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A note on generalized averaged Gaussian formulas

Miodrag M. Spalević

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Abstract We have recently proposed a very simple numerical method for constructing the averaged Gaussian quadrature formulas. These formulas exist in many more cases than the real positive Gauss–Kronrod formulas. In this note we try to answer whether the averaged Gaussian formulas are an adequate alternative to the corresponding Gauss–Kronrod quadrature formulas, to estimate the remainder term of a Gaussian rule.

Keywords Averaged gaussian quadrature formulas · Gauss–Kronrod quadrature formulas

1 Introduction

Let $d\sigma$ be a given positive measure on a bounded or an unbounded interval $[a, b] = \operatorname{supp}(d\sigma)$. If σ is an absolutely continuous function on $[a, b]$, then $d\sigma(x) = w(x)\,dx$, where w is a weight function. We call an *interpolatory quadrature formula* (abbreviated to q.f.) of the form

$$\int_a^b f(x)\,d\sigma(x) = Q_n[f] + R_n[f], \quad Q_n[f] = \sum_{j=1}^{n} \omega_j f(x_j), \tag{1}$$

where $x_1 < x_2 < \cdots < x_n$, $\omega_j \in \mathbb{R}$ $(j = 1, \ldots, n)$ and $R_n[f] = 0$ for $f \in \mathbb{P}_{2n-m-1}$ ($\mathbb{P}_n$ denotes the set of polynomials of degree at most n), $0 \le m \le n$, a $(2n - m - 1, n, d\sigma)$ q.f.. If in addition all quadrature weights ω_j, $j = 1, \ldots, n$, are positive, then it is called a *positive* $(2n - m - 1, n, d\sigma)$ q.f.. Furthermore, we

M. M. Spalević (✉)
Department of Mathematics and Informatics, Faculty of Science,
University of Kragujevac, P.O. Box 60, 34000 Kragujevac, Serbia
e-mail: spale@kg.ac.yu

say that a polynomial $t_n \in \mathbb{P}_n$ generates a $(2n-m-1, n, w)$ q.f. if t_n has n simple zeros $x_1 < x_2 < \cdots < x_n$, $t_n(x) = \prod_{j=1}^{n}(x - x_j)$, and if the interpolatory q.f. based on the nodes x_j, $j = 1, \ldots, n$, is a $(2n-m-1, n, d\sigma)$ q.f.. A $(2n-m-1, n, d\sigma)$ q.f. is *internal* if all its nodes belong to the closed interval $[a, b]$. A node not belonging to the interval $[a, b]$ is called *exterior node*.

Let us denote by p_k the monic polynomial of degree k, which is orthogonal to $\mathbb{P}_{k-1}$ with respect to $d\sigma$, i. e.

$$\int_a^b x^j p_k(x) d\sigma(x) = 0, \quad j = 0, 1, \ldots, k-1,$$

and let us recall that (p_k) satisfies a three-term recurrence relation of the form

$$p_{k+1}(x) = (x - \alpha_k) p_k(x) - \beta_k p_{k-1}(x), \quad k = 0, 1, \ldots, \tag{2}$$

where $p_{-1}(x) = 0$, $p_0(x) = 1$ and the β_k's have the property of being positive.

The unique interpolatory q.f. with ℓ nodes and the highest possible degree of exactness $2\ell - 1$ is the Gaussian formula with respect to the measure $d\sigma$,

$$Q_\ell^G[f] = \sum_{j=1}^{\ell} \omega_j^G f\left(x_j^G\right).$$

As shown by Golub and Welsch [9], the nodes of the q.f. Q_ℓ^G are the eigenvalues, and the weights are proportional to the squares of the first components of the eigenvectors, of the symmetric Jacobi tridiagonal matrix

$$J_\ell^G(d\sigma) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & \mathbf{0} \\ \sqrt{\beta_1} & \alpha_1 & \ddots & \\ & \ddots & \ddots & \sqrt{\beta_{\ell-1}} \\ \mathbf{0} & & \sqrt{\beta_{\ell-1}} & \alpha_{\ell-1} \end{bmatrix}.$$

In practice the common problem is to find some other q.f. for estimating the error of $Q_\ell^G[f]$. Typically, if it exists, the Gauss–Kronrod q.f. $Q_{2\ell+1}^{GK}$, with $2\ell + 1$ points and degree of exactness at least $3\ell + 1$ are used, under the assumption that the ℓ nodes of Q_ℓ^G are part of the $2\ell + 1$ nodes,

$$\int_a^b f(x)\, d\sigma(x) = Q_{2\ell+1}^{GK}[f] + R_{2\ell+1}^{GK}[f],$$

$$Q_{2\ell+1}^{GK}[f] = \sum_{j=1}^{\ell} \omega_j^{GK} f\left(x_j^G\right) + \sum_{k=1}^{\ell+1} \widetilde{\omega}_k^{GK} f\left(x_k^S\right). \tag{3}$$

The polynomial of degree $\ell + 1$, which vanishes at the $\ell + 1$ additional nodes x_k^S $(k = 1, \ldots, \ell + 1)$, the so-called Stieltjes polynomial, usually denoted by $E_{\ell+1}$, is characterized by an orthogonality relation with respect to a sign-changing weight. The efficient numerical methods for calculating the positive

Gauss–Kronrod q.f. are proposed by Laurie [14], and Calvetti et al. [2] (see also Monegato [16], and Gautschi [8]).

The existence of the positive Gauss–Kronrod q.f. depends on $d\sigma$, and there are several cases of non-existence known, e. g. for the Gauss–Laguerre and Gauss–Hermite cases [11]. Recently, for the Gegenbauer weight $w^{(\alpha,\alpha)}(x) = (1-x^2)^\alpha$, Peherstorfer and Petras [22] have shown nonexistence of Gauss–Kronrod formulas for ℓ sufficiently large and $\alpha > 5/2$. Analogous results for the Jacobi weight function $w^{(\alpha,\beta)}(x) = (1-x)^\alpha(1+x)^\beta$ can be found in their paper [23], particularly nonexistence for large ℓ of Gauss–Kronrod formulas when $\min(\alpha,\beta) \geq 0$ and $\max(\alpha,\beta) > 5/2$. In such cases it is of the interest to find an adequate alternative to the corresponding Gauss–Kronrod q.f.

An alternative approach are the Anti-Gaussian formulas in Laurie [13], which have been slightly generalized in Ehrich [6], and in the author's paper [24]. Such formulas always exist and are positive. However, for the polynomial degree of exactness in general only $\geq 2\ell+1$ can be guaranteed.

The observation in this note is essentially that the error of these generalized formulas for polynomials x^k, $k \leq 3\ell+1$, should be small. More precisely, the argument is based on the known characterization of these formulas by three-diagonal Jacobi matrices, and uses the characterization of positive q.f. by Peherstorfer in [20].

2 The optimal generalized averaged gaussian q.f. as an alternative to the corresponding Gauss–Kronrod q.f.

Let us remember, with little modification, Peherstorfer's impressive characterization results in the theory of positive interpolatory q.f. (1) (see [20, Theorem 3.2], and also [18, 19]).

A polynomial t_n generates a positive $(2n-1-m, n, d\sigma)$ q.f. $(0 \leq m \leq n)$ if and only if t_n can be generated by a three-term recurrence relation of the form

$$t_{j+1}(x) = (x-\tilde{\alpha}_j)t_j(x) - \tilde{\beta}_j t_{j-1}(x), \quad j = 0, 1, \ldots, n-1, \tag{4}$$

$t_{-1}(x) = 0$, $t_0(x) = 1$, with $\tilde{\alpha}_j \in \mathbb{R}$ and $\tilde{\beta}_j > 0$ for $j = 0, 1, \ldots, n-1$, and with

$$\tilde{\alpha}_j = \alpha_j \text{ for } j = 0, 1, \ldots, n-1-\left[\frac{m+1}{2}\right]; \quad \tilde{\beta}_j = \beta_j \text{ for } j = 0, 1, \ldots, n-1-\left[\frac{m}{2}\right]$$

and

$$\operatorname{sgn} t_j(a) = (-1)^j,\ t_j(b) > 0, \quad j = 1, \ldots, n,$$

which is again equivalent to the fact (see the proof of $d) \Longrightarrow a)$ in [20, Theorem 3.2]) that t_n can be represented in the form $(\ell := [(m+1)/2],\ n \geq 2\ell)$

$$t_n = g_\ell p_{n-\ell} - \tilde{\beta}_{n-\ell} g_{\ell-1} p_{n-\ell-1}, \tag{5}$$

where $g_{\ell-1}$ and g_ℓ are generated by a three-term recurrence relation of the form

$$g_{j+1}(x) = (x - \tilde{\alpha}_{n-1-j})g_j(x) - \tilde{\beta}_{n-j}g_{j-1}(x), \quad j = 0, 1, \ldots, \ell - 1,$$

$g_{-1}(x) = 0$, $g_0(x) = 1$, with $\tilde{\alpha}_{n-1-j} \in \mathbb{R}$ and $\tilde{\beta}_{n-j} > 0$ for $j = 0, 1, \ldots, \ell - 1$; $\tilde{\beta}_{n-\ell} > 0$, $\tilde{\beta}_{n-\ell} = \beta_{n-\ell}$ if $m = 2\ell - 1$; and

$$\operatorname{sgn} g_j(a) = (-1)^j, \ g_j(b) > 0, \quad j = 1, \ldots, \ell.$$

The corresponding Jacobi matrix is denoted by $J_n^P(d\sigma)$. It is well-known (see e. g. Gautschi [7]) that there is a one-to-one correspondence between Jacobi matrices and quadrature formulas with positive weights.

The following important sub-class of the quadrature formulas, just discussed, can be easily calculated, which is a consequence of the facts given in the proof of the Characterization Theorem (see [20, Theorem 3.2] for details, particularly in the part $(d) \Longrightarrow (a)$). Namely, consider the positive q.f. $(2n - 1 - m, n, d\sigma)$, i. e. Q_n^{GP}, in which

$$\begin{aligned} \tilde{\alpha}_{n-1-j} = \alpha_j \quad \text{and} \quad \tilde{\beta}_{n-j} = \beta_j \quad \text{for } j = 0, 1, \ldots, \ell - 1, \\ \tilde{\beta}_{n-\ell} = \beta_{n-\ell}\ (m = 2\ell - 1), \quad \text{i. e.,} \quad \tilde{\beta}_{n-\ell} = \beta_\ell\ (m = 2\ell)\,, \end{aligned} \tag{6}$$

which immediately yields

$$g_j \equiv p_j, \quad j = 1, \ldots, \ell.$$

Conversely, putting

$$g_\ell \equiv p_\ell \quad \text{and} \quad g_{\ell-1} \equiv p_{\ell-1} \tag{7}$$

the relations (6) follow. Hence if (7) or (6) holds, then (5) is reduced to

$$t_n = p_\ell p_{n-\ell} - \tilde{\beta}_{n-\ell} p_{\ell-1} p_{n-\ell-1}. \tag{8}$$

The Jacobi matrix in this case $J_n^{GP}(d\sigma)$ has the form

$$\begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & & & & & & \mathbf{0} \\ \sqrt{\beta_1} & \alpha_1 & \ddots & & & & & & & & \\ & \ddots & \ddots & \sqrt{\beta_{\ell-1}} & & & & & & & \\ & & \sqrt{\beta_{\ell-1}} & \alpha_{\ell-1} & \sqrt{\beta_\ell} & & & & & & \\ & & & \sqrt{\beta_\ell} & \alpha_\ell & \ddots & & & & & \\ & & & & \ddots & \ddots & \sqrt{\beta_{n-\ell-1}} & & & & \\ & & & & & \sqrt{\beta_{n-\ell-1}} & \alpha_{n-\ell-1} & \sqrt{\tilde{\beta}_{n-\ell}} & & & \\ & & & & & & \sqrt{\tilde{\beta}_{n-\ell}} & \alpha_{\ell-1} & \ddots & & \\ & & & & & & & \ddots & \ddots & \sqrt{\beta_1} & \\ \mathbf{0} & & & & & & & & \sqrt{\beta_1} & \alpha_0 & \end{bmatrix}.$$

The positive interpolatory q.f. which corresponds to the Jacobi matrix $J_n^{GP}(d\sigma)$ can be calculated by using the well-known software for Gauss quadrature formulas (see Golub and Welsch [9], and particularly the recent Gautschi's book [8]). The degree of exactness of this q.f. is $2n-2\ell$, or $2n-2\ell-1$, if $m=2\ell-1$, or $m=2\ell$, respectively. The weight coefficients in this q.f. are positive and the nodes are real and distinct.

The most interesting case $n=2\ell+1$ has been analyzed by Spalević [24]. In this case (8) is reduced to

$$t_n \equiv t_{2\ell+1} = p_\ell F_{\ell+1}\,,$$

where $F_{\ell+1}$ is the polynomial of degree $\ell+1$, defined by Franz Peherstorfer,

$$\begin{aligned} F_{\ell+1}(x) &= p_{\ell+1}(x) - \tilde{\beta}_{\ell+1} p_{\ell-1}(x) \\ &= (x-\alpha_\ell) p_\ell(x) - \hat{\beta}_\ell p_{\ell-1}(x), \end{aligned} \tag{9}$$

where $\hat{\beta}_\ell = \beta_\ell + \tilde{\beta}_{\ell+1}$.

Thus the optimal generalized averaged Gaussian q.f. $Q_{2\ell+1}^{GF}$, where $\tilde{\beta}_{\ell+1} = \beta_{\ell+1}$ $(n=2\ell+1,\ m=2\ell-1)$,

$$\int_a^b f(x)\,d\sigma(x) = Q_{2\ell+1}^{GF}[f] + R_{2\ell+1}^{GF}[f],$$

$$Q_{2\ell+1}^{GF}[f] = \sum_{j=1}^{\ell} \omega_j^{GF} f\left(x_j^G\right) + \sum_{k=1}^{\ell+1} \widetilde{\omega}_k^{GF} f\left(x_k^F\right), \tag{10}$$

which has degree of exactness at least $2\ell+2$ (that is $2\ell+3$ in a symmetric case, $d\sigma(-x) = d\sigma(x)$ on $[a,b]=[-c,c]$), is based on the zeros of $t_{2\ell+1} = p_\ell F_{\ell+1}$. x_j^G $(j=1,\ldots,\ell)$ denote the zeros of p_ℓ, i. e., the nodes in the corresponding Gauss q.f. Q_ℓ^G, and x_k^F $(k=1,\ldots,\ell+1)$ denote the zeros of $F_{\ell+1}$. In this case the Jacobi matrix $J_n^{GP}(d\sigma)$ is denoted by $J_{2\ell+1}^{GF}(d\sigma)$. A much shorter and more elementary argument of the same construction of $Q_{2\ell+1}^{GF}$ can be found in Spalević [24]. Ehrich [6] showed that $Q_{2\ell+1}^{GF}$ is the optimal stratified extension for Gauss–Laguerre and Gauss–Hermite q.f., in the corresponding cases. See also [10] for the Gauss–Gegenbauer q.f..

Note, if $\tilde{\beta}_{\ell+1} = \beta_\ell$, $(m=2\ell)$, i. e., $\hat{\beta}_\ell = 2\beta_\ell$ in (9), the corresponding positive q.f. has degree of exactness at least $2\ell+1$, hence it is the averaged Gaussian q.f. $Q_{2\ell+1}^{GA}$ introduced by Laurie [13], who obtained it by halving the sum of the Gauss q.f., based on the nodes of p_ℓ, and the anti-Gauss q.f., based on the nodes of $F_{\ell+1}$.

Since $\hat{\beta}_\ell > 0$, the zeros of p_ℓ and $F_{\ell+1}$ interlace. Therefore, the inner nodes x_k^F $(k=2,\ldots,\ell)$ are in $[a,b]$.

Investigations into these problem areas have recently attracted a lot of interest (see Calvetti and Reichel [3], Kim and Reichel [12]).

In the sequel, we will treat only the optimal averaged Gaussian q.f. $Q_{2\ell+1}^{GF}$, since similar conclusions can be derived for the averaged Gaussian q.f. $Q_{2\ell+1}^{GA}$ introduced by Laurie [13].

On the basis of the previous discussion we conclude that the optimal averaged Gaussian q.f. $Q_{2\ell+1}^{GF}$ has almost all desirable properties (which we looked for Gauss–Kronrod q.f.):

- The nodes of the ℓ-point Gaussian rule Q_ℓ^G are a subset of $Q_{2\ell+1}^{GF}$;
- The nodes of $Q_{2\ell+1}^{GF}$ are real, simple, distinct. Only two of them (x_1^F or $x_{\ell+1}^F$) may be outside of the interval $[a,b]$. The zeros of p_ℓ and $F_{\ell+1}$ interlace;
- The weight coefficients in $Q_{2\ell+1}^{GF}$ are positive;
- A very simple numerical method for constructing $Q_{2\ell+1}^{GF}$ has recently been proposed (cf. Spalević [24]).

Therefore, the optimal averaged Gaussian q.f. $Q_{2\ell+1}^{GF}$ could be an adequate alternative for the corresponding Gauss–Kronrod q.f. $Q_{2\ell+1}^{GK}$, especially if:

- The corresponding real positive Gauss–Kronrod q.f. $Q_{2\ell+1}^{GK}$ do not exist (cf. Kahaner and Monegato [11], Peherstorfer and Petras [22], Peherstorfer and Petras [23]), and
- The degree of exactness of the optimal averaged Gaussian q.f. $Q_{2\ell+1}^{GF}$ is greater than $2\ell+2$ (that is $2\ell+3$ in a symmetric case, $d\sigma(-x)=d\sigma(x)$ on $[a,b]=[-c,c]$).

In the rest of this note, we will concentrate our attention on the last request. More precisely, we shall demonstrate that from the computational point of view the degree of exactness of $Q_{2\ell+1}^{GF}$ can be considered to be $3\ell+1$ if the recurrence coefficients satisfy the conditions

$$\lim_{\ell\to\infty}\alpha_\ell = A, \qquad \lim_{\ell\to\infty}\beta_\ell = B, \tag{11}$$

where $A\in\mathbb{R}$, $B\in[0,+\infty)$. To this case of $d\sigma$, in particular, belong the cases with the Jacobi measures $d\sigma^{(\alpha,\beta)}(x)=w^{(\alpha,\beta)}(x)\,dx=(1-x)^\alpha(1+x)^\beta\,dx$, including the cases with the Gegenbauer measures $d\sigma^{(\alpha)}(x)=w^{(\alpha)}(x)\,dx=(1-x^2)^\alpha\,dx$. If (11) holds, then the interval $[a,b]=\operatorname{supp}(d\sigma)$ is bounded (cf. Chihara [4, Theorem 2.2 on p. 109]).

Let us return to the q.f. Q_n^{GP} discussed at the beginning of this section. Let $n=2\ell+1$. We take $\overline{\ell}$ to be $\left[\dfrac{\ell}{2}\right]$, or $(\ell+1)/2$ when ℓ is odd ($\ell\ge 3$). Therefore, in general $\ell\ge 2\overline{\ell}-1$. In these cases the conditions (6) are reduced to

$$\begin{aligned}\tilde{\alpha}_{n-1-j}=\alpha_j \quad \text{and} \quad \tilde{\beta}_{n-j}=\beta_j \quad \text{for } j=0,1,\ldots,\overline{\ell}-1,\\ \tilde{\beta}_{n-\overline{\ell}}=\beta_{n-\overline{\ell}}\;(\overline{m}=2\overline{\ell}-1), \quad \text{i.e.,} \quad \tilde{\beta}_{n-\overline{\ell}}=\beta_{\overline{\ell}}\;(\overline{m}=2\overline{\ell}),\end{aligned} \tag{12}$$

with $\overline{\ell}:=[(\overline{m}+1)/2]$, $n=2\ell+1\ge 2\overline{\ell}$ ($0\le\overline{m}\le n$). The corresponding positive q.f. $(2n-\overline{m}-1,n,d\sigma)$, i.e., $\overline{Q}_{2\ell+1}^{GP}$, where $n=2\ell+1$ has degree of exactness at least $3\ell+1$, and is based on the zeros of the polynomial $\overline{t}_n=p_{\overline{\ell}}p_{n-\overline{\ell}}-\tilde{\beta}_{n-\overline{\ell}}p_{\overline{\ell}-1}p_{n-\overline{\ell}-1}$. Its Jacobi matrix $J_n^{GP}(d\sigma)$ we denote by $\overline{J}_{2\ell+1}^{GP}(d\sigma)$. In the sequel we consider the case $\tilde{\beta}_{n-\overline{\ell}}=\beta_{n-\overline{\ell}}$ ($\overline{m}=2\overline{\ell}-1$), since the case $\tilde{\beta}_{n-\overline{\ell}}=\beta_{\overline{\ell}}$ ($\overline{m}=2\overline{\ell}$) can be treated in a similar way.

Let for instance the norm of an arbitrary matrix $\mathbf{C} = [c_{ij}]$ be defined by

$$\|\mathbf{C}\| = \max_i \left(\sum_j |c_{ij}| \right),$$

and let us consider the q.f. (1), i. e. Q_n, in the form of the vector $\mathbf{q}_n$, where

$$\mathbf{q}_n = \left[\mathbf{x}^T \; \omega^T \right], \tag{13}$$

where $\mathbf{x} = [x_1 \; x_2 \; \ldots \; x_n]^T$ is the vector of nodes, and $\omega = [\omega_1 \; \omega_2 \; \ldots \; \omega_n]^T$ is the vector of weight coefficients, in Q_n. Let the norm of the q.f. Q_n be defined by

$$\| Q_n \| = \|\mathbf{q}_n\| = \max\{\|\mathbf{x}\|, \|\omega\|\},$$

where $\|\mathbf{x}\| = \max_i |x_i|$, and $\|\omega\| = \max_i |\omega_i|$.

Observe that the map

$$\mathbf{H}_n^{-1} \; : \; J_n^P(d\sigma) \longmapsto \mathbf{q}_n^P$$

is continuous, namely

$$\begin{aligned} &\forall \varepsilon > 0, \exists \delta = \delta(\varepsilon) > 0, \forall J_n^{(1)P}(d\sigma), J_n^{(2)P}(d\sigma) : \\ &\left\| J_n^{(1)P}(d\sigma) - J_n^{(2)P}(d\sigma) \right\| < \delta \implies \left\| \mathbf{q}_n^{(1)P} - \mathbf{q}_n^{(2)P} \right\| < \varepsilon, \end{aligned} \tag{14}$$

where $J_n^{(i)P}(d\sigma)$, $\mathbf{q}_n^{(i)P}$ correspond to the positive q.f. $Q_n^{(i)P}$ $(i = 1, 2)$. This holds since the coefficients of the characteristic polynomial of matrix $J_n^P(d\sigma)$ depend continuously on the elements of matrix $J_n^P(d\sigma)$, on the basis of the definition of determinant. Further, it is well known that the zeros of an algebraic polynomial continuously depend on its coefficients. Finally, the weight coefficients in an interpolatory q.f. of type (1) continuously depend on its nodes.

The map $\mathbf{H}_n^{-1}$ is generally well conditioned (see Gautschi [8], as well as [1, Eq. 7 & Corollary 8]), and the calculation of Gauss-type quadrature formulas is a well-understood problem for which fully satisfactory methods are available when the recursion coefficients are known, as stressed in Laurie [15] and O'Leary et al. [17].

Consider the optimal averaged Gaussian q.f. $Q_{2\ell+1}^{GF}$, which has degree of exactness at least $2\ell + 2$, and the positive q.f. $\overline{Q}_{2\ell+1}^{GP}$ which has degree of exactness at least $3\ell + 1$. If the conditions (11) hold, i. e., if the sequences $(\alpha)_\ell$, $(\beta)_\ell$ are convergent, they are then Cauchy sequences, and in particular

$$\begin{aligned} &\forall \overline{\delta} > 0, \exists \overline{\ell} = \overline{\ell}(\overline{\delta}) \in \mathbb{N}, \forall \overline{j} \in \mathbb{N} : \\ &\;\overline{j} \geq \overline{\ell} \implies \left|\alpha_{j-h} - \alpha_{j+h}\right| < \overline{\delta}, \; \left|\sqrt{\beta_{j-h}} - \sqrt{\beta_{j+1+h}}\right| < \overline{\delta} \\ &(h = 1, 2, \ldots, j - \overline{j}), \end{aligned} \tag{15}$$

where $\overline{j} = [j/2]$, or $\overline{j} = (j + 1)/2$ (j (≥ 3) is odd).

Now in the case $\overline{j} = \overline{\ell}$, by putting $\overline{\delta} = \delta/3$, on the basis of (14), the fact that the map $\mathbf{H}_n^{-1}$ is well conditioned, (15), we conclude that for an arbitrary $\varepsilon > 0$ there exists sufficiently large $\overline{\ell}$ such that

$$\left\| \mathbf{q}_{2\ell+1}^{GF} - \overline{\mathbf{q}}_{2\ell+1}^{GP} \right\| < \varepsilon, \tag{16}$$

where $\mathbf{q}_{2\ell+1}^{GF}$, $\overline{\mathbf{q}}_{2\ell+1}^{GP}$ are the vectors of type (13) which correspond to the q.f. $Q_{2\ell+1}^{GF}$ and $\overline{Q}_{2\ell+1}^{GP}$, respectively.

From the computational point of view, on the basis of the previous analysis, we conclude as follows:

Let $\varepsilon = \frac{1}{2}10^{-k}$. If we round off the elements of the vector $\mathbf{q}_{2\ell+1}^{GF}$, that is of the optimal averaged Gaussian q.f. $Q_{2\ell+1}^{GF}$, on k decimal digits, we obtain the vector $\mathbf{q}_{2\ell+1}^{(0)GF}$, that is the q.f. $Q_{2\ell+1}^{(0)GF}$. Subject to (16) and the given absolute precision ε the q.f. $Q_{2\ell+1}^{(0)GF}$ represents the optimal averaged Gaussian q.f. which has degree of exactness at least $3\ell + 1$.

Therefore, we showed that from the computational point of view the q.f. $Q_{2\ell+1}^{GF}$ can be considered as an optimal substitute for the Gauss–Kronrod q.f., if the recurrence coefficients are convergent.

Remark 1 The interpolatory q.f. $Q_{2\ell+1}$ which contains as its subset all nodes of the Gauss q.f. Q_ℓ^G and has degree of exactness at least $3\ell + 1$ is uniquely given as the Gauss–Kronrod q.f. $Q_{2\ell+1}^{GK}$. We conclude that the corresponding Gauss–Kronrod q.f. $Q_{2\ell+1}^{GK}$ is the same as the q.f. $Q_{2\ell+1}^{(0)GF}$ up to the given absolute precision ε, if it is real and positive.

Remark 2 There are theoretical results which support the presented ideas. Indeed, for $w(x) = \sqrt{1-x^2}\, v(x)$, where v is *Lip* α and positive on $[-1, 1]$ it has been proved in [21, Corollary 10] that the Stieltjes polynomial is asymptotically of the form

$$E_{\ell+1}\left(x; \sqrt{1-x^2}\, v(x)\right) \simeq p_{\ell+1}\left(x; \frac{v(x)}{\sqrt{1-x^2}}\right).$$

Since under the above assumption on $v(x)$ the relation

$$p_{\ell+1}\left(x; \frac{v(x)}{\sqrt{1-x^2}}\right) \simeq p_{\ell+1}\left(x; \sqrt{1-x^2}\, v(x)\right) - \frac{1}{4} p_{\ell-1}\left(x; \sqrt{1-x^2}\, v(x)\right) \tag{17}$$

holds, the nodes of the Gauss–Kronrod q.f. are asymptotically the zeros of the polynomial

$$p_\ell(x; w)\left(p_{\ell+1}(x; w) - \frac{1}{4} p_{\ell-1}(x; w)\right)$$

which coincides with t_n (which generates the corresponding q.f. $Q_{2\ell+1}^{GF}$), as our assertion does, taking into account (11), with $A = 0$, $B = 1/4$, and the boundedness of $p_{\ell-1}(x)$ on $[-1, 1]$. Relation (17) follows by the asymptotic relation

$$\frac{\text{Im}\left\{z^{-(\ell+1)}\Phi_{2\ell+3}(z)\right\}}{\sin\varphi} - \frac{\text{Im}\left\{z^{-(\ell-1)}\Phi_{2\ell-1}(z)\right\}}{\sin\varphi} \simeq 2\text{Re}\left\{z^{-\ell}\Phi_{2\ell+1}(z)\right\}$$

where $\Phi_j(z) = z^j + \ldots$ is the orthogonal polynomial on the unit circle with respect to the weight function $v(\cos\varphi)$.

3 Numerical results

As we mentioned in the introduction (see also Laurie [13]), a common approach to estimate the modulus of remainder $|R_\ell[f]|$ in an interpolatory q.f. $Q_\ell[f]$ is to consider a second rule $Q_n[f]$ with $n > \ell$, and to take

$$|R_\ell[f]| \approx |Q_n[f] - Q_\ell[f]|,$$

provided n is such that this estimate is acceptable, i. e., sufficiently accurate. Usually $n = 2\ell + 1$, $Q_\ell[f] = Q_\ell^G[f]$. The cost, in terms of function evaluations, of this error estimate is $n + \ell > 2\ell$, unless the two sets of abscissas in $Q_\ell[f]$ and $Q_n[f]$ have common points. Particularly, if the second set of abscissas contains the first one then the total cost is only n. This is precisely the observation which leads to the Gauss–Kronrod q.f. (cf. [8, 16]) and averaged generalized Gaussian q.f. (cf. Spalević [24]).

In order to confirm the facts from Section 2 we made several tests. Some of the obtained results are displayed in this section. For the calculations we have used our numerical method (see Spalević [24]) and the Matlab routines which are downloadable from the web site http://www.cs.purdue.edu/archives/2002/wxg/codes/ and which are assembled as a companion piece to the book in [8].

Table 1 $\varrho(\ell)$ as a distance $Q_{2\ell+1}^{GF}$ of $Q_{2\ell+1}^{GK}$ in the Legendre case

ℓ	$\varrho(\ell)$	ℓ	$\varrho(\ell)$
3	1.732(−2)	65	4.191(−5)
4	6.903(−3)	70	3.602(−5)
5	6.631(−3)	75	3.153(−5)
7	3.445(−3)	80	2.764(−5)
8	2.293(−3)	85	2.458(−5)
10	1.539(−3)	90	2.187(−5)
12	1.102(−3)	95	1.969(−5)
15	7.673(−4)	100	1.774(−5)
20	4.193(−4)	125	1.140(−5)
25	2.793(−4)	150	7.915(−6)
30	1.911(−4)	200	4.461(−6)
35	1.433(−4)	250	2.858(−6)
40	1.088(−4)	300	1.986(−6)
45	8.705(−5)	350	1.460(−6)
50	7.007(−5)	400	1.118(−6)
55	5.843(−5)	450	8.838(−7)
60	4.887(−5)	500	7.160(−7)

Table 2 The corresponding quantities for the integrand $f_1(x) = \dfrac{x+1}{0.02+(x+1)^2}$ in the Legendre case

ℓ	R.Err.$_\ell(f_1)$	$D_\ell^{GK}(f_1)$	$D_\ell^{GF}(f_1)$
3	1.039(−3)	3.142(−1)	3.169(−1)
5	2.118(−4)	5.703(−2)	5.646(−2)
8	5.537(−6)	9.373(−3)	9.358(−3)
10	2.470(−7)	1.680(−4)	1.674(−4)
15	6.159(−10)	2.234(−5)	2.234(−5)
20	2.171(−11)	9.189(−7)	9.188(−7)
25	3.830(−13)	2.323(−8)	2.323(−8)
30	6.197(−15)	4.112(−10)	4.112(−10)
32	5.024(−16)	6.202(−11)	6.202(−11)

Table 3 The corresponding quantities for the integrand $\widetilde{f}(x) = (1+x)\log(1+x)$ in the Legendre case

ℓ	R.Err.$_\ell(\widetilde{f})$	$D_\ell^{GK}(\widetilde{f})$	$D_\ell^{GF}(\widetilde{f})$
3	1.970(−4)	7.242(−3)	7.318(−3)
10	3.195(−6)	8.206(−5)	8.330(−5)
25	9.874(−8)	2.338(−6)	2.376(−6)
50	6.454(−9)	1.518(−7)	1.543(−7)
100	4.127(−10)	9.674(−9)	9.834(−9)
300	5.161(−12)	1.210(−10)	1.230(−10)
500	6.632(−13)	1.572(−11)	1.598(−11)

Table 4 The corresponding quantities for the integrand $f_2(x) = e^{x^2}$ in the Gegenbauer case $w^{(-0.7)}(x) \equiv (1-x^2)^{-0.7}$ on $[-1, 1]$

ℓ	R.Err.$_\ell(f_2)$	$D_\ell^{GK}(f_2)$	$D_\ell^{GF}(f_2)$
3	2.200(−6)	4.097(−2)	4.095(−2)
4	2.343(−8)	2.467(−3)	2.466(−3)
5	3.586(−10)	1.207(−4)	1.207(−4)
6	5.700(−12)	4.961(−6)	4.961(−6)
7	9.236(−14)	1.754(−7)	1.754(−6)
8	1.376(−15)	5.442(−9)	5.442(−9)

Table 5 The corresponding quantities for the integrand $f_3(x) = e^{-x^{10}}$ in the Jacobi case $w^{(1/10,13/5)}(x) \equiv (1-x)^{1/10}(1+x)^{13/5}$ on $[-1, 1]$

ℓ	R.Err.$_\ell(f_3)$	$D_\ell^{GK}(f_3)$	$D_\ell^{GF}(f_3)$
3	2.102(−4)	2.225(−2)	2.281(−2)
5	1.370(−5)	5.566(−3)	5.603(−3)
7	7.023(−7)	2.039(−4)	2.058(−4)
9	1.718(−8)	2.934(−5)	2.930(−5)
11	3.038(−10)	2.538(−6)	2.539(−6)
13	2.779(−11)	6.061(−8)	6.054(−8)
14	–	–	2.995(−8)
15	–	–	1.338(−8)
17	–	–	1.068(−10)

Let us introduce the following quantities

$$\varrho(\ell) = \sqrt{\sum_{j=1}^{\ell} \left(\omega_j^{GK} - \omega_j^{GF}\right)^2 + \sum_{j=1}^{\ell+1} \left(\widetilde{\omega}_j^{GK} - \widetilde{\omega}_j^{GF}\right)^2 + \left(x_j^S - x_j^F\right)^2},$$

as a distance $Q_{2\ell+1}^{GF}$ of $Q_{2\ell+1}^{GK}$, and (f is a continuous function on $[a, b]$)

$$D_\ell^{GK}(f) = \left|Q_{2\ell+1}^{GK}[f] - Q_\ell^G[f]\right|,$$

$$D_\ell^{GF}(f) = \left|Q_{2\ell+1}^{GF}[f] - Q_\ell^G[f]\right|,$$

$$\text{R.Err.}_\ell(f) = \frac{\left|Q_{2\ell+1}^{GK}[f] - Q_{2\ell+1}^{GF}[f]\right|}{\left|Q_{2\ell+1}^{GK}[f]\right|}.$$

We have tested our q.f. for various functions, and the corresponding error estimates we have obtained behave very similarly to what we have reported in the paper. Very similar results are obtained when Laurie's formulas are used.

Consider first the Legendre weight function $w(x) \equiv 1$ on $[-1, 1]$. It is well known that both q.f. $Q_{2\ell+1}^{GK}$, $Q_{2\ell+1}^{GF}$ are internal, in this case. The corresponding numerical results for this case are displayed in Tables 1, and 2 when the integrand is $f_1(x) = (x+1)/(0.02 + (x+1)^2)$. The numbers in parentheses denote decimal exponents.

The integrand $f_1(x)$ is smooth, arbitrarily often differentiable in $[-1, 1]$, but has two poles in the complex plane close to the interval of integration. For the integrand $\widetilde{f}(x) = (1+x)\log(1+x)$, which is a non-smooth function in $[-1, 1]$, the corresponding numerical results are displayed in Table 3.

Consider secondly the Gegenbauer weight function $w(x) \equiv w^{(-0.7)}(x) \equiv (1-x^2)^{-0.7}$ on $[-1, 1]$. In this case, in both q.f. $Q_{2\ell+1}^{GK}$, $Q_{2\ell+1}^{GF}$, the first and the last node are real but outside of the interval $[-1, 1]$. On the basis of numerical results, the positive q.f. $Q_{2\ell+1}^{GK}$ there exists in this case. For the theoretical results see the recent paper by Ysern and Peherstorfer [5]. The corresponding numerical results for the integrand $f_2(x) = e^{x^2}$, and for this case, are displayed in Table 4.

Finally, consider the Jacobi weight function $w(x) \equiv w^{(1/10,13/5)}(x) \equiv (1-x)^{1/10}(1+x)^{13/5}$ on $[-1, 1]$. The corresponding optimal averaged Gaussian q.f. $Q_{2\ell+1}^{GF}$ in this case is internal (cf. Spalević [24]). Observe that the corresponding Gauss–Kronrod q.f. $Q_{2\ell+1}^{GK}$ do not exist for $\ell \geq 14$. The corresponding numerical results for the integrand $f_3(x) = e^{-x^{10}}$, and for this case, are displayed in Table 5.

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