

Error Estimates for Some Product Gauss Rules

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Abstract

Some integrals I^m over m -dimensional regions can be approximated by cubature formulas G_n^m constructed by the product of Gauss quadrature rules G_n . Using corresponding Gauss-Kronrod rules K_{2n+1} or corresponding generalized averaged Gauss rules \widehat{G}_{2n+1} instead of G_n , we construct cubature formulas K_{2n+1}^m and \widehat{G}_{2n+1}^m . In order to estimate the error $|I^m - G_n^m|$ we use the differences $|K_{2n+1}^m - G_n^m|$ and $|\widehat{G}_{2n+1}^m - G_n^m|$.

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1 Introduction

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

$$I(f) = \int_{\mathbb{R}} f(t) d\mu(t) \approx Q_n(f) = \sum_{k=1}^n \omega_k f(t_k).$$

The unique optimal interpolatory q.f. with n nodes and (algebraic) degree of exactness $2n - 1$ is Gauss q.f. G_n . The nodes of G_n are the eigenvalues and the weights are proportional to the squares of the first components of the corresponding eigenvectors of tridiagonal symmetric Jacobi matrix with diagonal elements $\alpha_0, \dots, \alpha_{n-1}$ and subdiagonal elements $\sqrt{\beta_1}, \dots, \sqrt{\beta_{n-1}}$, where α s and β s are coefficient of the three-term recurrence relation, satisfied by the monic orthogonal polynomials.

In order to (economically) estimate the error $|I - G_n|$ we can use the differences $|K_{2n+1} - G_n|$ and $|\widehat{G}_{2n+1} - G_n|$. K_{2n+1} is corresponding Gauss-Kronrod q.f. with degree of exactness $3n + 1$, and \widehat{G}_{2n+1} is corresponding generalized averaged Gauss q.f. with degree of exactness $2n + 2$, both with $2n + 1$ nodes (n nodes of G_n form a subset). K_{2n+1} has higher degree of exactness, but \widehat{G}_{2n+1} exists in some situations when K_{2n+1} does not and its numerical construction is simpler – Spalević in [2] proposed effective numerical procedure for constructing \widehat{G}_{2n+1} , where tridiagonal symmetric

matrix has diagonal elements $\alpha_0, \dots, \alpha_{n-1}; \alpha_n; \alpha_{n-1}, \dots, \alpha_0$ and subdiagonal elements $\sqrt{\beta_1}, \dots, \sqrt{\beta_{n-1}}; \sqrt{\beta_n}; \sqrt{\beta_{n+1}}; \sqrt{\beta_{n-1}}, \dots, \sqrt{\beta_1}$.

Some integrals $I^m = \int_{\Omega^m} f(\mathbf{x})\omega(\mathbf{x})d\mathbf{x}$, $\omega(\mathbf{x}) \geq 0$, $\mathbf{x} = (x_1, \dots, x_m) \in \mathbb{R}^m$, $m \geq 2$, over m -dimensional regions Ω^m , can be approximated by cubature formulas (c.f.) G_n^m constructed by the product of q.f. G_n . In order to estimate the error $|I^m - G_n^m|$ we first extend G_n^m to K_{2n+1}^m and \widehat{G}_{2n+1}^m , and than use the differences $|K_{2n+1}^m - G_n^m|$ and $|\widehat{G}_{2n+1}^m - G_n^m|$, where K_{2n+1}^m denotes c.f. constructed by the product of corresponding q.f. K_{2n+1} , and \widehat{G}_{2n+1}^m denotes c.f. constructed by the product of corresponding q.f. \widehat{G}_{2n+1} .

2 Main Results

In all considered cases we first introduce G_n^m constructed by the product of G_n (according to [1]). K_{2n+1}^m and \widehat{G}_{2n+1}^m can be introduced analogously, using corresponding K_{2n+1} and \widehat{G}_{2n+1} instead of G_n . In all examples we first solve I^m analytically, and than show results for $|I^m - G_n^m|$, $|I^m - K_{2n+1}^m|$, $|K_{2n+1}^m - G_n^m|$, $|I^m - \widehat{G}_{2n+1}^m|$, $|\widehat{G}_{2n+1}^m - G_n^m|$, for different values of n . All results are calculated with 40 significant decimal digits.

Cube: $C^m = \{\mathbf{x} \in \mathbb{R}^m \mid -1 \leq x_l \leq 1, l = 1, \dots, m\}$. Integral of each variable x_l , $l = 1, \dots, m$, can be approximated by n -point Gauss q.f. G_n with Legendre weight function $\omega(t) = 1$ on $[-1, 1]$,

$$\int_{-1}^1 \varphi(t)dt \approx \sum_{k=1}^n \omega_k \varphi(t_k),$$

which leads to c.f.

$$I^m \approx G_n^m = \sum_{k_1, \dots, k_m=1}^n \omega_{k_1} \cdots \omega_{k_m} \cdot f(t_{k_1}, \dots, t_{k_m}).$$

G_n^m has n^m , while corresponding K_{2n+1}^m and \widehat{G}_{2n+1}^m have $(2n+1)^m$ nodes. Selected results are shown in table 1.

Simplex: $T^m = \{\mathbf{x} \in \mathbb{R}^m \mid x_l \geq 0, l = 1, \dots, m, x_1 + \dots + x_m \leq 1\}$. Approximating integral of each variable x_l , $l = 1, \dots, m$, by n -point Gauss q.f. G_n with Jacobi weight function $\omega(t) = (1-t)^{m-l}$, $l = 1, \dots, m$, on $[0, 1]$,

$$\int_0^1 (1-t)^{m-l} \varphi(t)dt \approx \sum_{k=1}^n \omega_{k,m-l} \varphi(t_{k,m-l}), \quad l = 1, \dots, m,$$

we get c.f.

$$I^m \approx G_n^m = \sum_{k_1, \dots, k_m=1}^n \omega_{k_1, m-1} \cdots \omega_{k_m, 0} \cdot f(\Pi(k_1), \dots, \Pi(k_1, \dots, k_m)),$$

| | | | | | |
|--|-----------------|----------------------|------------------------|--------------------------------|----------------------------------|
| $I^2 = \int_{-1}^1 \int_{-1}^1 \cos(x_1 + x_2) dx_1 dx_2 = (2 \sin 1)^2 \approx 2.832\dots$ | | | | | |
| n | $ I^2 - G_n^2 $ | $ I^2 - K_{2n+1}^2 $ | $ K_{2n+1}^2 - G_n^2 $ | $ I^2 - \widehat{G}_{2n+1}^2 $ | $ \widehat{G}_{2n+1}^2 - G_n^2 $ |
| 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 |
| $I^7 = \int_{-1}^1 \dots \int_{-1}^1 \cos(x_1 + \dots + x_7) dx_1 \dots dx_7 = (2 \sin 1)^7 \approx 38.237\dots$ | | | | | |
| n | $ I^7 - G_n^7 $ | $ I^7 - K_{2n+1}^7 $ | $ K_{2n+1}^7 - G_n^7 $ | $ I^7 - \widehat{G}_{2n+1}^7 $ | $ \widehat{G}_{2n+1}^7 - G_n^7 $ |
| 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 |

Table 1: Selected results for integrals over m -dimensional cube.

| | | | | | |
|--|-----------------|----------------------|------------------------|--------------------------------|----------------------------------|
| $I^3 = \int_0^1 \int_0^{1-x_1} \int_0^{1-x_1-x_2} \frac{dx_1 dx_2 dx_3}{(1+x_1+x_2+x_3)^3} = \frac{8 \ln 2 - 5}{16} \approx 0.034\dots$ | | | | | |
| n | $ I^3 - G_n^3 $ | $ I^3 - K_{2n+1}^3 $ | $ K_{2n+1}^3 - G_n^3 $ | $ I^3 - \widehat{G}_{2n+1}^3 $ | $ \widehat{G}_{2n+1}^3 - G_n^3 $ |
| 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 |
| $I^4 = \int_0^1 \int_0^{1-x_1} \int_0^{1-x_1-x_2} \int_0^{1-x_1-x_2-x_3} \frac{dx_1 dx_2 dx_3 dx_4}{(1+x_1+x_2+x_3+x_4)^4} = \frac{24 \ln 2 - 16}{144} \approx 0.004\dots$ | | | | | |
| n | $ I^4 - G_n^4 $ | $ I^4 - K_{2n+1}^4 $ | $ K_{2n+1}^4 - G_n^4 $ | $ I^4 - \widehat{G}_{2n+1}^4 $ | $ \widehat{G}_{2n+1}^4 - G_n^4 $ |
| 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 2: Selected results for integrals over m -dimensional simplex.

$$\Pi(k_1) = t_{k_1, m-1},$$

$$\Pi(k_1, \dots, k_l) = (1 - t_{k_1, m-1}) \cdots (1 - t_{k_{l-1}, m-l+1}) t_{k_l, m-l}, \quad l = 2, \dots, m.$$

G_n^m has n^m , while corresponding K_{2n+1}^m and \widehat{G}_{2n+1}^m have $(2n+1)^m$ nodes.

Selected results are shown in table 2. In the cases of I^4 , $n = 4, 6$, q.f. K_{2n+1} doesn't exist and c.f. K_{2n+1}^4 can't be constructed.

Sphere: $S^m = \{\mathbf{x} \in \mathbb{R}^m \mid x_1^2 + \dots + x_m^2 = r^2\}$. If we introduce spherical coordinates $r, \varphi_1, \dots, \varphi_{m-1}$, than replace integral of variable φ_{m-1} by $(2n)$ -point rectangle formula and approximate integral of each variable φ_{m-l-2} , $l = 0, \dots, m-3$, by n -point Gauss q.f. G_n with Gegenbauer weight function $\omega(t) = (1-t^2)^{l/2}$, $l = 0, \dots, m-3$, on $[-1, 1]$,

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

| $S^3 : x_1^2 + x_2^2 + x_3^2 = 1, \quad I^3 = \int_{S^3} e^{x_1} d\mathbf{x} = 2\pi(e - 1/e) \approx 14.768\dots$ | | | | | |
|---|-----------------|----------------------|------------------------|--------------------------------|----------------------------------|
| n | $ I^3 - G_n^3 $ | $ I^3 - K_{2n+1}^3 $ | $ K_{2n+1}^3 - G_n^3 $ | $ I^3 - \widehat{G}_{2n+1}^3 $ | $ \widehat{G}_{2n+1}^3 - G_n^3 $ |
| 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 |

Table 3: Selected results for integrals over m -dimensional sphere.

we get c.f.

$$I^m \approx G_n^m = r^{m-1} \frac{\pi}{n} \sum_{k=1}^{2n} \sum_{k_1, \dots, k_{m-2}=1}^n \omega_{k_1, m-3} \cdots \omega_{k_{m-2}, 0} \cdot F\left(r, \varphi_{1, k_1}, \dots, \varphi_{m-2, k_{m-2}}, \frac{\pi}{n} k\right),$$

$$F(r, \varphi_1, \dots, \varphi_{m-1}) = f(r \cos \varphi_1, \dots, r \sin \varphi_1 \cdots \sin \varphi_{m-1}),$$

$$\varphi_{m-l-2, k} = \arccos t_{k, l}, \quad l = 0, \dots, m-3.$$

G_n^m has $2n^{m-1}$, while corresponding K_{2n+1}^m and \widehat{G}_{2n+1}^m have $2(2n+1)^{m-1}$ nodes.

Selected results are shown in table 3.

Ball: $B^m = \{\mathbf{x} \in \mathbb{R}^m \mid x_1^2 + \cdots + x_m^2 \leq 1\}$. I^m can be approximated by linear combination of n integrals over m -dimensional spheres of different radii,

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

If m is even, than $r_i^2 = \tau_i$, $2B_i r_i^{m-1} = \lambda_i$, $i = 1, \dots, n$, where τ_i and λ_i are nodes and weights of Gauss q.f.

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

If m is odd, than $r_i = \tau_i$, $B_i r_i^{m-1} = \lambda_i$, $i = 1, \dots, n$, where τ_i and λ_i are nodes and weights of Gauss q.f.

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

c.f. takes the form

$$I^m \approx G_n^m = \frac{\pi}{2n} \sum_{i=1}^n B_i r_i^{m-1} \sum_{k=1}^{4n} \sum_{k_1, \dots, k_{m-2}=1}^{2n} \omega_{k_1, m-3} \cdots \omega_{k_{m-2}, 0} \cdot F\left(r_i, \varphi_{1, k_1}, \dots, \varphi_{m-2, k_{m-2}}, \frac{\pi}{2n} k\right).$$

| $B^4 : x_1^2 + \dots + x_4^2 \leq 1, \quad I^4 = \int_{B^4} \sqrt{(x_2^2 + x_3^2 + x_4^2)^{17}} d\mathbf{x} = \frac{524288}{4849845} \pi \approx 0.339\dots$ | | | | | |
|--|-----------------|----------------------|------------------------|--------------------------------|----------------------------------|
| n | $ I^4 - G_n^4 $ | $ I^4 - K_{2n+1}^4 $ | $ K_{2n+1}^4 - G_n^4 $ | $ I^4 - \widehat{G}_{2n+1}^4 $ | $ \widehat{G}_{2n+1}^4 - G_n^4 $ |
| 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 |

Table 4: Selected results for integrals over m -dimensional ball.

G_n^m has $(2n)^m$, while corresponding K_{2n+1}^m and \widehat{G}_{2n+1}^m have $(4n+2)(4n+1)^{m-1}$ nodes.

Selected results are shown in table 4.

3 Conclusion

As expected, with the increase of n precision of all three c.f. G_n^m , K_{2n+1}^m , \widehat{G}_{2n+1}^m increases. Also expected, both K_{2n+1}^m and \widehat{G}_{2n+1}^m have better accuracy than G_n^m , while K_{2n+1}^m has better (or the same) accuracy than \widehat{G}_{2n+1}^m .

Both differences $|K_{2n+1}^m - G_n^m|$ and $|\widehat{G}_{2n+1}^m - G_n^m|$ give very good estimates of error $|I^m - G_n^m|$. \widehat{G}_{2n+1}^m exists in some situations when K_{2n+1}^m does not, and it's numerical construction is simpler than the construction of K_{2n+1}^m (since the construction of \widehat{G}_{2n+1}^m is simpler than the construction of K_{2n+1}^m). So, \widehat{G}_{2n+1}^m might be a better choice than K_{2n+1}^m for estimating error of G_n^m .

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