CONSTRUCTION OF GAUSS-KRONROD-HERMITE QUADRATURE AND CUBATURE FORMULAS

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Abstract. We study Gauss-Kronrod quadrature formula for Hermite weight function for the particular cases \( n = 1, 2, 3 \), we introduce a new Gauss-Kronrod-Hermite cubature formula and we describe the form of the weights and nodes.

1. Introduction. Quadrature and cubature rules of Gauss-Hermite type

Let us consider the weight function \( \rho(x) = e^{-x^2} \), defined and positive on \((-\infty, \infty)\). The quadrature rule of Gauss-Hermite type corresponding to this weight function is:

\[
\int_{\mathbb{R}} e^{-x^2} f(x) \, dx = \sum_{k=0}^{m} A_{m,k} f(a_k) + R_m[f].
\]  

(1)

The nodes \( a_k, k = 0, m \), the coefficients \( A_{m,k}, k = 0, m \) and the remainder term can be determined using the properties of Hermite orthogonal polynomials, defined as follows:

\[
H_m(x) = (-1)^m e^{x^2} \frac{d^m}{dx^m} [e^{-x^2}].
\]

(2)

It has been proved (see [1]) that:

(i) the nodes \( a_k, k = 0, m \), are the zeros of the Hermite orthogonal polynomial of degree \( m + 1 \);

(ii) the coefficients \( A_{m,k}, k = 0, m \) would be computed with the formula:

\[
A_{m,k} = \frac{2^{m+1} m! \sqrt{\pi}}{H_m(a_k) H_{m+1}'(a_k)}
\]

(3)

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(iii) the remainder term $R_m[f]$, for $f \in C^{2m+2}(\mathbb{R})$, has the representation:

$$R_m[f] = \frac{(m+1)! \sqrt{\pi} f^{(2m+2)}(\xi)}{2^{m+1}(2m+2)!} - \infty < \xi < \infty. \quad (4)$$

We also consider the Gauss-Hermite cubature rule of the form:

$$\int_{\mathbb{R}^2} P(x, y) f(x, y) dxdy = \sum_{i=0}^{m} \sum_{j=0}^{n} A_{i,j} f(x_i, y_j) + R_{m,n}[f]. \quad (5)$$

It has been proved (see [1]) that in this formula the coefficients are computed with:

$$A_{i,j} = A^{[1]}_{m,i} A^{[2]}_{n,j} = \frac{2^{m+1} m! \sqrt{\pi}}{H_m(x_i) H'_{m+1}(x_i)} \cdot \frac{2^{n+1} n! \sqrt{\pi}}{H_n(y_j) H'_{n+1}(y_j)}$$

where the nodes $x_i, i = 0, m$ and $y_j, j = 0, n$ are respectively the zeros of Hermite orthogonal polynomials $H_{m+1}, H_{n+1}$.

If $f \in C^{m+1,n+1}(\mathbb{R}^2)$ then the remainder term has the expression:

$$R_{m,n}[f] = \pi \frac{(m+1)!}{2^{m+1}(2m+2)!} f^{(2m+2,0)}(\xi_1, \eta_1) + \pi \frac{(n+1)!}{2^{n+1}(2n+2)!} f^{(0,2n+2)}(\xi_2, \eta_2)$$

$$- \frac{\sqrt{\pi} (m+1)!}{2^{m+1}(2m+2)!} \cdot \frac{\sqrt{\pi} (n+1)!}{2^{n+1}(2n+2)!} f^{(2m+2,2n+2)}(\xi_3, \eta_3). \quad (7)$$

2. Study upon the quadrature rule of Gauss-Kronrod type with Hermite weight function

In this section we consider the Gauss-Kronrod quadrature formula with Hermite weight function $\rho(x) = e^{-x^2}$, nonnegative and defined on $\mathbb{R}$

$$\int_{\mathbb{R}} \rho(x) f(x) dx = \sum_{i=1}^{m} \sigma_i f(x_i) + \sum_{k=1}^{m+1} \sigma_k f(x_k^*) + R_m[f] \quad (8)$$

where $x_i = x_i^{(m)}$ are the Gaussian nodes (i.e. the zeros of $H_m(\cdot, \rho)$, the $m$th degree orthogonal polynomial relative to the measure $\sigma(t) = \rho(t) dt$ on $\mathbb{R}$) and the nodes $x_k^*$ (the Kronrod nodes) and weights $\sigma_i = \sigma_i^{(m)}$, $\sigma_k = \sigma_k^{(m)}$ are determined such that (8) has maximum degree of exactness $3m + 1$, i.e.

$$R_m[f] = 0, \forall f \in P_{3m+1}. \quad (9)$$

It is well known that $x_k^*$ must be the zeros of the (monic) orthogonal polynomial $H_{m+1}^*$ of degree $m + 1$ relative to the measure $\rho^*(x) = H_m(x, \rho)\rho(x)$ on $\mathbb{R}$. 112
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Even through \(H_m\), and hence \(\rho^*\), changes sign on \(\mathbb{R}\), it is known that \(H_{m+1}^*\) exists uniquely (see e.g. [3]). There is no guarantee, however, that the zeros \(x_k^*\) of \(H_{m+1}^*\) are real, neither that the interlacing property of Gauss nodes with nodes of Kronrod type holds.

We study in the following the cases \(m = 1, m = 2\) and \(m = 3\), i.e. we check the existence of quadrature rules with 3, 5 and 7 nodes.

For case \(m = 1\) we found the Gauss-Kronrod quadrature formula with 3 nodes:

\[
\int_{\mathbb{R}} e^{-x^2} f(x) dx = \frac{\sqrt{\pi}}{6} f\left(-\frac{\sqrt{3}}{2}\right) + \frac{2\sqrt{\pi}}{3} f(0) + \frac{\sqrt{\pi}}{6} f\left(\frac{\sqrt{3}}{2}\right) + R_2[f]
\]

where \(H_1(x) = x\) represent the Hermite polynomial with zeros \(x_1 = 0\) and the polynomial \(H_2^*(x) = x^2 - \frac{3}{2}\) has been determined from the orthogonality condition:

\[
\int_{\mathbb{R}} e^{-x^2} H_2^*(x) H_1(x) x^k dx = 0, \quad k = 0, 1.
\]

For the computation of the coefficients we used the formula (see [5])

\[
\sigma_i = \gamma_i + \frac{\|H_m\|_{d\rho}^2}{H_{m+1}^*(x_i) H_m^*(x_i)}, \quad i = 1, 2, \ldots, m
\]

and

\[
\sigma_k^* = \frac{\|H_m\|_{d\sigma}^2}{H_m(x_k^*) H_{m+1}^*(x_k^*)}, \quad k = 1, 2, \ldots, m + 1
\]

where \(\gamma_i = \gamma_i^{(m)}\) are the Christoffel numbers (i.e. the weights in the Gaussian quadrature rule and \(\| \cdot \|_{d\rho}\) the \(L_2\)-norm for the weight function).

One can observe that all the zeros of polynomial \(H_2^*\) are real and they interlace with the zero of polynomial \(H_1\).

For the case \(m = 2\), one gets the following quadrature formula

\[
\int_{\mathbb{R}} e^{-x^2} f(x) dx = \\
= \frac{\sqrt{\pi}}{30} \left[ f(-\sqrt{3}) + 9f\left(-\frac{\sqrt{2}}{2}\right) + 10f(0) + 9f\left(\frac{\sqrt{2}}{2}\right) + f(\sqrt{3}) \right] + R_2[f].
\]

Here one can observe that all the nodes are real and the interlacing property is satisfied. All the coefficients of formula are positive.
If \( m = 3 \) Stieltjes polynomial, respective \( H^*_4 \) has two real zeros and two complex zeros, fact that doesn’t assure us the existence of Gauss-Kronrod quadrature formula in this case.

3. Construction of Gauss-Kronrod-Hermite type cubature formula

Let \( f : \mathbb{R}^2 \rightarrow \mathbb{R} \) be a integrable Riemann function. Applying the Gauss-Kronrod quadrature formula with Hermite measure

\[
\int_{\mathbb{R}} e^{-x^2} f(x, y) dx = \sum_{i=1}^{m} A_{m,i} f(x_i, y) + \sum_{k=1}^{m+1} A_{m,k}^* f(x_k^*, y) + R_m[f]
\]

which will multiply with measure \( \rho(y) = e^{-y^2} \), obtaining the measure \( p(x, y) = e^{-(x^2+y^2)} \) of the double integrals, after that we integrate, term by term and we obtain:

\[
\int_{\mathbb{R}^2} e^{-(x^2+y^2)} f(x, y) dx dy = \sum_{i=1}^{m} A_{m,i} \int_{\mathbb{R}} e^{-y^2} f(x_i, y) dy + \sum_{k=1}^{m+1} A_{m,k}^* e^{-y^2} f(x_k^*, y) +
\]

\[
+ R_m[f] \int_{\mathbb{R}} e^{-y^2} dy.
\]

For the integrals above we apply again one of quadrature rule of Gauss-Kronrod type:

\[
\int e^{-y^2} f(x_i, y) dy = \sum_{j=1}^{n} A_{n,j} f(x_i, y_j) + \sum_{l=1}^{n+1} A_{n,l}^* f(x_i, y_l^*) + R_n[f]
\]

and

\[
\int e^{-y^2} f(x_k^*, y) dy = \sum_{j=1}^{n} A_{n,j} f(x_k^*, y_j) + \sum_{l=1}^{n+1} A_{n,l}^* f(x_k^*, y_l^*) + R_n[f]
\]

respectively.

From here, it results the cubature rule:

\[
\int_{\mathbb{R}^2} e^{-(x^2+y^2)} f(x, y) dx dy \approx \sum_{i=1}^{m} \sum_{j=1}^{n} A_{m,i} A_{n,j} f(x_i, y_j)
\]

\[
+ \sum_{i=1}^{m} \sum_{l=1}^{n+1} A_{m,i} A_{n,l}^* f(x_i, y_l^*) + \sum_{k=1}^{m+1} \sum_{j=1}^{n} A_{m,k}^* A_{n,j} f(x_k^*, y_j)
\]

\[
+ \sum_{k=1}^{m+1} \sum_{l=1}^{n+1} A_{m,k}^* A_{n,l}^* f(x_k^*, y_l^*)
\]
with Gauss nodes \((x_i, y_j), i = \overline{1, m}, j = \overline{1, n}\) and Kronrod nodes \((x^*_k, y^*_l), k = \overline{1, m + 1}, l = \overline{1, n + 1}\), respectively mixed nodes of form \((x^*_k, y^*_l)\) and \((x_i, y_j)\).

The coefficients of Gauss-Kronrod-Hermite type cubature rules could be determined from:

\[ A_{i,j} = A_{m,i} A_{n,j}, \quad A^*_{i,l} = A_{m,i} A^*_n l, \]
\[ A^*_{k,j} = A^*_{m,k} A_{n,j}, \quad A^*_{k,l} = A^*_{m,k} A^*_{n,l} \]

where

\[ A_{m,i} = \gamma_i + \frac{\|H_m\|^2}{H_{m+1}(x_i) H_n'(x_i)}, \quad i = \overline{1, m} \]
\[ A_{n,j} = \gamma_j + \frac{\|H_n\|^2}{H_{n+1}(y_j) H_n'(y_j)}, \quad j = \overline{1, n} \]
\[ A^*_{n,l} = \frac{\|H_n\|^2}{H_n(y^*_l) H_n'(y^*_l)}, \quad l = \overline{1, m + 1} \]
\[ A^*_{m,k} = \frac{\|H_m\|^2}{H_m(x^*_k) H_{m+1}(x^*_k)}, \quad k = \overline{1, m + 1}. \]

4. Example

1. For the case \(m = n = 1\) we have:

\[
\int \int_{\mathbb{R}^2} e^{-(x^2+y^2)} dxdy \simeq (A_{1,1})^2 f(x_1, y_1) + A_{1,1} A^*_{1,1} f(x_1, y^*_1) + A_{1,1} A^*_{1,2} f(x_1, y^*_2) + 
+A^*_{1,1} A_{1,1} f(x^*_1, y_1) + A^*_{1,2} A_{1,1} f(x^*_2, y_1) + (A^*_{1,1})^2 f(x^*_1, y^*_1) + A^*_{1,1} A^*_{1,2} f(x^*_1, y^*_2) + 
+A^*_{1,2} A^*_{1,1} f(x^*_2, y^*_1) + (A^*_{1,2})^2 f(x^*_2, y^*_2),
\]

where \(x_1 = 0 = y_1\) and \(x^*_1 = -\sqrt{\frac{3}{2}} = y^*_1, x^*_2 = \sqrt{\frac{3}{2}} = y^*_2\).

The values of the weights of this formula are:

\[ A_{1,1} = \frac{2\sqrt{\pi}}{3} \quad \text{respectively} \quad A^*_{1,1} = \frac{\sqrt{\pi}}{6} = A^*_{1,2}. \]

From here result the following cubature formula:

\[ \int \int_{\mathbb{R}^2} e^{-(x^2+y^2)} f(x, y) dxdy \simeq \frac{4\pi}{9} f(0, 0) + 
+\frac{\pi}{9} \left[ f\left(0, -\sqrt{\frac{3}{2}}\right) + f\left(0, \sqrt{\frac{3}{2}}\right) + f\left(-\sqrt{\frac{3}{2}}, 0\right) + f\left(\sqrt{\frac{3}{2}}, 0\right) \right] + \]

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where the gaussian nodes are:

\[ x_{n}1, x_{n}2 \] representing the Kronrod nodes.

For \( f(x, y) = x^2y^2 \) we have

\[
\int \int_{\mathbb{R}^2} e^{-(x^2+y^2)}x^2y^2dxdy = \int_{\mathbb{R}} x^2e^{-x^2}dx \int_{\mathbb{R}} y^2e^{-y^2}dy = \int_{\mathbb{R}} \frac{\sqrt{\pi}}{2} \cdot \frac{\sqrt{\pi}}{2} = \frac{\pi}{4}
\]

representing the exact value of this integral.

Applying cubature formula we obtain:

\[
\int \int_{\mathbb{R}^2} e^{-(x^2+y^2)}x^2y^2dxdy = \frac{\pi}{35} \left[ \frac{3}{2} \cdot \frac{3}{2} + \frac{3}{2} \cdot \frac{3}{2} + \frac{3}{2} \cdot \frac{3}{2} + \frac{3}{2} \cdot \frac{3}{2} \right] = \frac{\pi}{36} \cdot 4 \cdot \frac{9}{4} = \frac{\pi}{4}
\]

2. For the case \( m = n = 2 \) we have:

\[
\int \int_{\mathbb{R}^2} e^{-(x^2+y^2)}f(x, y)dxdy \simeq (A_{2,1})^2f(x_1, y_1) + A_{2,1}A_{2,2}f(x_1, y_2) + A_{2,2}A_{2,1}f(x_2, y_1) + A_{2,2}f(x_2, y_2) + A_{2,2}A_{2,2}f(x_1, y_1) + A_{2,1}A_{2,2}f(x_1, y_2) + A_{2,2}A_{2,3}f(x_2, y_1)
\]

where the gaussian nodes are: \( x_1 = -\frac{\sqrt{3}}{2} = y_1 \) and \( x_2 = \frac{\sqrt{3}}{2} = y_2 \) the roots of the orthogonal polynomial of Hermite type: \( H_2(x) = x^2 - \frac{1}{2} \). The Stieltjes polynomial is: \( H_3^2(x) = x^2 - 3 \) with the roots: \( x_1^* = -\sqrt{3} = y_1^* \), \( x_2^* = 0 = y_2^* \), \( x_3^* = \sqrt{3} = y_3^* \), representing the Kronrod nodes.

The values of the weights of this formula are:

\[ A_{2,1} = 3\frac{\sqrt{\pi}}{10} = A_{2,2} \]

and

\[ A_{2,1}^* = \frac{\sqrt{\pi}}{30} = A_{2,3}^* \quad A_{2,2}^* = \frac{\sqrt{\pi}}{3} \]

\[
\int \int_{\mathbb{R}^2} e^{-(x^2+y^2)}f(x, y)dxdy =
\]

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\[
\begin{align*}
&= \frac{9\pi}{100} \left[ f \left( -\frac{\sqrt{2}}{2}, -\frac{\sqrt{3}}{2} \right) + f \left( -\frac{\sqrt{2}}{2}, \frac{\sqrt{3}}{2} \right) + f \left( \frac{\sqrt{2}}{2}, -\frac{\sqrt{3}}{2} \right) + f \left( \frac{\sqrt{2}}{2}, \frac{\sqrt{3}}{2} \right) \right] + \\
&\quad + \frac{\pi}{100} \left[ f \left( -\frac{\sqrt{2}}{2}, -\sqrt{3} \right) + f \left( -\frac{\sqrt{2}}{2}, \sqrt{3} \right) + f \left( \frac{\sqrt{2}}{2}, -\sqrt{3} \right) + f \left( \frac{\sqrt{2}}{2}, \sqrt{3} \right) \right] + \\
&\quad + f \left( -\sqrt{3}, -\frac{\sqrt{2}}{2} \right) + f \left( -\sqrt{3}, \frac{\sqrt{2}}{2} \right) + f \left( \sqrt{3}, -\frac{\sqrt{2}}{2} \right) + f \left( \sqrt{3}, \frac{\sqrt{2}}{2} \right) \right] + \\
&\quad + \frac{\pi}{10} \left[ f \left( -\frac{\sqrt{2}}{2}, 0 \right) + f \left( \frac{\sqrt{2}}{2}, 0 \right) + f \left( 0, -\frac{\sqrt{2}}{2} \right) + f \left( 0, \frac{\sqrt{2}}{2} \right) \right] + \\
&\quad + \frac{\pi}{90} \left[ f \left( -\sqrt{3}, -\sqrt{3} \right) + f \left( -\sqrt{3}, \sqrt{3} \right) + f \left( \sqrt{3}, -\sqrt{3} \right) + f \left( \sqrt{3}, \sqrt{3} \right) \right] + \\
&\quad + \frac{\pi}{90} \left[ f \left( -\sqrt{3}, 0 \right) + f \left( 0, -\sqrt{3} \right) + f \left( 0, \sqrt{3} \right) + f \left( \sqrt{3}, 0 \right) \right] + \frac{\pi}{9} f(0,0).
\end{align*}
\]

References


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