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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:

$$\int_{\mathbb{R}} e^{-x^2} f(x)dx = \sum_{k=0}^{m} A_{m,k} f(a_k) + R_m[f]. \tag{1}$$

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

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

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

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

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

$$A_{m,k} = \frac{2^{m+1} m! \sqrt{\pi}}{H_m(a_k) H'_{m+1}(a_k)} \tag{3}$$

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

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

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

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

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

$$A_{i,j} = A^{[1]}_{m,i} A^{[2]}_{n,j} = \frac{2^{m+1} m! \sqrt{\pi}}{H_m(x_i) H'_{m+1}(x_i)} \cdot \frac{2^{n+1} n! \sqrt{\pi}}{H_n(y_j) H'_{m+1}(y_j)} \tag{6}$$

where the nodes x_i, $i = \overline{0,m}$ and y_j, $j = \overline{0,n}$ 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:

$$R_{m,n}[f] = \frac{\pi(m+1)!}{2^{m+1}(2m+2)!} f^{(2m+2,0)}(\xi_1, \eta_1) + \frac{\pi(n+1)!}{2^{n+1}(2n+2)!} f^{(0,2n+2)}(\xi_2, \eta_2) \tag{7}$$
$$- \frac{\sqrt{\pi}(m+1)!}{2^{m+1}(2m+2)!} \cdot \frac{\sqrt{\pi}(n+1)!}{2^{n+1}(2n+2)!} f^{(2m+2,2n+2)}(\xi_3, \eta_3).$$

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 $\mathbb{R}$

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

where $x_i = x_i^{(m)}$ are the Gaussian nodes (i.e. the zeros of $H_m(\cdot, \rho)$, the mth degree orthogonal polynomial relative to the measure $d\sigma(t) = \rho(t)dt$ 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.

$$R_m[f] = 0, \ \forall\ f \in \mathbf{P}_{3m+1}. \tag{9}$$

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 $\mathbb{R}$.

Even through H_m, and hence ρ^*, 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 $H^*_2(x) = x^2 - \dfrac{3}{2}$ 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])

$$\sigma_i = \gamma_i + \frac{\|H_m\|^2_{d\rho}}{H^*_{m+1}(x_i) H'_m(x_i)}, \quad i = 1, 2, \ldots, m$$

and

$$\sigma^*_k = \frac{\|H_m\|^2_{d\sigma}}{H_m(x^*_k) H^{*1}_{m+1}(x^*_k)}, \quad k = 1, 2, \ldots, m+1$$

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 $f : \mathbb{R}^2 \to \mathbb{R}$ 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:

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

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

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:

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

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

$$+ \sum_{k=1}^{m+1} \sum_{l-1}^{n+1} A_{m,k}^* A_{n,l}^* f(x_k^*, y_l^*)$$

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_j) and (x_i, y_l^*).

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

$$A_{m,i} = \gamma_i + \frac{\|H_m\|^2}{H_{m+1}^*(x_i)H_n'(x_i)}, \quad i = \overline{1,m}$$

$$A_{n,j} = \gamma_j + \frac{\|H_n\|^2}{H_{n+1}^*(y_j)H_n'(y_j)}, \quad j = \overline{1,n}$$

$$A_{n,l}^* = \frac{\|H_n\|^2}{H_n(y_l^*)H_{n+1}^{*\prime}(y_l^*)}, \quad l = \overline{1,m+1}$$

$$A_{m,k}^* = \frac{\|H_m\|^2}{H_m(x_k^*)H_{m+1}'(x_k^*)}, \quad k = \overline{1,m+1}.$$

4. **Example**

1. For the case $m = n = 1$ we have:

$$\iint_{\mathbb{R}^2} e^{-(x^2+y^2)}dxdy \simeq (A_{1,1})^2 f(x_1,y_1) + A_{1,1}A_{1,1}^* f(x_1,y_1^*) + A_{1,1}A_{1,2}^* f(x_1,y_2^*)+$$

$$+A_{1,1}^*A_{1,1}f(x_1^*,y_1) + A_{1,2}^*A_{1,1}f(x_2^*,y_1) + (A_{1,1}^*)^2 f(x_1^*,y_1^*) + A_{1,1}^*A_{1,2}^* f(x_1^*,y_2^*)+$$

$$+A_{1,2}^*A_{1,1}^* f(x_2^*,y_1^*) + (A_{1,2}^*)^2 f(x_2^*,y_2^*),$$

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:

$$\iint_{\mathbb{R}^2} e^{-(x^2+y^2)} f(x,y)dxdy \simeq \frac{4\pi}{9} f(0,0)+$$

$$+\frac{\pi}{9}\left[f\left(0,-\sqrt{\frac{3}{2}}\right) + f\left(0,\sqrt{\frac{3}{2}}\right) + f\left(-\sqrt{\frac{3}{2}},0\right) + f\left(\sqrt{\frac{3}{2}},0\right)\right] +$$

$$+\frac{\pi}{36}\left[f\left(-\sqrt{\frac{3}{2}},-\sqrt{\frac{3}{2}}\right)+f\left(-\sqrt{\frac{3}{2}},\sqrt{\frac{3}{2}}\right)+f\left(\sqrt{\frac{3}{2}},-\sqrt{\frac{3}{2}}\right)+f\left(\sqrt{\frac{3}{2}},\sqrt{\frac{3}{2}}\right)\right].$$

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

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

representing the exact value of this integral.

Applying cubature formula we obtain:

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

2. For the case $m=n=2$ we have:

$$\iint_{\mathbb{R}^2} e^{-(x^2+y^2)}f(x,y)dxdy\simeq (A_{2,1})^2f(x_1,y_1)+A_{2,1}A_{2,2}f(x_1,y_2)+A_{2,2}A_{2,1}f(x_2,y_1)+$$

$$+(A_{2,2})^2f(x_2,y_2)+A_{2,1}A^*_{2,1}f(x_1,y^*_1)+A_{2,1}A^*_{2,2}f(x_1,y^*_2)+A_{2,1}A^*_{2,3}f(x_1,y^*_3)+$$

$$+A_{2,2}A^*_{2,1}f(x_2,y^*_1)+A_{2,2}A^*_{2,2}f(x_2,y^*_2)+A_{2,2}A^*_{2,3}f(x_2,y^*_3)+$$

$$+A^*_{2,1}A_{2,1}f(x^*_1,y_1)+A^*_{2,1}A_{2,2}f(x^*_1,y_2)+A^*_{2,2}A_{2,1}f(x^*_2,y_1)+A^*_{2,2}A_{2,2}f(x^*_2,y_2)+$$

$$+A^*_{2,3}A_{2,1}f(x^*_3,y_1)+A^*_{2,3}A_{2,2}f(x^*_3,y_2)+(A^*_{2,1})^2f(x^*_1,y^*_1)+A^*_{2,1}A^*_{2,2}f(x^*_1,y^*_2)+$$

$$+A^*_{2,1}A^*_{2,3}f(x^*_1,y^*_3)+A^*_{2,2}A^*_{2,1}f(x^*_2,y^*_1)+(A^*_{2,2})^2f(x^*_2,y^*_2)+A^*_{2,2}A^*_{2,3}f(x^*_2,y^*_3)+$$

$$+A^*_{2,3}A^*_{2,1}f(x^*_3,y^*_1)+A^*_{2,3}A^*_{2,2}f(x^*_3,y^*_2)+(A^*_{2,3})^2f(x^*_3,y^*_3),$$

where the gaussian nodes are: $x_1=-\frac{\sqrt{2}}{2}=y_1$ and $x_2=\frac{\sqrt{2}}{2}=y_2$ the roots of the orthogonal polynomial of Hermite type: $H_2(x)=x^2-\frac{1}{2}$. The Stieltjes polynomial is: $H^*_3(x)=x(x^2-3)$ 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:

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

and

$$A^*_{2,1}=\frac{\sqrt{\pi}}{30}=A^*_{2,3},\quad A^*_{2,2}=\frac{\sqrt{\pi}}{3}.$$

$$\iint_{\mathbb{R}^2} e^{-(x^2+y^2)}f(x,y)dxdy=$$

$$= \frac{9\pi}{100}\left[f\left(-\frac{\sqrt{2}}{2},-\frac{\sqrt{2}}{2}\right)+f\left(-\frac{\sqrt{2}}{2},\frac{\sqrt{2}}{2}\right)+f\left(\frac{\sqrt{2}}{2},-\frac{\sqrt{2}}{2}\right)+f\left(\frac{\sqrt{2}}{2},\frac{\sqrt{2}}{2}\right)\right]+$$
$$+\frac{\pi}{100}\left[f\left(-\frac{\sqrt{2}}{2},-\sqrt{3}\right)+f\left(-\frac{\sqrt{2}}{2},\sqrt{3}\right)+f\left(\frac{\sqrt{2}}{2},-\sqrt{3}\right)+f\left(-\frac{\sqrt{2}}{2},\sqrt{3}\right)+\right.$$
$$\left.+f\left(-\sqrt{3},-\frac{\sqrt{2}}{2},\right)+f\left(-\sqrt{3},\frac{\sqrt{2}}{2},\right)+f\left(\sqrt{3},-\frac{\sqrt{2}}{2},\right)+f\left(\sqrt{3},\frac{\sqrt{2}}{2},\right)\right]+$$
$$+\frac{\pi}{10}\left[f\left(-\frac{\sqrt{2}}{2},0\right)+f\left(\frac{\sqrt{2}}{2},0\right)+f\left(0,-\frac{\sqrt{2}}{2}\right)+f\left(0,\frac{\sqrt{2}}{2}\right)\right]+$$
$$+\frac{\pi}{900}\left[f\left(-\sqrt{3},-\sqrt{3}\right)+f\left(-\sqrt{3},\sqrt{3}\right)+f\left(\sqrt{3},-\sqrt{3}\right)+f\left(\sqrt{3},\sqrt{3}\right)\right]+$$
$$+\frac{\pi}{90}\left[f\left(-\sqrt{3},0\right)+f\left(0,-\sqrt{3}\right)+f\left(0,\sqrt{3}\right)+f\left(\sqrt{3},0\right)\right]+\frac{\pi}{9}f(0,0).$$

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