-smooth functions, as long as the lack of smoothness is confined to a known function $\psi(x)$. For this reason, we call f a function with a *confined singularity.*

The existence of generalized Gaussian quadrature rules dates back to Markov in the study of Chebyshev sets [21]. A more recent treatise is given in [15]. It follows from this theory that a quadrature rule with n points exists that integrates $2n$ basis functions ϕ_k exactly,

$$\sum_{j=1}^n w_j \phi_k(x_j) = \int_a^b w(x)\phi_k(x)\,\mathrm{d}x, \qquad k = 1,\ldots,2n, \tag{1}$$

if $\{\phi_k\}_{k=1}^{2n}$ is a Chebyshev set. Functions of the form $x^k + x^l\psi(x)$ are only a special case of this more general setting (albeit possibly a limiting special case if $\psi(x)$ is unbounded [20]).

One of the advantages listed above of classical Gauss-type properties has long been missing: an efficient construction algorithm. Generalized Gaussian quadrature rules were described for special cases only in literature, for example in [11, 24, 7]. Two generally applicable numerical methods for computing these rules were first described in [20, 30]. These authors also introduced the name *generalized Gaussian quadrature*. The proposed methods essentially consist of a continuation approach combined with Newton's method to solve the set of $2n$ nonlinear equations (1) for the $2n$ unknowns w_j and x_j. Although not as efficient as orthogonal polynomial-based methods for classical rules, generalized Gaussian quadrature rules can be computed with reasonable efficiency for almost any basis set $\{\phi_k\}$. The results are particularly useful in integral equation methods, that require the evaluation of a large number of integrals with well-understood singular behaviour [26, 17, 16, 2].

The purpose of this paper is to analyze generalized Gaussian quadrature rules in the setting of functions with a confined singularity. Though more limited than the general theory, this setting is already most useful in applications. We provide error estimates for generalized Gaussian quadrature rules in §3. Next, in §4 we characterize generalized Gaussian quadrature rules in terms of two sequences of functions $R_n(x)$ and $S_n(x)$, that obey certain orthogonality properties and that vanish at the quadrature points. This theory is comparable to the theory in multivariate cubature formulae more than to the theory of univariate Gaussian quadrature [3, 6, 5]. We discuss scaling invariance of the quadrature rules in §5 and we briefly outline three approaches for the numerical construction of the rules in §6. We end with some numerical examples in §7.

2 Preliminaries

We consider in this paper the numerical approximation of the integral

$$I[f] := \int_a^b w(x) f(x)\, \mathrm{d}x, \tag{2}$$

where $w(x) > 0$, $x \in [a, b]$, by a quadrature rule $Q[\cdot]$ with n points and weights of the form

$$Q[f] := \sum_{j=1}^{n} w_j f(x_j). \tag{3}$$

This approximation carries an error

$$\epsilon[f] := |\ I[f] - Q[f]\ |.$$

2.1 Functions with a confined singularity

We assume that the function f has the form

$$f(x) = u(x) + v(x)\psi(x), \tag{4}$$

where u and v lie in $C^k[a, b]$ for some sufficiently large k. We make no assumptions on the smoothness of the function ψ, except that it is possibly unbounded only in one of the endpoints a or b.[1] This most basic case is, arguably, also the most useful case in applications, as it covers integrands with a singularity or near singularity at one of the endpoints. We note for example that all rules constructed in [20] fit this pattern.

[1] This condition appears in the proof of Theorem 3.4. It may conceivably be lifted to allow singularities at both endpoints at the cost of having less nice error estimates.

We introduce some more notation. We denote by P_m the set of polynomials up to degree m and we define P_{-1} to be the empty set. The sets of functions T_m, $m = 0, 1, \ldots$, are defined by

$$T_m := \begin{cases} \{\, 1,\, \psi,\, x,\, x\,\psi, \ldots,\, x^{l-1}\,\psi,\, x^l\,\}, & m = 2l \text{ is even}, \\ \{\, 1,\, \psi,\, x,\, x\,\psi, \ldots,\, x^{l-1}\,\psi,\, x^l,\, x^l\psi\,\}, & m = 2l+1 \text{ is odd}. \end{cases} \tag{5}$$

They form the sequence $\{1\}$, $\{1, \psi\}$, $\{1, \psi, x\}$, $\{1, \psi, x, x\psi\}$, ... The corresponding function spaces are defined as

$$V_m := \operatorname{span}\{T_m\}, \qquad m = 0, 1, \ldots$$

Note that the functions in V_m are not in general square integrable, because $\psi(x)^2$ may not be integrable on $[a, b]$.

2.2 Existence of the quadrature rule

We assume in this paper that the function ψ is such that a generalized Gaussian quadrature rule exists for all n. That is, we assume that

$$Q[\phi] = I[\phi], \qquad \forall \phi \in T_{2n-1}. \tag{6}$$

Expression (6) leads to a set of $2n$ nonlinear equations in w_j and x_j – it corresponds exactly to expression (1) in our new notation.

Existence and uniqueness of the quadrature rule is guaranteed if T_{2n-1} is a Chebyshev set on $[a, b]$. This is a side-result of a more general theory on the geometric properties of the *moment spaces* that are induced by a Chebyshev set (see [21, 15]). More recently, it was proved in [20] that existence and uniqueness is guaranteed if T_{2n-1} is a Chebyshev set on any closed subinterval of (a, b). The latter generalization allows unbounded singularities at the endpoints. It should be mentioned that these results yield sufficient, but not necessary conditions.

In both cases, we can define an interpolation operator $\mathcal{P}_{\mathbf{x}}$ for a set of points $\mathbf{x} = \{x_j\}_{j=1}^n$ such that $\mathcal{P}_{\mathbf{x}}[f] \in V_{n-1}$ and

$$(\mathcal{P}_{\mathbf{x}}[f])(x_j) = f(x_j), \qquad j = 1, \ldots, n. \tag{7}$$

Assuming that T_{n-1} is a Chebyshev set on all closed subsets of (a, b), this operator is the identity on V_{n-1} for all sets $\mathbf{x}$ with $x_j \in (a, b)$, $j = 1, \ldots, n$.

Note that the choice of $\psi(x)$ is not as free as the choice of the weight function $w(x)$. Any weight function that satisfies $w(x) > 0$ on $[a, b]$ will do. On the other hand, it is known that the function $\psi(x)$ should be either monotonuously increasing or decreasing, in order to obtain a Chebyshev set. The main choices the authors have in mind are $\psi(x) = \log(x + \delta)$ and $\psi(x) = (x + \delta)^\alpha$, with $\alpha > -1$ and where δ determines the location of the singularity.

3 Error estimates

The central result in this section is the error estimate, proved in Theorem 3.4,

$$\epsilon[f] \leq \frac{1}{(n-1)!}\,(b-a)^n\, \left(W \|u^{(n)}\|_\infty + (2WC_\psi + W_\psi)\|v^{(n)}\|_\infty \right),$$

with the constants defined as in the theorem and depending only on the weight function $w(x)$ and the singularity function $\psi(x)$. The estimate shows that the convergence of the quadrature rule is unaffected by the unboundedness or the lack of smoothness of the singularity function ψ, even though ψ is evaluated implicitly in f and the smooth functions u and v are unknown.

3.1 The Peano kernel

Error estimates for interpolatory quadrature rules are most often given in terms of a derivative of f, with the order of the derivative depending on the polynomial degree of the rule. These estimates can be obtained from error estimates for polynomial interpolation or from the Peano kernel theorem. General error estimates for interpolation by Chebyshev sets are not available. The specific form of the function spaces V_{2n-1} however enables the use of the Peano kernel theorem [23]. For a functional $L[f]$ and an integer $k \geq 0$, the Peano kernel is defined by

$$K(\theta) = \frac{1}{k!} L_x[\,(x-\theta)_+^k\,], \tag{8}$$

with

$$(x-\theta)_+^k = \begin{cases} (x-\theta)^k, & x \geq \theta, \\ 0, & x < \theta. \end{cases} \tag{9}$$

The notation $L_x[\cdot]$ indicates that the functional L operates on a function of x. In the following Theorem, $\mathcal{V}[a,b]$ is the space of real-valued function on $[a,b]$ that are of bounded variation.

Theorem 3.1 (Peano kernel [23])**.** *Let k be any non-negative integer, and let L be a bounded linear functional from $\mathcal{V}[a,b]$ to $\mathbb{R}$, such that $L[f]$ is zero when f is in P_k, and such that the function $K(\theta)$, $a \leq \theta \leq b$, defined by equation (8), is of bounded variation. Then, if f is in $C^{k+1}[a,b]$, the functional $L[f]$ has the value*

$$L[f] = \int_a^b K(\theta) f^{(k+1)}(\theta)\,\mathrm{d}\theta. \tag{10}$$

The proof is based on an expression for the remainder in a Taylor series of f. An estimate follows of the form

$$|L[f]| \leq \|K\|_1 \|f^{(k+1)}\|_\infty. \tag{11}$$

In the following section, from Theorem 3.1 we will obtain bounds for the error $L[f] := I[f] - Q[f]$ in terms of a derivative of f.

3.2 Functions with a confined singularity

Let us first apply the Peano kernel theorem to smooth functions $f(x) = u(x)$. The operator

$$L_1[u] := I[u] - Q[u] \tag{12}$$

defines the error in the numerical approximation of the integral $I[u]$ by a generalized Gaussian quadrature rule with n points.

Lemma 3.2. *For $u \in C^n[a,b]$, we have*

$$|I[u] - Q[u]| \leq \frac{1}{(n-1)!}\, W\,(b-a)^n \|u^{(n)}\|_\infty,$$

where $W := \int_a^b w(x)\,\mathrm{d}x$.

Proof. The quadrature rule is exact for polynomials up to degree $n-1$. Thus, the Peano kernel (8) is given by

$$K(\theta) = \frac{1}{(n-1)!}\left(I[\,(x-\theta)_+^{n-1}\,] - Q[\,(x-\theta)_+^{n-1}\,]\right). \tag{13}$$

We have, for $\theta \in [a,b]$,

$$\begin{aligned} I[(x-\theta)_+^{n-1}] &= \int_a^b w(x)(x-\theta)_+^{n-1}\,\mathrm{d}x = \int_\theta^b w(x)(x-\theta)^{n-1}\,\mathrm{d}x \\ &\leq W(b-\theta)^{n-1} \leq W(b-a)^{n-1}. \end{aligned}$$

We also have

$$\begin{aligned} Q[(x-\theta)_+^{n-1}] &= \sum_{j=1}^n w_j(x_j-\theta)_+^{n-1} \\ &\leq \sum_{j=1}^n w_j(b-\theta)^{n-1} \leq W(b-\theta)^{n-1} \leq W(b-a)^{n-1}. \end{aligned}$$

Note that in the latter derivation we have used the fact that the weights are all positive and that they sum up to W. Given that both $I[\,(x-\theta)_+^{n-1}\,]$ and $Q[\,(x-\theta)_+^{n-1}\,]$ in (13) are positive, we have

$$|K(\theta)| \leq \frac{1}{(n-1)!} W(b-a)^{n-1}.$$

It follows that

$$\|K\|_1 = \int_a^b |K(\theta)|\,\mathrm{d}\theta \leq \frac{1}{(n-1)!}\int_a^b W(b-a)^{n-1}\,\mathrm{d}\theta = \frac{1}{(n-1)!} W(b-a)^n.$$

The result now follows from the general error estimate (11). □

Next, we establish an error estimate for functions of the form $f(x) = \psi(x)v(x)$, where $v(x)$ is a smooth function. Define the linear functional

$$L_2[v] := I[\psi v] - Q[\psi v].$$

This functional is exact for polynomials up to degree $n-1$ and, hence, we can again invoke the Peano kernel theorem.

Lemma 3.3. *If $v \in C^n[a,b]$ and if $\psi(x) > 0, \forall x \in (a,b)$, we have*

$$|L_2[v]| \leq \frac{1}{(n-1)!}\, W_\psi\,(b-a)^n \|v^{(n)}\|_\infty,$$

where $W_\psi := \int_a^b w(x)\psi(x)\,\mathrm{d}x$.

Proof. The result follows from Lemma 3.2 by defining a weight function of the form $w(x)\psi(x)$. Note that, since $\psi(x)$ is in this lemma assumed to be positive, we indeed have

$$\sum_{j=1}^{n} w_j \psi(x_j) = \int_a^b w(x)\psi(x)\,\mathrm{d}x = W_\psi,$$

with all terms in the summation positive, as required in the proof of Lemma 3.2. □

We can now state the central result of this section.

Theorem 3.4. *Assume $f(x) = u(x) + v(x)\psi(x)$ with $u, v \in C^n[a, b]$. Then we have*

$$\epsilon[f] \leq \frac{1}{(n-1)!}(b-a)^n \left(W \|u^{(n)}\|_\infty + (2WC_\psi + W_\psi)\|v^{(n)}\|_\infty \right), \tag{14}$$

with constants W and W_ψ as defined in Lemma 3.2 and Lemma 3.3, and with

$$C_\psi \geq \min(|\sup_{x\in[a,b]} \psi(x)|\,,\,|\inf_{x\in[a,b]} \psi(x)|) \geq 0 \tag{15}$$

a positive and bounded constant.

Proof. We can not immediately invoke Lemma 3.3 because the function $\psi(x)$ is not necessarily positive on the open interval (a, b). We will construct a function $\tilde{\psi}(x) = A\psi(x) + B$ that is positive on (a, b). Define the values $M^+ = \sup_{x\in[a,b]} \psi(x)$ and $M^- = \inf_{x\in[a,b]} \psi(x)$. Next, define

$$\tilde{\psi}(x) := \begin{cases} \psi(x) - M^-, & \text{if } |M^-| \leq |M^+|, \\ -\psi(x) + M^+, & \text{otherwise.} \end{cases}$$

By our assumption that $\psi(x)$ can be unbounded in at most one endpoint, at least one of M^+ or M^- is finite. We have thus written $\tilde{\psi}(x) = A\psi(x) + B$, with $A = \pm 1$ and $|B| \leq C_\psi$ where C_ψ is finite. By construction, we have $\tilde{\psi}(x) \geq 0$, for $x \in (a, b)$.

We rewrite the function $f(x)$ in terms of $\tilde{\psi}(x)$, using that $1/A = A$,

$$f(x) = u(x) - \frac{B}{A}v(x) + \frac{1}{A}v(x)(A\psi(x) + B) = u(x) - ABv(x) + Av(x)\tilde{\psi}(x).$$

Note that if u and v are polynomials of degree k, than $u(x) - ABv(x)$ and $Av(x)$ are also polynomials of degree k. This means that the generalized Gaussian quadrature rules constructed using either $\psi(x)$ or $\tilde{\psi}(x)$ are the same.

We now apply Lemma 3.2, noting that $C_\psi > |AB| = |B|$,

$$|I[u - ABv] - Q[u - ABv]| \leq \frac{1}{(n-1)!} W\,(b-a)^n (\|u^{(n)}\|_\infty + C_\psi \|v^{(n)}\|_\infty).$$

Lemma 3.3 leads to

$$|I[\tilde{\psi}Av] - Q[\tilde{\psi}Av]| \leq \frac{1}{(n-1)!} W_{\tilde{\psi}}\,(b-a)^n \|v^{(n)}\|_\infty.$$

We also have

$$W_{\tilde{\psi}} = \int_a^b w(x)(A\psi(x) + B)\,\mathrm{d}x \leq W_\psi + C_\psi W.$$

The combination of the above inequalities proves the result. □

The importance of Theorem 3.4 is that it shows that the convergence of $Q[f]$ to $I[f]$ depends only on the smoothness of $u(x)$ and $v(x)$, irrespective of the lack of smoothness in $\psi(x)$. An advantage of the current method of proof is that the constants in the error estimate (14) are entirely explicit in their dependence on the functions $w(x)$ and $\psi(x)$.

3.3 Functions with multiple singularities

We digress briefly from the case of functions with a single confined singularity to note that the error estimates readily extend to the case of functions with multiple singularities. Consider m functions $\psi_m(x)$ and a function $f(x)$ with multiple singularities of the form

$$f(x) = \sum_{m=1}^{M} u_m(x)\psi_m(x), \tag{16}$$

where $u_m(x)$ are smooth functions, $m = 1, \ldots, M$. The function f may for example have singularities in both endpoints of the integration interval $[a, b]$. One is led to consider a quadrature rule $Q[f] = \sum_{j=1}^{n} w_j f(x_j)$ that satisfies

$$Q[x^k\psi_m] = I[x^k\psi_m], \qquad k = 0, \ldots, n_m - 1, \quad m = 1, \ldots .M. \tag{17}$$

In the following, we forego the existence question in favour of deriving error estimates. We assume for simplicity that all $\psi_m(x) \geq 0$ and moreover that the quadrature rule has positive weights.

Lemma 3.5. *Assume that all $\psi_m(x) \geq 0$, $\forall x \in [a, b]$, and define $L_m[u] := Q[u\psi_m] - I[u\psi_m]$. Then for $u \in C^{n_m}[a, b]$ we have*

$$|L_m[u]| \leq \frac{1}{(n_m - 1)!} W_{\psi_m} (b - a)^{n_m} \|u^{(n_m)}\|_\infty,$$

where $W_{\psi_m} = \int_a^b w(x)\psi_m(x)\,\mathrm{d}x$.

The proof of this Lemma is exactly like that of Lemma 3.3.

Theorem 3.6. *Let $Q[f] = \sum_{j=1}^{n} w_j f(x_j)$ satisfy conditions* (17) *for certain $n_m > 0$, $m = 1, \ldots, M$, and let $w_j > 0$, $j = 1, \ldots, n$ and $\psi_m(x) \geq 0$, $m = 1, \ldots, M$. Then for functions f of the form* (16) *we have*

$$|I[f] - Q[f]| \leq \sum_{m=1}^{m} \frac{1}{(n_m - 1)!} W_{\psi_m} (b - a)^{n_m} \|u^{(n_m)}\|_\infty, \tag{18}$$

with W_{ψ_m} defined as in Lemma 3.5.

Proof. We can write

$$L[f] - Q[f] = \sum_{m=1}^{m} L_m[u_m],$$

where the linear operators L_m are as in Lemma 3.5. The result follows immediately from Lemma 3.5 and from

$$\sum_{m=1}^{m} L_m[u_m] \leq \sum_{m=1}^{m} |L_m[u_m]|.$$

□

Note that the assumption $\psi_m(x) \geq 0$ simplifies the error estimate (18) compared to the previous estimate (14). This comes at a cost of having slightly less general results.

4 A theory of generalized Gaussian quadrature

4.1 Orthogonal polynomials

It is well known that the points of a classical Gaussian rule are the roots of a polynomial $p_n(x)$ of degree n that is uniquely determined, up to a constant factor, by the orthogonality conditions

$$\int_a^b w(x)\, x^k\, p_n(x)\, \mathrm{d}x = 0, \qquad k = 0, \ldots, n-1. \tag{19}$$

Let us denote the classical Gaussian quadrature rule relative to the weight function $w(x)$ by $Q^G[\cdot]$. The concept of orthogonality derives from an inner product, which is not available in the generalized setting. This, however, is not an essential argument in the characterization of Q^G by p_n. An alternative and more general point of view is that the quadrature rule Q^G is characterized by a set of functions that vanish at the quadrature points. This set in turn is characterized by p_n. The meaning of these statements is clarified in the following Lemma.

Lemma 4.1. *Let $I[f]$ be a linear, continuous functional defined on a vector space F of functions on $[a,b]$ and consider a quadrature rule $Q[f] = \sum_{j=1}^n w_j f(x_j)$. For a subspace $F_1 \subset F$, define*

$$F_0 = \{f_0 \in F_1 : f_0(x_j) = 0,\ j = 1, \ldots, n\}.$$

A necessary and sufficient condition for the existence of a quadrature rule that is exact for all $f \in F_1$ is

$$f_0 \in F_0 \Rightarrow I[f_0] = 0. \tag{20}$$

Proof. This is only a special case of Theorem 3.1 in [3] (with short proof). □

An interpolatory quadrature rule with n points x_j is based on interpolating n given function values by a polynomial of degree $n-1$. It is obvious that such rules can be exact for polynomials of degree up to $n-1$, as the function to integrate is recovered exactly by the interpolation. Lemma 4.1 gives conditions for exactness in a larger space F_1: the functional $I[f]$ has to vanish for all functions in F_1 that vanish at the quadrature points.

Consider for example the space $F_1 = P_{2n-1}$ of polynomials up to degree $2n-1$. Each polynomial that vanishes at all quadrature points can be factorized into a polynomial multiple of p_n. The space F_0 can therefore be characterized in terms of p_n by

$$F_0 \equiv \operatorname{span}\{p_n(x) x^k\}_{k=0}^{n-1}. \tag{21}$$

Condition (20) now corresponds exactly to the orthogonality conditions (19).

4.2 Characterizing generalized Gaussian quadrature rules

We return to the setting of a function f with a confined singularity of the form (4). Define the space of all functions in V_{2n-1} vanishing at a set $\mathbf{x} = \{x_j\}_{j=1}^n$ of n distinct points in (a, b) as

$$F_0(\mathbf{x}) := \{f \in V_{2n-1} | f(x_j) = 0,\ j = 1, \ldots, n\}. \tag{22}$$

The space $F_0(\mathbf{x})$ can not be characterized in terms of a single polynomial that vanishes at the points x_j as in (21). It can, however, be characterized in terms of two different functions $R_n(x)$ and $S_n(x)$ that vanish at the set of points. The space $F_0(\mathbf{x})$ then consists of a linear combination of polynomial multiples of $R_n(x)$ and $S_n(x)$. We show this first for the case where $n = 2l$ is even.

Lemma 4.2. *If $n = 2l$ is even, then each $f_0 \in F_0(\mathbf{x})$ can be written as*

$$f_0(x) = p(x)R_n(x) + q(x)S_n(x), \tag{23}$$

with $p, q \in P_{l-1}$ and where

$$R_n(x) = x^l - \mathcal{P}_{\mathbf{x}}[x^l], \qquad S_n(x) = x^l\psi(x) - \mathcal{P}_{\mathbf{x}}[x^l\psi]. \tag{24}$$

Conversely, each function of the form (23) with $p, q \in P_{l-1}$ lies in $F_0(\mathbf{x})$.

Proof. Recall that $\mathcal{P}_{\mathbf{x}}$ is an interpolation operator, that is defined by (7). It follows from the construction that $R_n(x_j) = S_n(x_j) = 0$. It follows in turn that any function of the form $p(x)R_n(x) + q(x)S_n(x) \in F_0(\mathbf{x})$ for $p, q \in P_{l-1}$. It remains to show that all functions $f_0 \in F_0(\mathbf{x})$ can be written this way.

We prove the decomposition by construction with a procedure similar to polynomial long division. Any function $f_0 \in F_0(\mathbf{x}) \subset V_{2n-1}$ can be written in the basis T_{2n-1} as

$$f_0(x) = \sum_{k=0}^{n-1} a_k x^k + \sum_{k=0}^{n-1} b_k x^k \psi(x),$$

with suitable coefficients a_k and b_k. We define the function $f_1(x)$ by

$$f_1(x) = f_0(x) - a_{n-1}x^{l-1}R_n(x) - b_{n-1}x^{l-1}\psi(x)S_n(x).$$

Note that we now have $f_1 \in V_{2n-3}$, so we can write

$$f_1(x) = \sum_{k=0}^{n-2} c_k x^k + \sum_{k=0}^{n-2} d_k x^k \psi(x).$$

with suitable coefficients c_k and d_k. We define $f_2(x)$ by

$$f_2(x) = f_1(x) - c_{n-2}x^{l-2}R_n(x) - b_{n-2}x^{l-2}\psi(x)S_n(x),$$

and so on. The procedure can be performed l times until we arrive at

$$f_0(x) = p(x)R_n(x) + q(x)S_n(x) + f_l(x),$$

where $p(x)$ and $q(x)$ are polynomials of degree $l - 1$ and $f_l \in V_{2n-1-2l} = V_{n-1}$. However, since $f_0(x_j) = 0$ we must have $f_l(x_j) = 0$. Therefore $\mathcal{P}_{\mathbf{x}}[f_l] \equiv 0$, which is only possible if $f_l(x) \equiv 0$. □

The case where n is odd is analogous, with small differences in the degree of polynomials involved only.

Lemma 4.3. *If $n = 2l - 1$ is odd, then each $f_0 \in F_0(\mathbf{x})$ can be written as*

$$f_0(x) = p(x)R_n(x) + q(x)S_n(x), \tag{25}$$

with $p(x) \in P_{l-2}$ and $q(x) \in P_{l-1}$, and where

$$R_n(x) = x^l - \mathcal{P}_{\mathbf{x}}[x^l], \qquad S_n(x) = x^{l-1}\psi(x) - \mathcal{P}_{\mathbf{x}}[x^{l-1}\psi]. \tag{26}$$

Conversely, each function of the form (25) *with $p(x) \in P_{l-2}$ and $q(x) \in P_{l-1}$ lies in $F_0(\mathbf{x})$.*

From Lemmas 4.2 and 4.3 a set of quadrature points x_j can be characterized as the common roots of the functions $R_n(x)$ and $S_n(x)$. Given a set of points $\mathbf{x}$, the weights of an interpolatory quadrature rule are found easily. Denote the n Lagrange functions by $\mathcal{L}_j(x) \in P_{n-1}$, $j = 1, \ldots, n$, i.e.

$$\mathcal{L}_j(x_{j'}) = \delta_{j-j'}, \qquad j, j' = 1, \ldots, n.$$

Then we have

$$w_j = I[\mathcal{L}_j]. \tag{27}$$

For any set of points $\mathbf{x}$, expression (27) yields a quadrature rule that is exact on V_{n-1} by construction. For the set of generalized Gaussian quadrature points, the rule is exact on V_{2n-1}. Assembling our results, we can prove the following theorem.

Theorem 4.4. *Let $\mathbf{x} = \{x_j\}_{j=1}^n$ be a set of n distinct points in (a, b) and define a quadrature rule $Q[f] = \sum_{j=1}^n w_j f(x_j)$ with weights given by* (27). *We have $Q[f] = I[f]$ for all $f \in V_{2n-1}$ if and only if*

$$I[x^k R_n] = 0, \qquad k = 0, \ldots, l-1, \tag{28}$$

$$I[x^k S_n] = 0, \qquad k = 0, \ldots, l-1, \tag{29}$$

if $n = 2l$ is even, and

$$I[x^k R_n] = 0, \qquad k = 0, \ldots, l-2, \tag{30}$$

$$I[x^k S_n] = 0, \qquad k = 0, \ldots, l-1, \tag{31}$$

if $n = 2l - 1$ is odd. The functions $R_n(x)$ and $S_n(x)$ are defined by (24) *for even n and by* (26) *for odd n.*

Proof. We consider only the case where $n = 2l$ is even. The case of odd n is proven in an analogous manner.

Assume for the first direction of the 'if and only if' statement that $\mathbf{x}$ is such that $Q[f]$ is exact on V_{2n-1}. It follows from the necessary condition in Lemma 4.1 that we should have

$$I[f_0] = 0, \qquad \forall f_0 \in F_0.$$

From Lemma 4.2, we may write $f_0(x) = p(x)R_n(x) + q(x)S_n(x)$. The functions $R_n(x)$ and $S_n(x)$ are well defined. We should have $I[f_0] = 0$ for all $p \in P_{l-1}$ and for all $q \in P_{l-1}$. This corresponds exactly to conditions (28)–(29).

Conversely, assume that for a given set $\mathbf{x}$ the conditions (28)–(29) hold. In that case, we have from Lemma 4.2 that $I[f_0] = 0$, for all $f_0 \in F_0$. This, according to Lemma 4.1, is a sufficient condition for the result. □

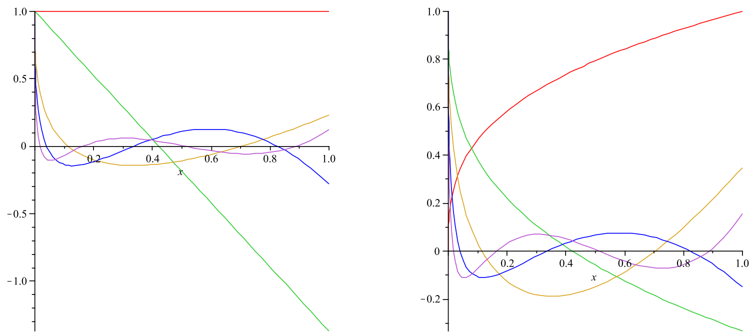

Figure 1: Plots of the functions $R_n(x)$ (left panel) and $S_n(x)$ (right panel) for $n = 0, \ldots, 4$, corresponding to the singularity function $\psi(x) = x^{1/3}$ on $[0, 1]$. The functions have been normalized such that $R_n(0) = Q_n(0) = 1$. Moreover, we have set $R_0(x) = x$ and $S_0(x) = x^{1/3}$.

Example 4.5. *The functions $R_n(x)$ and $Q_n(x)$ are illustrated in Figure 1 for the case $\psi(x) = x^{1/3}$ on the integration interval* $[0, 1]$.

The functions $R_n(x)$ and $S_n(x)$ retain some orthogonality properties: they are orthogonal to polynomials up to a degree of approximately $n/2$. They are not orthogonal to each other: recall that the product of two functions in V_m for some m may not be integrable, depending on the type of singularity. Yet, the functions $R_n(x)$ and $S_n(x)$ are not independent, as one completely characterizes the other and vice-versa through their common roots at the quadrature points. Denote by $\mathcal{R}(f)$ the set of roots of $f(x)$ on (a, b), for any f with n distinct roots. Then we have the nonlinear relations

$$R_n(x) = x^l - \mathcal{P}_{\mathcal{R}(S_n)}[x^l], \qquad \text{with } l = \left\lceil \frac{n}{2} \right\rceil, \tag{32}$$

and

$$S_n(x) = x^{l'}\psi(x) - \mathcal{P}_{\mathcal{R}(R_n)}[x^{l'}\psi], \qquad \text{with } l' = \left\lfloor \frac{n}{2} \right\rfloor. \tag{33}$$

4.3 Discrete orthogonality

In this section we attempt to further clarify the difference between classical Gaussian quadrature rules, connected to orthogonal polynomials, and generalized Gaussian quadrature rules, connected to the functions $R_n(x)$ and $S_n(x)$. We will show that the functions $R_n(x)$ and $S_n(x)$ are orthogonal to all functions in V_{n-1} with respect to a discrete scalar product, defined in terms of the points x_j and weights w_j of the generalized Gaussian quadrature rule as

$$u_n(f, g) := \sum_{j=1}^{n} w_j f(x_j) g(x_j). \tag{34}$$

Lemma 4.6. *The bilinear form* (34) *is a real scalar product on V_{n-1}.*

Proof. The form is linear and symmetric. It is positive, $u_n(f, f) \geq 0$, because the weights are all (strictly) positive. Finally, it is nondegenerate because

$u_n(f,f) = 0$ implies $f(x_j) = 0$, $j = 1,\ldots,n$ and, since no nonzero function in V_{n-1} vanishes at n distinct points, this in turn implies $f(x) \equiv 0$. □

Consider next the following sequence of orthogonal functions $r_{n,k}(x)$. Denote by $\{\phi_j\}_{j=0}^{n-1}$ a basis for V_{n-1}, for example $1, \psi, x, x\psi, \ldots$. Set

$$r_{n,0}(x) := \phi_0(x), \tag{35}$$

and define iteratively

$$r_{n,k}(x) = \phi_k(x) - \sum_{j=0}^{k-1} \frac{u_n(\phi_k, r_{n,j})}{u_n(r_{n,j}, r_{n,j})} r_{n,j}(x), \qquad k = 1,\ldots,n-1. \tag{36}$$

This Gram-Schmidt procedure leads to well-defined functions $r_{n,k}(x)$ that are orthogonal with respect to u_n.

Next, define the functions

$$r_{n,n}(x) = x^l - \sum_{j=0}^{n-1} \frac{u_n(x^l, r_{n,j})}{u_n(r_{n,j}, r_{n,j})} r_{n,j}(x), \tag{37}$$

with $l = \lceil \frac{n}{2} \rceil$ and

$$s_{n,n}(x) = x^{l'}\psi(x) - \sum_{j=0}^{n-1} \frac{u_n(x^{l'}\psi, r_{n,j})}{u_n(r_{n,j}, r_{n,j})} r_{n,j}(x), \tag{38}$$

with $l' = \lfloor \frac{n}{2} \rfloor$.

Theorem 4.7. *We have $R_n(x) = r_{n,n}(x)$ and $S_n(x) = s_{n,n}(x)$.*

Proof. We have by construction that

$$u_n(r_{n,n}, g) = 0, \quad \forall g \in V_{n-1}. \tag{39}$$

Construct the functions $g_j \in V_{n-1}$ such that $g_j(x_i) = \delta_{i,j}$, $i,j = 1,\ldots,n$. This is always possible, because T_{n-1} is a Chebyshev set. It follows from the definition (34) and from the property (39) that

$$u_n(r_{n,n}, g_j) = w_j r_{n,n}(x_j) = 0.$$

This implies that $r_{n,n}(x_j) = 0$, $j = 1,\ldots,n$. We also have by construction that $r_{n,n}(x) \in \operatorname{span}(T_{n-1} \cup \{x^l\})$. Moreover, $r_{n,n}(x)$ is nonzero because the basis function x^l has coefficient 1.

The function $R_n(x) = x^l - \mathcal{P}_{\mathbf{x}}(x^l)$ is nonzero, has coefficient 1 with x^l and vanishes at the quadrature points. This function is unique, because $\mathcal{P}_{\mathbf{x}}$ is invertible on V_{n-1}. It follows that $r_{n,n}(x) = R_n(x)$.

The proof for the statement $S_n(x) = s_{n,n}(x)$ is analogous. □

Theorem 4.7 implies that both $R_n(x)$ and $S_n(x)$ can be found by a Gram-Schmidt procedure applied to a basis of V_{n-1} using the scalar product u_n. As the scalar product itself is defined in terms of the quadrature rule however, this only implicitly determines R_n and S_n. In contrast, consider a similar scalar product for classical Gaussian quadrature rules. This scalar product u_n^G can be defined as in (34), but using the points and weights of the classical Gaussian quadrature rule. The bilinear form u_n^G coincides with the L_2 inner product for polynomial f and g up to certain degree,

$$u_n^G(f,g) = \int_a^b w(x)f(x)g(x)\,\mathrm{d}x, \qquad \forall f \in P_n, \forall g \in P_{n-1}.$$

All computations in the Gram-Schmidt procedure can be performed explicitly, leading to $p_n(x)$. Alternatively, of course, one can employ the three-term recurrence formula of orthogonal polynomials. Both schemes are not available in the setting of generalized Gaussian quadrature.

Example 4.8. *An exception to the general case is given by the special case $\psi(x) = \sqrt{x}$. In that case, it is easy to verify that the product of two functions in V_{n-1} lies in V_{2n-1}. The scalar product u_n then coincides with the L_2 inner product because the quadrature rule is exact on V_{2n-1}. The Gram-Schmidt procedure can be performed and $R_n(x)$ can be determined explicitly for all n.*

In this case the generalized Gaussian quadrature rule is closely related to a classical Gaussian quadrature rule with the weight function $w(y) = 2y$. Indeed, consider the substitution $x = y^2$,

$$\int_0^1 f(x)\,\mathrm{d}x = \int_0^1 2yf(y^2)\,\mathrm{d}y.$$

For any $f(x) = u(x) + v(x)\sqrt{x}$ with polynomial u and v, the function $f(y^2)$ is simply a polynomial in y. The generalized Gaussian quadrature rule with points x_j can also be obtained from the classical Gaussian rule with weight function $2y$ and quadrature points y_j by $x_j = y_j^2$.

5 Scaling of the quadrature rule

One additional useful property of generalized Gaussian quadrature is that they are invariant to a scaling of the integration interval for a wide variety of functions ψ with a singularity at one of the endpoints. Consider, without loss of generality, a singularity function $\psi(x)$ with a singularity at $x = 0$, and define the integral

$$I_b[f] := \int_0^b f(x)\,\mathrm{d}x. \tag{40}$$

We show that for many cases of practical interest, the generalized Gaussian quadrature rule for I_b is invariant to a scaling of b, up to a simple scaling of the weights and quadrature points expressed in (42) below.

5.1 Scaling invariant rules

Assume that $f(x) = u(x)+v(x)\psi(x)$ on $[0,b]$. We are interested in the points $x_{j,b}$ and weights $w_{j,b}$ of a generalized Gaussian quadrature rule on $[0,b]$. Rescaling the interval to $[0,1]$ by letting $x = bt$, we note that $(bt)^\alpha = b^\alpha t^\alpha$ and that $\log(bt) = \log b + \log t$. This motivates the following lemma.

Lemma 5.1. *If*

$$\psi(bt) = A_b\psi(t) + B_b. \tag{41}$$

then

$$w_{j,b} = b\, w_{j,1}, \qquad \textit{and} \qquad x_{j,b} = bx_{j,1}. \tag{42}$$

Proof. We rescale the interval to $[0,1]$. We have $I_b[f] = b\, I_1[\tilde{f}]$ with

$$\tilde{f}(t) = f(bt) = u(bt) + v(bt)\psi(bt).$$

Using (42) we write

$$\tilde{f}(t) = u(bt) + A_b v(bt) + B_b v(bt)\psi(t) =: \tilde{u}(t) + \tilde{v}(t)\psi(t).$$

Note that if u and v are polynomials of degree $n-1$, then $\tilde{u}(t) = u(bt) + A_b v(bt)$ and $\tilde{v}(t) = B_b v(bt)$ are also polynomials of the same degree. Therefore, if the points and weights $x_{j,1}$ and $w_{j,1}$ are a generalized Gaussian quadrature rule on $[0,1]$, then the scaled points and weights given by (42) are a generalized Gaussian quadrature rule on $[0,b]$ for the integral (40). □

Note that, contrary to alternative approaches where the singularity function $\psi(x)$ has been included into a weight function (see, for example, [14]), in generalized Gaussian quadrature it is not necessary to know the constants A_b and B_b. One only evaluates the function $f(x)$ on $[0,b]$ in the points $bx_{j,1}$.

5.2 Nearly scaling invariant quadrature rules

We say that singularity functions satisfying (41) give rise to *scaling invariant* quadrature rules because exactness is retained for $f(x) = u(x) + v(x)\psi(x)$, $x \in [0,b]$, when $u(x)$ and $v(x)$ are polynomials of sufficiently small degree. Less restrictive conditions on ψ than those of Lemma 5.1 may still yield useful results however, as the following lemma shows.

Lemma 5.2. *Assume that*

$$\psi(bt) = p(t,b)\psi(t) + q(t,b). \tag{43}$$

Then for $f(x) = u(x) + v(x)\psi(x)$, $x \in [0,b]$, *we have*

$$\left| I_b[f] - \sum_{j=1}^{n} w_{j,b} f(x_{j,b}) \right| \le \frac{1}{(n-1)!} \left(W\|\tilde{u}^{(n)}\|_\infty + (2WC_\psi + W_\psi)\|\tilde{v}^{(n)}\|_\infty \right)$$

with $\tilde{u}(t) = b[u(bt) + q(t,b)]$, $\tilde{v}(t) = bv(bt)p(t,b)$, $t \in [0,1]$ *and with* $w_{j,b}$ *and* $x_{j,b}$ *given by* (42).

Proof. Letting $x = bt$, we obtain

$$\int_0^b f(x)\,\mathrm{d}x = b\int_0^1 [u(bt) + q(t,b) + v(bt)p(t,b)\psi(t)]\,\mathrm{d}t.$$

We then apply Theorem 3.4 using the definitions of $\tilde{u}$ and $\tilde{v}$. □

This Lemma shows that if $p(t,b)$ and $q(t,b)$ are smooth functions, in the sense that they are sufficiently differentiable and have small derivatives, then the scaled quadrature rule carries small error. The rule is in general no longer exact however for polynomial u and v. As before, explicit knowledge of the functions $p(t,b)$ and $q(t,b)$ is not required, one simply evaluates $f(x)$.

5.3 Nearly singular integrals

Generalized Gaussian quadrature rules loose some of their appeal in the setting of nearly singular integrals. Consider for example the integral

$$\int_0^1 u(x) + v(x)\psi(x+\delta)\,\mathrm{d}x$$

with $\delta \geq 0$. Let us first note that convergence is not the issue. A generalized Gaussian quadrature rule exists for each value of δ, with the quadrature points $x_j(\delta)$ and weights $w_j(\delta)$ depending on δ. Following Theorem 3.4, the quadrature error is small uniformly in δ if the quantities

$$W_\psi = \int_0^1 w(x)\psi(x+\delta)\,\mathrm{d}x,$$

and

$$\min(\,|\sup_{x\in[0,1]} \psi(x+\delta)|\,,\,|\inf_{x\in[0,1]} \psi(x+\delta)|\,)$$

are bounded in δ, or grow only slowly with δ. This can be readily verified for many singularity functions $\psi(x)$ of interest.

Issues may arise in applications however if integrals appear with a range of values of δ. The points $x_j(\delta_1)$ and $x_j(\delta_2)$ are not related by a simple scaling in this setting. The quadrature rule has to be constructed for each separate value of δ. One can conceivably approximate the functions $x_j(\delta)$ and $w_j(\delta)$ a priori as a function of δ. This approximation is a current subject of further study.

6 Numerical construction methods

A numerical method for the construction of generalized Gaussian quadrature rules was first described in [20]. Starting from a known classical Gaussian quadrature rule, a continuation process is started where the polynomial basis functions are transformed smoothly into the desired Chebyshev set of functions $\{\phi_k\}_{k=1}^{2n}$. At each intermediate stage in the process, generalized Gaussian quadrature rules are computed via Newton's method by solving a set of n nonlinear equations in the unknowns x_{nj} (thereby assuming that this intermediate rule exists, which in general need not be the case). The continuation is necessary to provide starting points for the final computation that are sufficiently close to the true solution, in order to ensure the convergence of Newton's method for the quadrature rule one is interested in.

A different approach was proposed in [30] by performing continuation on the weight function. There, the authors solve a nonlinear system of $2n$ equations,

$$w_1\phi_k(x_1) + w_2\phi_k(x_2) + \ldots + w_n\phi_k(x_n) = I_\delta[\phi_k], \qquad k = 1, \ldots, 2n, \qquad (44)$$

where the weight function depends on the continuation parameter δ. The size of the system is larger, with $2n$ equations rather than n, but the Jacobian assumes a much simpler form and the method is reported to be more robust.

In this section, we briefly outline three separate approaches for the computation of generalized Gaussian quadrature rules in our framework of functions with an isolated singularity in $\psi(x)$.

6.1 Exploiting orthogonality

The function R_n completely characterizes the generalized Gaussian quadrature rule. In the case of even n, $n = 2l$, let

$$R_n(x) = x^l + \sum_{k=0}^{l-1} a_k x^k + \sum_{k=0}^{l-1} b_k x^k \psi(x).$$

This form has n unknowns. However, the function R_n satisfies $l = n/2$ orthogonality conditions (28) that result in linear relations in the unknown coefficients a_k and b_k. We may therefore write l coefficients in terms of the l other coefficients. The remaining l degrees of freedom are used to satisfy the orthogonality conditions (29) for S_n.

This approach reduces the size of the nonlinear system of equations from $2n$ to $n/2$ equations. In principle, this is a substantial reduction. However, the Jacobian of this system of equations is rather involved. The method in particular requires an implementation of the mapping from R_n to S_n as given by (33). As a result, we found that in practice it is faster to solve the larger set of equations in all cases we considered. An easier method to exploit the existence of the functions R_n and S_n numerically does not seem apparent.

6.2 A bootstrapping algorithm

From the general theory of Chebyshev sets, one knows that the quadrature points x_{nj} of various n interlace, i.e.,

$$x_{nj} \in (x_{n+1,j}, x_{n+1,j+1}).$$

From this, we construct starting points $x^*_{n+1,j}$ as follows. Having computed $x_{n,j}$, we set

$$\begin{aligned} x^*_{n+1,1} &= (a + x_{n,1})/2, \\ x^*_{n+1,j} &= (x_{n,j-1} + x_{n,j})/2, \qquad j = 2, \ldots, n, \\ x^*_{n+1,n+1} &= (x_{n,n} + b)/2. \end{aligned} \tag{45}$$

Newton's method is then used to solve the set of equations (44) with $\mathbf{x}^*$ as starting points and starting weights computed from (27).

A small, yet crucial difference with [30] is that we use Newton's method with damping [23]. Here, a damping parameter is used to restrict the size of the step in each iteration. The occasional lack of convergence of Newton's method without damping appears to be remedied by a small number of initial iterations with damping. This approach has the clear advantage that no continuation is necessary. Even though the approach requires the computation of all lower order quadrature rules Q_m, for $m = 1, \ldots, n$, we found it to be fastest in practice. The initial rule Q_1 is easily computed analytically.

In principle, convergence of this approach is not guaranteed, not even when the damping parameter goes to zero. However, we found that the approach converged for all examples that the authors have implemented so far. Note that this is the method we have used in all numerical examples of this paper.

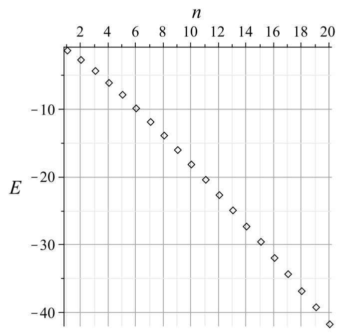

Figure 2: Absolute error E in the approximation of I_1 by a generalized Gaussian quadrature rule with n points. The error is shown in base-10 logarithmic scale.

6.3 A continuation method

If the function $\psi(x)$ is a smooth function away from $x = 0$, an alternative continuation approach becomes viable. One can perform continuation on the parameter δ, for functions of the form

$$f(x) = u(x) + v(x)\psi(x + \delta).$$

For large δ, the span of the basis T_{n-1} is close to the span of a polynomial basis. For increasing δ the generalized Gaussian quadrature rule therefore converges to the classical Gaussian quadrature rule. Starting from the classical Gaussian quadrature rule and sufficiently large δ, continuation on δ may be performed until δ has the desired (small) value. Convergence is guaranteed in this approach by taking sufficiently small steps.

7 Examples

We end this paper with three numerical examples. We used the bootstrapping method described in §6.2 to compute all quadrature rules with the following damping approach. If Newton's method without damping failed to converge, we started a new iteration from the starting values using a damping factor 1/2 in the first five iterations only. This process was repeated, halving the damping factor of the first five iterations after each restart, until convergence was achieved. No examples failed to converge with this approach. The majority of computations did not require any damping. Computations were performed in Maple in high precision arithmetic in order to illustrate the convergence to high accuracy. The evaluation of the quadrature rules was also replicated for all examples in IEEE double precision in Matlab to confirm stability of the computations up to machine precision (this is not shown in the figures).

As our first example, consider the integral

$$I_1 := \int_0^1 H_0^{(1)}(x)\,\mathrm{d}x,$$

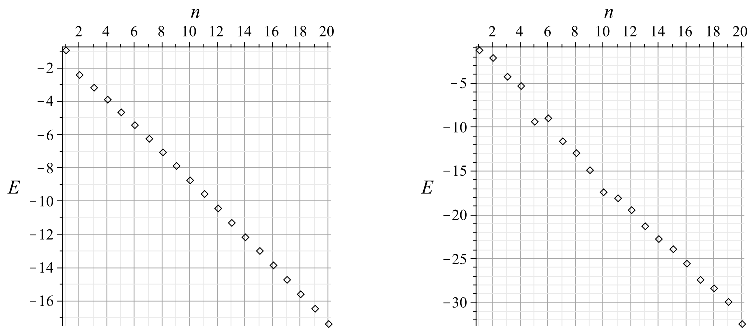

Figure 3: Absolute error (in base-10 logarithmic scale) of generalized Gaussian quadrature for a logarithmically singular integral with exponential decay (left panel) and for a nearly singular integral involving a square root (right panel).

where $H_0^{(1)}(x)$ is the Hankel function of the first kind and order zero. The integrand has the form $u(x)+v(x)\log(x)$, but it is not straightforward to obtain expressions for u and v [1]. The convergence rate is shown in Figure 2. Machine accuracy in double precision is obtained approximately at $n=9$ points.

In the second example we consider the integral

$$I_2 = \int_0^\infty x H_1^{(1)}(x) e^{-(1+i)x}\,\mathrm{d}x,$$

where $H_1^{(1)}$ is the Hankel function of the first kind of order zero. Integrals of this type appeared in computational models for scattering phenomena [13], for the evaluation of oscillatory integrals using a steepest-descent approach [12]. The integrand is continuous at $x=0$ but has a logarithmic singularity in its derivatives. It decays like e^{-x} for large x. We constructed generalized Gaussian quadrature rules with the singularity function $\psi(x)=\log(x)$ and the weight function $w(x)=e^{-x}$. The results are shown in the left panel of Figure 3. The starting values (45) were slightly modified in this case, because the right endpoint of the integration interval is infinite. As a starting value for the rightmost quadrature point, we used

$$\begin{aligned} x_{2,2}^* &= x_{1,1} + 2, \\ x_{n+1,n+1}^* &= x_{n,n} + (x_{n,n} - x_{n-1,n-1}), \quad n = 2, \ldots. \end{aligned}$$

In the third example we consider the integral

$$I_3 := \int_0^1 \sqrt{0.01 + x + x^2}(\cos(x) + \sin(x))\,\mathrm{d}x.$$

This example illustrates both the advantages and disadvantages of generalized Gaussian quadrature for nearly singular integrals. The integral behaves as $u(x)\sqrt{x-\epsilon}+v(x)$ for $x \to \epsilon$ where $\epsilon = -0.0101\ldots$ is the root of

$$0.01 + x + x^2 = 0$$

closest to the interval $[0,1]$. Convergence is illustrated in the right panel of Figure 3 using $\psi(x) = \sqrt{x+\epsilon}$. Similar, though slightly worse results were obtained by using $\epsilon = 0.01$. The disadvantages for nearly singular integrals are that best results are obtained with a sharp estimate of ϵ and that the quadrature rule depends on ϵ. The advantage is that convergence is very rapid. Machine accuracy in double precision is reached approximately at $n = 9$ points.

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