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Error Estimates for Certain Cubature Formulae

Davorka Jandrlić[a], Miodrag Spalević[a], Jelena Tomanović[a]

[a]*Department of Mathematics, Faculty of mechanical engineering, University of Belgrade, Serbia*

Dedicated to Prof. Walter Gautschi on the occasion of his 90th anniversary

Abstract. We estimate the errors of selected cubature formulae constructed by the product of Gauss quadrature rules. The cases of multiple and (hyper-)surface integrals over n-dimensional cube, simplex, sphere and ball are considered. The error estimates are obtained as the absolute value of the difference between cubature formula constructed by the product of Gauss quadrature rules and cubature formula constructed by the product of corresponding Gauss-Kronrod or corresponding generalized averaged Gaussian quadrature rules. Generalized averaged Gaussian quadrature rule $\widehat{G}_{2l+1}$ is $(2l+1)$-point quadrature formula. It has $2l+1$ nodes and the nodes of the corresponding Gauss rule G_l with l nodes form a subset, similar to the situation for the $(2l+1)$-point Gauss-Kronrod rule H_{2l+1} associated with G_l. The advantages of $\widehat{G}_{2l+1}$ are that it exists also when H_{2l+1} does not, and that the numerical construction of $\widehat{G}_{2l+1}$, based on recently proposed effective numerical procedure, is simpler than the construction of H_{2l+1}.

1. Introduction

Assume that $d\sigma$ is a nonnegative measure on an interval $[a,b] = \mathrm{supp}(d\sigma)$, and $d\sigma(t) = \omega(t)dt$ on $[a,b]$, where ω is a weight function.

Consider the l point quadrature formula (q.f.) of the form

$$I(f) = \int_a^b f(t)d\sigma(t) = Q_l(f) + R_l(f), \quad Q_l(f) = \sum_{j=1}^{l} \omega_j f(t_j), \tag{1}$$

with nodes $t_1 < t_2 < ... < t_l$ and weights $\omega_j \in \mathbb{R}$, $j = 1,2,...,l$. If all ω_j are positive, than (1) is called positive quadrature formula.

The q.f. (1) is said to have (algebraic) degree of exactness d if $R_l(f) = 0$ for all $f \in \mathcal{P}_d$, where $\mathcal{P}_d$ denotes the set of all (algebraic) polynomials of degree at most d. The q.f. (1) with $d = l-1$ is called interpolatory.

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Email addresses: djandrlic@mas.bg.ac.rs (Davorka Jandrlić), mspalevic@mas.bg.ac.rs (Miodrag Spalević), jtomanovic@mas.bg.ac.rs (Jelena Tomanović)

The unique optimal interpolatory q.f. with l nodes is Gauss formula

$$I(f) = \int_a^b f(t)d\sigma(t) = G_l(f) + R_l^G(f), \quad G_l(f) = \sum_{j=1}^{l} \omega_j^G f(t_j^G).$$

It has degree of exactnes $2l-1$ and is named after Gauss who discovered it in the case $d\sigma(t) = dt$ (see [8]).

Let $\pi_k(\cdot)$, $k = 0, 1, 2, \ldots$ be the monic orthogonal polynomials with respect to the measure $d\sigma$. They satisfy the three-term recurrence relation

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t), \quad k = 0, 1, 2, \ldots,$$

where $\pi_{-1}(t) = 0$, $\pi_0(t) = 1$, $\alpha_k \in \mathbb{R}$, $\beta_k > 0$ (for details see Gautschi [9]).

The $l \times l$ Jacobi matrix is tridiagonal symmetric matrix

$$J_l^G(d\sigma) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \mathbf{0} \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{\beta_{l-2}} & \alpha_{l-2} & \sqrt{\beta_{l-1}} \\ \mathbf{0} & & & \sqrt{\beta_{l-1}} & \alpha_{l-1} \end{bmatrix}.$$

The nodes of G_l are the eigenvalues and the weights are proportional to the squares of the first components of the corresponding eigenvectors of the Jacobi matrix $J_l^G(d\sigma)$ (see Wilf [28]). The nodes and weights of G_l can be conveniently computed by the Golub-Welsch algorithm [12].

An important task in practical calculations is to (economically) estimate the error $|(I - G_l)(f)|$ of the Gauss q.f. G_l. Of our interest are two formulae which can be used in this purpose.

One of them is $(2l+1)$-point Gauss-Kronrod q.f.

$$I(f) = \int_a^b f(t)d\sigma(t) = H_{2l+1}(f) + R_{2l+1}^H(f), \quad H_{2l+1}(f) = \sum_{j=1}^{l} \omega_j^H f(t_j^G) + \sum_{k=1}^{l+1} \tilde{\omega}_k^H f(t_k^S),$$

which has degree of precision $3l+1$. The error of G_l can be estimeted by the difference $|(H_{2l+1} - G_l)(f)|$.

H_{2l+1} has $2l+1$ nodes and the l nodes of the corresponding Gauss rule G_l form a subset. Additional $l+1$ nodes should alternate with the Gauss nodes and be choosen, together with all weights, in such a manner as to achive maximum degree of exactness. It turns out that the additional nodes are zeros of the Stieltjes polynomials (first considered by Stieltjes in the case $d\sigma(t) = dt$, see [2]), which are orthogonal with respect to a variable-sign weight function.

The idea of such error estimation (in the case $d\sigma(t) = dt$) was first put forward by Kronrod [14]. For historical details see Gautschi [11], while an overview on Gauss-Kronrod formulas can be found in Notaris [18].

Laurie [15] and Calvetti at al. [3] proposed the efficient numerical methods for calculating the positive Gauss-Kronrod q.f. (see also Monegato [16] and Gautschi [9], jointly with [10]).

There are several known cases of nonexistance of the positive Gauss-Kronrod q.f. For the Gegenbauer measure $d\sigma^{(\alpha,\alpha)}(t) = (1-t^2)^\alpha dt$, Peherstorfer and Petras [21] have shown nonexistance of Gauss-Kronrod formulae for sufficiently large l and $\alpha > 5/2$. In their paper [22] can be found analogous results for the Jacobi measure $d\sigma^{(\alpha,\beta)}(t) = (1-t)^\alpha(1+t)^\beta dt$, in particular nonexistence of Gauss-Kronrod formulae for large l when $\min(\alpha, \beta) \geq 0$ and $\max(\alpha, \beta) > 5/2$. Kahaner and Monegato [13] shown that Kronrod extension does not exist in some cases of Gauss-Laguerre and Gauss-Hermite formulae.

In the situations when Gauss-Kronrod formula doesn't exist, it is of interest to find adequate alternative and this alternative can be $(2l+1)$-point generalized averaged Gaussian q.f.

$$I(f) = \int_a^b f(t)d\sigma(t) = \widehat{G}_{2l+1}(f) + R_{2l+1}^{\widehat{G}}(f),$$

with degree of precision $2l+2$. The difference $|(\widehat{G}_{2l+1} - G_l)(f)|$ can also be used as the error estimation of G_l.

Same as H_{2l+1}, formula $\widehat{G}_{2l+1}$ has $2l+1$ nodes and the nodes of the corresponding Gauss rule G_l with l nodes form a subset. The Jacobi matrix of $\widehat{G}_{2l+1}$ is also tridiagonal symmetric matrix of the form

$$J^{\widehat{G}}_{2l+1}(d\sigma) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & & & & \mathbf{0} \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & & & & \\ & \ddots & \ddots & \ddots & & & & & \\ & & \sqrt{\beta_{l-1}} & \alpha_{l-1} & \sqrt{\beta_l} & & & & \\ & & & \sqrt{\beta_l} & \alpha_l & \sqrt{\beta_{l+1}} & & & \\ & & & & \sqrt{\beta_{l+1}} & \alpha_{l-1} & \sqrt{\beta_{l-1}} & & \\ & & & & & \sqrt{\beta_{l-1}} & \alpha_{l-2} & \sqrt{\beta_{l-2}} & \\ & & & & & & \ddots & \ddots & \ddots \\ & & & & & & \sqrt{\beta_2} & \alpha_1 & \sqrt{\beta_1} \\ \mathbf{0} & & & & & & & \sqrt{\beta_1} & \alpha_0 \end{bmatrix}.$$

Spalević [24] (see also [25], [26]) proposed a very simple and effective method for constructing the generalized averaged Gaussian q.f. by following the results on caracterization of the positive q.f. by Peherstorfer [19] (see also [20]).

The adventages of $\widehat{G}_{2l+1}$ are that it exists in some situations when H_{2l+1} does not, and that it's numerical construction in [24] is simpler than the construction of H_{2l+1} in [15] (see also [9], jointly with [10]).

Now, let $\Omega^n \subset \mathbb{R}^n$ and $\omega(\boldsymbol{x}) \geq 0$ for all $\boldsymbol{x} = (x_1, x_2, ..., x_n) \in \mathbb{R}^n$, $n \geq 2$. Consider the cubature formula (c.f.) of the form

$$I^n(f) = \int_{\Omega^n} f(\boldsymbol{x})\omega(\boldsymbol{x})d\boldsymbol{x} = Q^n_L(f) + R^n_L(f), \quad Q^n_L(f) = \sum_{j=1}^{L} \omega_j f(\boldsymbol{x}_j), \tag{2}$$

with $\boldsymbol{x}_j \in \mathbb{R}^n$, $\omega_j \in \mathbb{R}$, $j = 1, 2, ..., L$. The c.f. (2) is said to have (algebraic) degree of exactness d if $R^n_L(f) = 0$ for all $f \in \mathcal{P}^n_d$, where $\mathcal{P}^n_d$ denotes the set of all (algebraic) polynomials in n variables of degree at most d.

There are several encyclopedic works on multiple numerical integration, like Mysovskikh [17] and Stroud [27]. Stroud's work was continued by Cools and Rabinowitz, see [4] and [6]. Something about c.f. can be found also in [1], [5], [7] and [23].

Some multiple integration rules (also called cubature rules or cubature formulae) can be constructed by the product of Gauss q.f. The c.f. which approximate integral over n-dimensional region constructed by the product of l-point Gauss q.f. will be denoted by G^n_l. In the next chapters we consider the formulas G^n_l for integrals over n-dimensional cube, simplex, sphere and ball, by following results from Mysovskikh [17].

In order to estimate the error of G^n_l we first extend it to H^n_{2l+1} and $\widehat{G}^n_{2l+1}$, and than use the differences $|(H^n_{2l+1} - G^n_l)(f)|$ and $|(\widehat{G}^n_{2l+1} - G^n_l)(f)|$ as error estimates, where H^n_{2l+1} denotes c.f. constructed by the product of corresponding Gauss-Kronrod q.f., and $\widehat{G}^n_{2l+1}$ denotes c.f. constructed by the product of corresponding generalized averaged Gaussian q.f.

In all examples we first solve I^n analytically, and than show results for $|I^n - G^n_l|$, $|I^n - H^n_{2l+1}|$, $|H^n_{2l+1} - G^n_l|$, $|I^n - \widehat{G}^n_{2l+1}|$ and $|\widehat{G}^n_{2l+1} - G^n_l|$ for different values of n and l. All results are calculated with 40 significant decimal digits.

2. Error estimates for integrals over *n*-dimensional cube

The simplest situation which will be considered is the case of integral over n-dimensional cube,

$$I^n = \int_{K^n} f(\boldsymbol{x})d\boldsymbol{x}, \quad K^n = \{\boldsymbol{x} \in \mathbb{R}^n \mid -1 \leq x_i \leq 1,\ i = 1, 2, ..., n\},$$

which can be written in the form

$$I^n = \int_{-1}^{1} dx_1 \int_{-1}^{1} dx_2 ... \int_{-1}^{1} f(x_1, x_2, ..., x_n) dx_n.$$

Integral of each variable on the right side of previous equation can be approximated by l-point Gauss q.f. G_l with Legendre weight function $\omega(t) = 1$ on $[-1, 1]$,

$$\int_{-1}^{1} \varphi(t)dt \approx \sum_{j=1}^{l} \omega_j^G \varphi(t_j^G),$$

which leads to l^n-point c.f.

$$I^n \approx G_l^n = \sum_{j_1, j_2, ..., j_n = 1}^{l} \omega_{j_1}^G \omega_{j_2}^G ... \omega_{j_n}^G f(t_{j_1}^G, t_{j_2}^G, ..., t_{j_n}^G).$$

Analogously, using $(2l+1)$-point q.f. H_{2l+1} or $\widehat{G}_{2l+1}$,

$$\int_{-1}^{1} \varphi(t)dt \approx \sum_{j=1}^{2l+1} \omega_j^H \varphi(t_j^H), \qquad \int_{-1}^{1} \varphi(t)dt \approx \sum_{j=1}^{2l+1} \omega_j^{\widehat{G}} \varphi(t_j^{\widehat{G}})$$

instead of G_l, we get $(2l+1)^n$-point c.f.

$$I^n \approx H_{2l+1}^n = \sum_{j_1, j_2, ..., j_n = 1}^{2l+1} \omega_{j_1}^H \omega_{j_2}^H ... \omega_{j_n}^H f(t_{j_1}^H, t_{j_2}^H, ..., t_{j_n}^H), \qquad I^n \approx \widehat{G}_{2l+1}^n = \sum_{j_1, j_2, ..., j_n = 1}^{2l+1} \omega_{j_1}^{\widehat{G}} \omega_{j_2}^{\widehat{G}} ... \omega_{j_n}^{\widehat{G}} f(t_{j_1}^{\widehat{G}}, t_{j_2}^{\widehat{G}}, ..., t_{j_n}^{\widehat{G}}).$$

Example 2.1. *In Table 2.1 are shown selected results on error estimates of G_l^n for certain integrals over cube. We consider the cases of $l = 2, 4, 6$ for $n = 1, 2, 3, 5$, the cases of $l = 2, 4$ for $n = 7$, and the case of $l = 2$ for $n = 10$ (notice that l is number of nodes of Gauss q.f.; for expamle, the number of nodes of corresponding c.f. H_{2l+1}^n or $\widehat{G}_{2l+1}^n$ with $l = 4$ and $n = 7$ is $(2l+1)^n = 9^7 = 4782969$). In all cases both H_{2l+1}^n and $\widehat{G}_{2l+1}^n$ have better accuracy than G_l^n, and both $|(H_{2l+1}^n - G_l^n)(f)|$ and $|(\widehat{G}_{2l+1}^n - G_l^n)(f)|$ give good error estimates of G_l^n.*

Example 2.2. *In this example we consider 2-dimensional integral and take a slightly different approach. Integral of variable x_2 is approximated by l-point Gauss q.f. with Legendre weight function $\omega(t) = 1$ on $[-1, 1]$,*

$$\int_{-1}^{1} \varphi(t)dt \approx \sum_{j2=1}^{l} \omega_{j2}^G \varphi(t_{j2}^G),$$

while integral of variable x_1 is approximated by l-point Gauss q.f. with Jacobi weight function $\omega(t) = (1+t)^4$ on $[-1, 1]$,

$$\int_{-1}^{1} \varphi(t)(1+t)^4 dt \approx \sum_{j1=1}^{l} \omega_{j1}^G \varphi(t_{j1}^G).$$

Gauss-Kronrod q.f. with Jacobi weight function $\omega(t) = (1+t)^4$ on $[-1, 1]$ doesn't exist for any $l = 2, 4, 6$ (see [22]) and c.f. H_{2l+1}^2 can't be constructed. On the other hand, corresponding generalized averaged Gaussian q.f. does exist. The results are shown in Table 2.2, and again we have good error estimates.

In Table 2.3 are shown results for the same integral, but here $f(x_1, x_2) = (1+x_1)^4 \cos(x_1+x_2)$ and $\omega(x_1) = \omega(x_2) = 1$ (Gauss-Kronrod q.f. exists in this situation). Both $|(H_{2l+1}^n - G_l^n)(f)|$ and $|(\widehat{G}_{2l+1}^n - G_l^n)(f)|$ give good error estimates of G_l^n, but notice that G_l^n with $\omega(x_1) = (1+x_1)^4$ has better accuracy than G_l^n with $\omega(x_1) = 1$, and also $\widehat{G}_{2l+1}^2$ with $\omega(x_1) = (1+x_1)^4$ has better accuracy than $\widehat{G}_{2l+1}^2$ with $\omega(x_1) = 1$. $\widehat{G}_{2l+1}^2$ with $\omega(x_1) = (1+x_1)^4$ for $l = 2, 4$ has even better accuracy than H_{2l+1}^2 (with $\omega(x_1) = 1$).

$I^1 = \int_{-1}^{1} \cos(x_1)dx_1 = 2\sin 1 \approx 1.682...$					
l	$\lvert I^1 - G_l^1\rvert$	$\lvert I^1 - H_{2l+1}^1\rvert$	$\lvert H_{2l+1}^1 - G_l^1\rvert$	$\lvert I^1 - \widehat{G}_{2l+1}^1\rvert$	$\lvert \widehat{G}_{2l+1}^1 - G_l^1\rvert$
2	7.118e-03	8.850e-08	7.118e-03	8.850e-08	7.118e-03
4	2.809e-07	1.127e-16	2.809e-07	3.226e-14	2.809e-07
6	1.514e-12	2.451e-26	1.514e-12	1.347e-20	1.514e-12
$I^2 = \int_{-1}^{1}\int_{-1}^{1} \cos(x_1 + x_2)dx_1dx_2 = (2\sin 1)^2 \approx 2.832...$					
l	$\lvert I^2 - G_l^2\rvert$	$\lvert I^2 - H_{2l+1}^2\rvert$	$\lvert H_{2l+1}^2 - G_l^2\rvert$	$\lvert I^2 - \widehat{G}_{2l+1}^2\rvert$	$\lvert \widehat{G}_{2l+1}^2 - G_l^2\rvert$
2	2.391e-02	2.979e-07	2.391e-02	2.979e-07	2.391e-02
4	9.455e-07	3.794e-16	9.455e-07	1.086e-13	9.455e-07
6	5.095e-12	8.249e-26	5.095e-12	4.534e-20	5.095e-12
$I^3 = \int_{-1}^{1}\int_{-1}^{1}\int_{-1}^{1} \cos(x_1 + x_2 + x_3)dx_1dx_2dx_3 = (2\sin 1)^3 \approx 4.766...$					
l	$\lvert I^3 - G_l^3\rvert$	$\lvert I^3 - H_{2l+1}^3\rvert$	$\lvert H_{2l+1}^3 - G_l^3\rvert$	$\lvert I^3 - \widehat{G}_{2l+1}^3\rvert$	$\lvert \widehat{G}_{2l+1}^3 - G_l^3\rvert$
2	6.023e-02	7.520e-07	6.023e-02	7.520e-07	6.023e-02
4	2.387e-06	9.577e-16	2.387e-06	2.741e-13	2.387e-06
6	1.286e-11	2.082e-25	1.286e-11	1.145e-19	1.286e-11
$I^5 = \int_{-1}^{1}...\int_{-1}^{1} \cos(x_1 + \cdots + x_5)dx_1...dx_5 = (2\sin 1)^5 \approx 13.500...$					
l	$\lvert I^5 - G_l^5\rvert$	$\lvert I^5 - H_{2l+1}^5\rvert$	$\lvert H_{2l+1}^5 - G_l^5\rvert$	$\lvert I^5 - \widehat{G}_{2l+1}^5\rvert$	$\lvert \widehat{G}_{2l+1}^5 - G_l^5\rvert$
2	2.831e-01	3.550e-06	2.831e-01	3.550e-06	2.831e-01
4	1.127e-05	4.521e-15	1.127e-05	1.294e-12	1.127e-05
6	6.072e-11	9.830e-25	6.072e-11	5.403e-19	6.072e-11
$I^7 = \int_{-1}^{1}...\int_{-1}^{1} \cos(x_1 + \cdots + x_7)dx_1...dx_7 = (2\sin 1)^7 \approx 38.237...$					
l	$\lvert I^7 - G_l^7\rvert$	$\lvert I^7 - H_{2l+1}^7\rvert$	$\lvert H_{2l+1}^7 - G_l^7\rvert$	$\lvert I^7 - \widehat{G}_{2l+1}^7\rvert$	$\lvert \widehat{G}_{2l+1}^7 - G_l^7\rvert$
2	1.118	1.408e-05	1.118	1.408e-05	1.118
4	4.468e-05	1.792e-14	4.468e-05	5.131e-12	4.468e-05
$I^{10} = \int_{-1}^{1}...\int_{-1}^{1} \cos(x_1 + \cdots + x_{10})dx_1...dx_{10} = (2\sin 1)^{10} \approx 182.260...$					
l	$\lvert I^{10} - G_l^{10}\rvert$	$\lvert I^{10} - H_{2l+1}^{10}\rvert$	$\lvert H_{2l+1}^{10} - G_l^{10}\rvert$	$\lvert I^{10} - \widehat{G}_{2l+1}^{10}\rvert$	$\lvert \widehat{G}_{2l+1}^{10} - G_l^{10}\rvert$
2	7.564	9.584e-05	7.564	9.584e-05	7.564

Table 2.1: Example 2.1

$I^2 = \int_{-1}^{1}\int_{-1}^{1}(1 + x_1)^4 \cos(x_1 + x_2)dx_1dx_2 = 16(1 - \sin 2 - \cos 2) \approx 8.109...$					
l	$\lvert I^2 - G_l^2\rvert$	$\lvert I^2 - H_{2l+1}^2\rvert$	$\lvert H_{2l+1}^2 - G_l^2\rvert$	$\lvert I^2 - \widehat{G}_{2l+1}^2\rvert$	$\lvert \widehat{G}_{2l+1}^2 - G_l^2\rvert$
2	3.880e-02	-	-	6.634e-07	3.880e-02
4	1.454e-06	-	-	4.310e-13	1.454e-06
6	7.700e-12	-	-	2.115e-19	7.700e-12

Table 2.2: Example 2.2a) with $\omega(x_1) = (1 + x_1)^4$, $\omega(x_2) = 1$.

$I^2 = \int_{-1}^{1}\int_{-1}^{1}(1 + x_1)^4 \cos(x_1 + x_2)dx_1dx_2 = 16(1 - \sin 2 - \cos 2) \approx 8.109...$					
l	$\lvert I^2 - G_l^2\rvert$	$\lvert I^2 - H_{2l+1}^2\rvert$	$\lvert H_{2l+1}^2 - G_l^2\rvert$	$\lvert I^2 - \widehat{G}_{2l+1}^2\rvert$	$\lvert \widehat{G}_{2l+1}^2 - G_l^2\rvert$
2	6.276e-01	1.930e-04	6.274e-01	1.930e-04	6.274e-01
4	6.008e-04	4.263-12	6.008e-04	5.874e-10	6.008e-04
6	2.772e-08	4.669e-21	2.772e-08	9.469e-16	2.772e-08

Table 2.3: Example 2.2b) with $\omega(x_1) = \omega(x_2) = 1$.

3. Error estimates for integrals over *n*-dimensional simplex

Consider the integral over n-dimensional simplex

$$I^n = \int_{T^n} f(\mathbf{x})d\mathbf{x}, \quad T^n = \{\mathbf{x} \in \mathbb{R}^n \mid x_i \geq 0,\ i = 1, 2, ..., n,\ x_1 + x_2 + \cdots + x_n \leq 1\}.$$

Approximating integral of variable $x_n, x_{n-1}, ..., x_1$ by l-point Gauss q.f. G_l with Jacobi weight function $\omega(t) = (1-t)^{m-1}dt$, $m = n, n-1, ..., 1$, on $[0, 1]$,

$$\int_0^1 (1-t)^{m-1}\varphi(t)dt \approx \sum_{j=1}^{l} \omega^G_{j,m-1}\varphi(t^G_{j,m-1}), \quad m = n, n-1, ..., 1,$$

leads to l^n-point c.f.

$$I^n \approx G^n_l = \sum_{j_1, j_2, ..., j_n = 1}^{l} \omega^G_{j_1,n-1}\omega^G_{j_2,n-2}...\omega^G_{j_n,0} f(\Pi^G(j_1), \Pi^G(j_1, j_2), ..., \Pi^G(j_1, j_2, ..., j_n)),$$

$$\Pi^G(j_1) = t^G_{j_1,n-1}, \quad \Pi^G(j_1, j_2, ..., j_m) = (1 - t^G_{j_1,n-1})(1 - t^G_{j_2,n-2})...(1 - t^G_{j_{m-1},n-m+1})t^G_{j_m,n-m}, \quad m = 2, 3, ..., n.$$

Using corresponding $(2l+1)$-point q.f. H_{2l+1} or $\widehat{G}_{2l+1}$ instead of G_l, we get $(2l+1)^n$-point c.f.

$$I^n \approx H^n_{2l+1} = \sum_{j_1, j_2, ..., j_n = 1}^{2l+1} \omega^H_{j_1,n-1}\omega^H_{j_2,n-2}...\omega^H_{j_n,0} f(\Pi^H(j_1), \Pi^H(j_1, j_2), ..., \Pi^H(j_1, j_2, ..., j_n)),$$

$$I^n \approx \widehat{G}^n_{2l+1} = \sum_{j_1, j_2, ..., j_n = 1}^{2l+1} \omega^{\widehat{G}}_{j_1,n-1}\omega^{\widehat{G}}_{j_2,n-2}...\omega^{\widehat{G}}_{j_n,0} f(\Pi^{\widehat{G}}(j_1), \Pi^{\widehat{G}}(j_1, j_2), ..., \Pi^{\widehat{G}}(j_1, j_2, ..., j_n)).$$

Example 3.1. *In Table 3.1 are shown selected results on error estimates of G^n_l for certain integrals over simplex. Both $|(H^n_{2l+1} - G^n_l)(f)|$ and $|(\widehat{G}^n_{2l+1} - G^n_l)(f)|$ give good error estimates of G^n_l. Notice that in all cases H^n_{2l+1} has better (or the same for $n = 1$, $l = 2$) accuracy than $\widehat{G}^n_{2l+1}$, but in cases $n = 4$, $l = 4, 6$, q.f. H_{2l+1} doesn't exist and c.f. H^n_{2l+1} can't be constructed.*

4. Error estimates for integrals over *n*-dimensional sphere

Now we consider the integral over n-dimensional sphere

$$I^n = \int_{S^n} f(\mathbf{x})d\mathbf{x}, \quad S^n = \{\mathbf{x} \in \mathbb{R}^n \mid x_1^2 + x_2^2 + \cdots + x_n^2 = r^2\}.$$

Let r be radial coordinate, and $\varphi_1, \varphi_2, ..., \varphi_{n-1}$ angular coordinates of n-dimensional spherical coordinate system, where $0 \leq \varphi_j \leq \pi$, $j = 1, 2, ..., n-2$, $0 \leq \varphi_{n-1} \leq 2\pi$. Cartesian coordinates $x_1, x_2, ..., x_n$ may be computed from $r, \varphi_1, \varphi_2, ..., \varphi_{n-1}$ with

$$\begin{aligned}
x_1 &= r\cos\varphi_1, \\
x_2 &= r\sin\varphi_1\cos\varphi_2, \\
x_3 &= r\sin\varphi_1\sin\varphi_2\cos\varphi_3, \\
&\vdots \\
x_{n-2} &= r\sin\varphi_1\sin\varphi_2...\sin\varphi_{n-3}\cos\varphi_{n-2}, \\
x_{n-1} &= r\sin\varphi_1\sin\varphi_2...\sin\varphi_{n-3}\sin\varphi_{n-2}\cos\varphi_{n-1}, \\
x_n &= r\sin\varphi_1\sin\varphi_2...\sin\varphi_{n-3}\sin\varphi_{n-2}\sin\varphi_{n-1},
\end{aligned}$$

$I^1 = \int_0^1 \frac{dx_1}{1+x_1} = \ln 2 \approx 0.693...$					
l	$\lvert I^1 - G_l^1\rvert$	$\lvert I^1 - H_{2l+1}^1\rvert$	$\lvert H_{2l+1}^1 - G_l^1\rvert$	$\lvert I^1 - \widehat{G}_{2l+1}^1\rvert$	$\lvert \widehat{G}_{2l+1}^1 - G_l^1\rvert$
2	8.395e-04	2.179e-07	8.397e-04	2.179e-07	8.397e-04
4	7.631e-07	1.322e-12	7.631e-07	1.636e-11	7.631e-07
6	6.734e-10	1.228e-17	6.734e-10	3.983e-15	6.734e-10
$I^2 = \int_0^1 \int_0^{1-x_1} \frac{dx_1 dx_2}{(1+x_1+x_2)^2} = \frac{2\ln 2 - 1}{2} \approx 0.193...$					
l	$\lvert I^2 - G_l^2\rvert$	$\lvert I^2 - H_{2l+1}^2\rvert$	$\lvert H_{2l+1}^2 - G_l^2\rvert$	$\lvert I^2 - \widehat{G}_{2l+1}^2\rvert$	$\lvert \widehat{G}_{2l+1}^2 - G_l^2\rvert$
2	4.973e-04	8.995e-08	4.974e-04	1.865e-07	4.975e-04
4	4.914e-07	4.446e-13	4.914e-07	1.996e-11	4.914e-07
6	4.406e-10	2.702e-18	4.406e-10	5.529e-15	4.406e-10
$I^3 = \int_0^1 \int_0^{1-x_1} \int_0^{1-x_1-x_2} \frac{dx_1 dx_2 dx_3}{(1+x_1+x_2+x_3)^3} = \frac{8\ln 2 - 5}{16} \approx 0.034...$					
l	$\lvert I^3 - G_l^3\rvert$	$\lvert I^3 - H_{2l+1}^3\rvert$	$\lvert H_{2l+1}^3 - G_l^3\rvert$	$\lvert I^3 - \widehat{G}_{2l+1}^3\rvert$	$\lvert \widehat{G}_{2l+1}^3 - G_l^3\rvert$
2	1.237e-04	1.353e-08	1.237e-04	6.196e-08	1.237e-04
4	1.285e-07	2.513e-14	1.285e-07	7.961e-12	1.285e-07
6	1.167e-10	2.024e-18	1.167e-10	2.337e-15	1.167e-10
$I^4 = \int_0^1 \int_0^{1-x_1} \int_0^{1-x_1-x_2} \int_0^{1-x_1-x_2-x_3} \frac{dx_1 dx_2 dx_3 dx_4}{(1+x_1+x_2+x_3+x_4)^4} = \frac{24\ln 2 - 16}{144} \approx 0.004...$					
l	$\lvert I^4 - G_l^4\rvert$	$\lvert I^4 - H_{2l+1}^4\rvert$	$\lvert H_{2l+1}^4 - G_l^4\rvert$	$\lvert I^4 - \widehat{G}_{2l+1}^4\rvert$	$\lvert \widehat{G}_{2l+1}^4 - G_l^4\rvert$
2	1.959e-05	1.131e-09	1.959e-05	1.179e-08	1.960e-05
4	2.111e-08	-	-	1.661e-12	2.111e-08
6	1.937e-11	-	-	5.015e-16	1.937e-11

Table 3.1: Example 3.1

where volume element is

$$d\boldsymbol{x} = r^{n-1} \sin^{n-2}\varphi_1 \sin^{n-3}\varphi_2 ... \sin\varphi_{n-1} d\varphi_1 d\varphi_2 ... d\varphi_{n-1}.$$

Than, I^n is equal to integral over $(n-1)$-dimensional parallelepiped,

$$I^n = r^{n-1} \int_0^{\pi} ... \int_0^{\pi} \int_0^{2\pi} f(r\cos\varphi_1, r\sin\varphi_1\cos\varphi_2, ..., r\sin\varphi_1\sin\varphi_2 ... \sin\varphi_{n-1}) \sin^{n-2}\varphi_1 \sin^{n-3}\varphi_2 ... \sin\varphi_{n-1} d\varphi_1 d\varphi_2 ... d\varphi_{n-1}.$$

If we replace integral of variable φ_{n-1} with $(2l)$-point rectangle formula,

$$\int_a^b \varphi(t)dt \approx h \sum_{j=1}^{2l} \varphi(t_1 + (j-1)h), \quad h = (b-a)/(2l), \quad t_1 \in [a, a+h],$$

and approximate integral of each variable $\varphi_{n-2}, \varphi_{n-1}, ..., \varphi_1$ by Gauss q.f. G_l with Gegenbauer weight function $\omega(t) = (1-t^2)^{m/2}$, $m = n-3, n-2, ..., 0$, on $[-1, 1]$,

$$\int_{-1}^{1} (1-t^2)^{m/2} \varphi(t)dt \approx \sum_{j=1}^{l} \omega_{j,m}^G \varphi(t_{j,m}^G), \quad m = n-3, n-2, ..., 0,$$

we get c.f. with $2l^{n-1}$ nodes,

$$\begin{aligned} &I^n \approx G_l^n = r^{n-1} \frac{\pi}{l} \sum_{j=1}^{2l} \sum_{j_1, j_2, ..., j_{n-2}=1}^{l} \omega_{j_1,n-3}^G \omega_{j_2,n-4}^G ... \omega_{j_{n-2},0}^G F(r, \varphi_{1,j_1}^G, \varphi_{2,j_2}^G, ..., \varphi_{n-2,j_{n-2}}^G, \frac{\pi}{l} j), \\ &F(r, \varphi_1, \varphi_2, ..., \varphi_{n-1}) = f(r\cos\varphi_1, r\sin\varphi_1\cos\varphi_2, ..., r\sin\varphi_1\sin\varphi_2 ... \sin\varphi_{n-1}), \\ &\varphi_{n-m-2,j}^G = \arccos t_{j,m}^G, \quad m = 0, 1, ..., n-3. \end{aligned} \tag{3}$$

$S^3: x_1^2+x_2^2+x_3^2=1,\quad I^3=\int_{S^3} e^{x_1} d\boldsymbol{x} = 2\pi(e-1/e) \approx 14.768...$					
l	$\lvert I^3-G_l^3\rvert$	$\lvert I^3-H_{2l+1}^3\rvert$	$\lvert H_{2l+1}^3-G_l^3\rvert$	$\lvert I^3-\widehat{G}_{2l+1}^3\rvert$	$\lvert\widehat{G}_{2l+1}^3-G_l^3\rvert$
2	4.842e-02	5.748e-07	4.842e-02	5.748e-07	4.842e-02
4	1.854e-06	7.429e-16	1.854e-06	2.123e-13	1.854e-06
6	9.855e-12	1.583e-25	9.855e-12	8.746e-20	9.855e-12
$S^3: x_1^2+x_2^2+x_3^2=4,\quad I^3=\int_{S^3} e^{x_1} d\boldsymbol{x} = 4\pi(e^2-1/e^2) \approx 91.152...$					
l	$\lvert I^3-G_l^3\rvert$	$\lvert I^3-H_{2l+1}^3\rvert$	$\lvert H_{2l+1}^3-G_l^3\rvert$	$\lvert I^3-\widehat{G}_{2l+1}^3\rvert$	$\lvert\widehat{G}_{2l+1}^3-G_l^3\rvert$
2	3.484	6.184e-04	3.485	6.184e-04	3.485
4	2.044e-03	5.225e-11	2.044e-03	3.729e-09	2.044e-03
6	1.703e-07	6.922e-19	1.703e-07	2.408e-14	1.703e-07
8	3.873e-12	2.086e-27	3.873e-12	8.727e-20	3.873e-12
$S^3: x_1^2+x_2^2+x_3^2=9,\quad I^3=\int_{S^3} e^{x_1} d\boldsymbol{x} = 6\pi(e^3-1/e^3) \approx 377.664...$					
l	$\lvert I^3-G_l^3\rvert$	$\lvert I^3-H_{2l+1}^3\rvert$	$\lvert H_{2l+1}^3-G_l^3\rvert$	$\lvert I^3-\widehat{G}_{2l+1}^3\rvert$	$\lvert\widehat{G}_{2l+1}^3-G_l^3\rvert$
2	4.803e+01	3.866e-02	4.807e+01	3.866e-02	4.807e+01
4	1.331e-01	3.852e-08	1.331e-01	1.222e-06	1.331e-01
6	5.428e-05	5.550e-15	5.428e-05	3.860e-11	5.428e-05
8	6.132e-09	1.871e-22	6.132e-09	6.962e-16	6.132e-09
$S^3: x_1^2+x_2^2+x_3^2=16,\quad I^3=\int_{S^3} e^{x_1} d\boldsymbol{x} = 8\pi(e^4-1/e^4) \approx 1371.740...$					
l	$\lvert I^3-G_l^3\rvert$	$\lvert I^3-H_{2l+1}^3\rvert$	$\lvert H_{2l+1}^3-G_l^3\rvert$	$\lvert I^3-\widehat{G}_{2l+1}^3\rvert$	$\lvert\widehat{G}_{2l+1}^3-G_l^3\rvert$
2	3.496e+02	7.667e-01	3.503e+02	7.667e-01	3.503e+02
4	2.796	4.495e-06	2.796	8.052e-05	2.796
6	3.443e-03	3.426e-12	3.443e-03	7.669e-09	3.443e-03
8	1.197e-06	6.329e-19	1.197e-06	4.269e-13	1.197e-06
10	1.592e-10	3.534e-26	1.592e-10	1.344e-17	1.592e-10

Table 4.1: Example 4.1

Using corresponding $(2l+1)$-point q.f. H_{2l+1} or $\widehat{G}_{2l+1}$ instead of G_l, we get c.f. with $2(2l+1)^{n-1}$ nodes,

$$I^n \approx H_{2l+1}^n = r^{n-1}\frac{\pi}{2l+1}\sum_{j=1}^{2(2l+1)}\sum_{j_1,j_2,\dots,j_{n-2}=1}^{2l+1}\omega_{j_1,n-3}^H\omega_{j_2,n-4}^H\dots\omega_{j_{n-2},0}^H F(r,\varphi_{1,j_1}^H,\varphi_{2,j_2}^H,\dots,\varphi_{n-2,j_{n-2}}^H,\frac{\pi}{2l+1}j),$$

$$I^n \approx \widehat{G}_{2l+1}^n = r^{n-1}\frac{\pi}{2l+1}\sum_{j=1}^{2(2l+1)}\sum_{j_1,j_2,\dots,j_{n-2}=1}^{2l+1}\omega_{j_1,n-3}^{\widehat{G}}\omega_{j_2,n-4}^{\widehat{G}}\dots\omega_{j_{n-2},0}^{\widehat{G}} F(r,\varphi_{1,j_1}^{\widehat{G}},\varphi_{2,j_2}^{\widehat{G}},\dots,\varphi_{n-2,j_{n-2}}^{\widehat{G}},\frac{\pi}{2l+1}j).$$

According to [21], Gauss-Kronrod q.f. H_{2l+1} with Gegenbauer weight function $\omega(t)=(1-t^2)^\alpha$ doesn't exist for sufficiently large l and $\alpha>5/2$. In construction of c.f. H_{2l+1}^n we use weight function $\omega(t)=(1-t^2)^{m/2}$, $m=n-3,n-2,\dots,0$. So, if integral over n-dimensional sphere is considered with $n>8$, for sufficiently large l c.f. H_{2l+1}^n can't be constructed.

Example 4.1. *Consider the sphere $S^3: x_1^2+x_2^2+x_3^2=r^2$ and surface integral $I^3=\int_{S^3} e^{x_1} d\boldsymbol{x} = 2r\pi(e^r-1/e^r)$. In Table 4.1 selected results for $r=1,2,3,4$ are shown. Both $\lvert(H_{2l+1}^n-G_l^n)(f)\rvert$ and $\lvert(\widehat{G}_{2l+1}^n-G_l^n)(f)\rvert$ give good error estimates of G_l^n.*

5. Error estimates for integrals over *n*-dimensional ball

Integral over n-dimensional ball,

$$I^n = \int_{B^n} f(\boldsymbol{x})d\boldsymbol{x}, \quad B^n = \{\boldsymbol{x} \in \mathbb{R}^n \mid x_1^2 + x_2^2 + \cdots + x_n^2 \leq 1\}$$

can be approximated by the sume of integrals over n-dimensional spheres,

$$I^n \approx \sum_{i=1}^{l} B_i \int_{S_i^n} f(\boldsymbol{x})d\boldsymbol{x}, \quad S_i^n = \{\boldsymbol{x} \in \mathbb{R}^n \mid x_1^2 + x_2^2 + \cdots + x_n^2 = r_i^2\}.$$

If n is even, than

$$(r_i^G)^2 = \tau_i^G, \quad 2B_i^G(r_i^G)^{n-1} = \lambda_i^G, \quad i = 1, 2, ..., l,$$

where τ_i^G and λ_i^G are nodes and weights of Gauss q.f.

$$\int_0^1 t^{n/2-1}\varphi(t)dt \approx \sum_{i=1}^{l} \lambda_i^G \varphi(\tau_i^G).$$

If n is odd, than

$$r_i^G = \tau_i^G, \quad B_i^G(r_i^G)^{n-1} = \lambda_i^G, \quad i = 1, 2, ..., l,$$

where τ_i^G and λ_i^G are nodes and weights of Gauss q.f.

$$\int_{-1}^1 t^{n-1}\varphi(t)dt \approx \sum_{\substack{i=-l \\ i\neq 0}}^{l} \lambda_i^G \varphi(\tau_i^G).$$

According to (3), $(2l)^n$-point c.f. takes the form

$$I^n \approx G_l^n = \sum_{i=1}^{l} B_i^G(r_i^G)^{n-1}\frac{\pi}{2l}\sum_{j=1}^{4l}\sum_{j_1,j_2,...,j_{n-2}=1}^{2l} \omega_{j_1,n-3}^G\omega_{j_2,n-4}^G...\omega_{j_{n-2},0}^G F(r_i^G, \varphi_{1,j_1}^G, \varphi_{2,j_2}^G, ..., \varphi_{n-2,j_{n-2}}^G, \frac{\pi}{2l}j).$$

For error estimates we extend it to $((4l + 2)(4l + 1)^{n-1})$-point c.f.

$$I^n \approx H_{2l+1}^n = \sum_{i=1}^{2l+1} B_i^H(r_i^H)^{n-1}\frac{\pi}{4l+1}\sum_{j=1}^{8l+2}\sum_{j_1,j_2,...,j_{n-2}=1}^{4l+1} \omega_{j_1,n-3}^H\omega_{j_2,n-4}^H...\omega_{j_{n-2},0}^H F(r_i^H, \varphi_{1,j_1}^H, \varphi_{2,j_2}^H, ..., \varphi_{n-2,j_{n-2}}^H, \frac{\pi}{4l+1}j),$$

$$I^n \approx \widehat{G}_{2l+1}^n = \sum_{i=1}^{2l+1} B_i^{\widehat{G}}(r_i^{\widehat{G}})^{n-1}\frac{\pi}{4l+1}\sum_{j=1}^{8l+2}\sum_{j_1,j_2,...,j_{n-2}=1}^{4l+1} \omega_{j_1,n-3}^{\widehat{G}}\omega_{j_2,n-4}^{\widehat{G}}...\omega_{j_{n-2},0}^{\widehat{G}} F(r_i^{\widehat{G}}, \varphi_{1,j_1}^{\widehat{G}}, \varphi_{2,j_2}^{\widehat{G}}, ..., \varphi_{n-2,j_{n-2}}^{\widehat{G}}, \frac{\pi}{4l+1}j).$$

Example 5.1. *In Table 5.1 are shown selected results on error estimates of G_l^n for integral $I^4 = \int_{B^4} \sqrt{(x_2^2 + x_3^2 + x_4^2)^{17}}d\boldsymbol{x}$, $B^4 : x_1^2 + x_2^2 + x_3^2 + x_4^2 \leq 1$. Again, both $|(H_{2l+1}^n - G_l^n)(f)|$ and $|(\widehat{G}_{2l+1}^n - G_l^n)(f)|$ give good error estimates of G_l^n.*

$B^4 : x_1^2 + x_2^2 + x_3^2 + x_4^2 \le 1, \quad I^4 = \int_{B^4} \sqrt{(x_2^2 + x_3^2 + x_4^2)^{17}} d\boldsymbol{x} = 524288\pi/4849845 \approx 0.339...$					
l	$\lvert I^4 - G_l^4\rvert$	$\lvert I^4 - H_{2l+1}^4\rvert$	$\lvert H_{2l+1}^4 - G_l^4\rvert$	$\lvert I^4 - \widehat{G}_{2l+1}^4\rvert$	$\lvert\widehat{G}_{2l+1}^4 - G_l^4\rvert$
2	1.084e-01	7.329e-06	1.084e-01	6.606e-05	1.084e-01
4	9.084e-05	9.728e-13	9.084e-05	4.984e-11	9.084e-05
6	4.369e-10	3.459e-16	4.369e-10	1.409e-14	4.369e-10
8	6.133e-13	1.283e-18	6.133e-13	5.122e-17	6.133e-13

Table 5.1: Example 5.1

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