

Degree optimal average quadrature rules for the generalized Hermite weight function

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Abstract

For the practical estimation of the error of Gauss quadrature rules Gauss-Kronrod rules are widely used; but, it is well known that for the generalized Hermite weight function, $\omega_\alpha(x) = |x|^{2\alpha} \exp(-x^2)$ over $[-\infty, \infty]$, real positive Gauss-Kronrod rules do not exist. Among the alternatives which are available in the literature, the anti-Gauss and average rules introduced by Laurie, and their modified versions, are of particular interest. In this paper, we investigate the properties of the modified anti-Gauss and average quadrature rules for ω_α , and we determine the degree optimal average rules by proving that for each n -point Gauss rule for ω_α there exists a unique average rule with the precise degree of exactness $2n+3$. We also give some numerical examples to test the performance of the average rules obtained in this paper.

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1 Introduction

Let $\omega(x)$ be a given nonnegative weight function over an interval $[a, b]$ and let

$$Q_n f := \sum_{k=1}^n w_k f(x_k) \quad (1)$$

be an n -point quadrature rule (or quadrature formula) for the integral

$$I f := \int_a^b \omega(x) f(x) dx. \quad (2)$$

Here the interval $[a, b]$ may be finite or infinite. We assume that the moments $\mu_m = I x^m$ exist and are finite for all $m \in \mathbf{N}$. In the above formula x_k and w_k ,

which depend on n and ω , are called the nodes and weights of the quadrature rule Q_n respectively. To make the terminology precise we shall say: The quadrature rule (1) is *real* if its nodes and weights are all real, and it is positive if its weights are all positive.

The algebraic *degree* of exactness of the quadrature rule Q_n is defined by

$$\deg(Q_n) = \sup\{s \mid R_n p = 0 \quad \forall p \in \mathbf{P}_s\}, \quad (3)$$

where \mathbf{P}_s denotes the set of polynomials of degree at most s and

$$R_n f := I f - Q_n f. \quad (4)$$

The unique quadrature rule with n -nodes and highest possible degree of exactness $2n - 1$ is the *Gauss rule*

$$\mathcal{G}_n f := \sum_{k=1}^n w_k f(x_k) \quad (5)$$

whose nodes and weights are uniquely determined by the requirement that

$$R_n^G f := I f - \mathcal{G}_n f = 0 \quad \forall f \in \mathbf{P}_{2n-1}. \quad (6)$$

It can be shown that the error of the Gauss rule (5) can be expressed as

$$R_n^G f = \frac{f^{(2n)}(\xi)}{(2n)!} \int_a^b \omega(x) \prod_{k=1}^n (x - x_k)^2 dx \quad \text{for some } \xi \in (a, b), \quad (7)$$

see e.g. [20]. Unfortunately, it is frequently not possible to use this error formula to determine how to choose n so as to achieve specified accuracy for a given integral of the form (2), because the $2n$ th derivative, in general, is difficult to estimate. Therefore, it is not easy to find an accurate estimate of the error by using (7) when f is some function that has not been subjected to very much analysis. A common approach to estimate the error in practice is to consider a second rule \mathcal{A} of degree greater than $2n - 1$ and to use $\mathcal{A}f - \mathcal{G}_n f$ (see e.g. [5, 13, 15]). It can be shown that any such quadrature rule requires at least $n + 1$ additional nodes.

Several possibilities for constructing a rule \mathcal{A} with $n + 1$ extra points (for unbounded intervals) have been singled out in the literature:

- The $(n + 1)$ -point Gauss quadrature rule, $\mathcal{A} = \mathcal{G}_{n+1}$. However, it has been noted in [1] that this procedure can be unreliable.
- For certain weight functions (including the Legendre weight) it is possible to find a $(2n + 1)$ -point rule Q_{2n+1}^K of degree at least $3n + 1$, with node set containing all the nodes of \mathcal{G}_n . Such a quadrature rule (if it exists) is

called *Gauss-Kronrod rule* associated with \mathcal{G}_n or *Kronrod extension* of \mathcal{G}_n . For Gauss-Kronrod type quadrature rules, see [2, 7, 11, 14, 15] and the references therein. The difference $Q_{2n+1}^K - \mathcal{G}_n$ is used to estimate the error of \mathcal{G}_n . Gauss-Kronrod rules are of optimal degree (as an extension of \mathcal{G}_n with $n+1$ additional simple nodes) and therefore have found widespread acceptance as components of automatic quadrature algorithms. However, for some weight functions (such as the Laguerre and Hermite weight functions) real positive Gauss-Kronrod rules do not exist for all n .

- In cases where no real positive Gauss-Kronrod rule exists, it is possible to find a *suboptimal* extension that is, a $(2n+1)$ -point rule of degree greater than $2n$ but less than $3n+1$, by gradually reducing the degree aimed at until an extension is to exist [1, 17, 18].

It is well known that for the generalized Hermite weight function ω_α^H ,

$$\omega_\alpha^H(x) = |x|^{2\alpha} \exp(-x^2), \quad x \in [-\infty, \infty], \quad 2\alpha > -1, \quad (8)$$

real positive Gauss-Kronrod rules do not exist in general. For example, for the classical Hermite weight function ω_0^H real positive Gauss-Kronrod rules exist only for $n = 1, 2$ (see [10]). Several authors considered modified quadrature extensions of the Gauss-Hermite formulas for specific values of n (see e.g. [1, 17, 18]). As a different approach, Laurie [13] introduced the so-called anti-Gauss rules and corresponding average rules to estimate the error of the Gauss quadrature rules. The anti-Gauss and average rules and their modified versions introduced by Ehrlich [6], which will be defined below, exist for any nonnegative weight function.

The $(n+1)$ -point modified *anti-Gauss rule* [6] (see also [3, 13])

$$\tilde{\mathcal{G}}_{n+1,\gamma} f := \sum_{k=1}^{n+1} \tilde{w}_k f(\tilde{x}_k), \quad \gamma > -1, \quad (9)$$

is defined uniquely, for each value of the parameter $\gamma > -1$, by the relation

$$(I - \tilde{\mathcal{G}}_{n+1,\gamma})p = -(1 + \gamma)(I - \mathcal{G}_n)p \quad \forall p \in \mathbf{P}_{2n+1} \quad (10)$$

and the corresponding modified *average rule* is defined as

$$\mathcal{L}_{2n+1,\gamma} := \frac{1}{2 + \gamma} \left\{ (1 + \gamma) \mathcal{G}_n + \tilde{\mathcal{G}}_{n+1,\gamma} \right\}, \quad \gamma > -1, \quad (11)$$

which is a *stratified type extension* of \mathcal{G}_n . (For stratified and related quadrature rules, see [12, 19]). Note that when $\gamma = 0$, the modified anti-Gauss and average rules given by (9) and (11) agree with the anti-Gauss and average rules introduced by Laurie in [13]. Ehrlich [6] investigated the properties of

(9) and (11) for the Laguerre and classical Hermite weight functions, and he obtained the degree optimal average rules for these weights.

Throughout this paper the error of anti-Gauss rule (9) will be denoted by

$$\tilde{R}_{n+1,\gamma}f := If - \tilde{\mathcal{G}}_{n+1,\gamma}f. \quad (12)$$

It can be shown that the nodes of $\tilde{\mathcal{G}}_{n+1,\gamma}$ are interlaced by those of \mathcal{G}_n , see Theorem 3.1 in Section 3, which implies that the anti-Gauss rules and corresponding average rules always exist, and therefore at worst two nodes of the anti-Gauss rules may be exterior to the interval of integration. Moreover, these rules can easily be constructed, see Lemma 2.1 in Section 2. Because of the relation (10), the Gauss and modified anti-Gauss rules have errors of opposite sign for many integrands f (see [3] for details). This means that the exact value of the integral is bracketed by the values obtained by \mathcal{G}_n and $\tilde{\mathcal{G}}_{n+1,\gamma}$. On the other hand, from (10) and (11) we get

$$\mathcal{L}_{2n+1,\gamma}f - \mathcal{G}_nf = \frac{\tilde{\mathcal{G}}_{n+1,\gamma}f - \mathcal{G}_nf}{2 + \gamma} = (I - \mathcal{G}_n)f, \quad \forall f \in \mathbf{P}_{2n+1}. \quad (13)$$

Therefore, by this relation and the reasons stated above in this paragraph, the modified anti-Gauss rule $\tilde{\mathcal{G}}_{n+1,\gamma}$ (although its degree is equal to $2n - 1$) and corresponding average rule (11) can be used to estimate the error of the Gauss rule \mathcal{G}_n for any nonnegative weight function.

From (10) and (11) it follows that

$$R_{2n+1,\gamma}f := If - \mathcal{L}_{2n+1,\gamma}f = 0 \quad \forall f \in \mathbf{P}_{2n+1}. \quad (14)$$

Hence the degree of $\mathcal{L}_{2n+1,\gamma}$ is (at least) $2n+1$ for any value of $\gamma > -1$. This means that the degree of this rule may be greater than $2n+1$ for some value(s) of γ . Ehrich [6] proved that for the classical Hermite weight function there exists a unique value of γ , namely $\gamma = 1/n$, such that the corresponding modified average rule has the precise degree of exactness $2n + 3$. He also obtained a similar result for the generalized Laguerre measure [6, Theorem 3].

The main purpose of this paper is to determine the modified average rules of the highest possible degree associated with the generalized Hermite weight function (8), and to investigate the properties of these and related modified anti-Gauss and average rules.

The paper is organized as follows. In Section 2 some properties of the modified anti-Gauss rules for a general weight function are given. In Section 3 the modified anti-Gauss and corresponding average rules associated with the generalized Hermite weight function (8) are investigated and it is shown that there is a unique value of γ , $\gamma = \gamma^*(n, \alpha)$, such that the corresponding average rule has the precise degree of exactness $2n + 3$. Finally in the last section, to show the performance of the anti-Gauss and average quadrature rules with γ^* , some numerical examples are given.

2 Some properties of modified anti-Gauss rules

Associated with the n -point Gauss rule (5), consider the symmetric tridiagonal $n \times n$ matrix, known as the Jacobi matrix of order n ,

$$T_n = \begin{bmatrix} a_0 & \sqrt{b_1} & & \mathbf{0} \\ \sqrt{b_1} & a_1 & \ddots & \\ & \ddots & \ddots & \sqrt{b_{n-1}} \\ \mathbf{0} & & \sqrt{b_{n-1}} & a_{n-1} \end{bmatrix} \tag{15}$$

where a_k, b_k are given by the following relations

$$\begin{aligned} p_{-1} &= 0, & p_0 &= 1, \\ p_{k+1} &= (x - a_k)p_k - b_k p_{k-1}, & k &= 0, 1, \dots, \end{aligned} \tag{16}$$

$$b_0 = I[p_0], \quad b_{k+1} = \frac{I[p_{k+1}^2]}{I[p_k^2]}, \quad a_k = \frac{I[xp_k^2]}{I[p_k^2]}, \quad k = 0, 1, 2, \dots \tag{17}$$

It is well known that the nodes x_k of the n -point Gauss rule are the roots of the orthogonal polynomial p_n obtained by the relations (16)-(17). It is also well known that these nodes are the eigenvalues of the matrix (15) and the weights are given by $w_k = b_0 v_{k,1}^2$, where $v_{k,1}$ is the first component of the normalized eigenvector \mathbf{v}_k corresponding to the eigenvalue x_k (see e.g. [9, 20]).

Let $\{a_k, b_k\}$ be the coefficients in (17) to obtain the orthogonal polynomials $p_k(x)$, and T_n be the Jacobi matrix (15). Then we have

Lemma 2.1 *The nodes \tilde{x}_k and weights \tilde{w}_k of the anti-Gauss rule (9) are*

$$\tilde{x}_k = \lambda_k, \quad \tilde{w}_k = b_0(\tilde{v}_{k,1})^2, \quad k = 1, 2, \dots, n + 1, \tag{18}$$

where λ_k are the eigenvalues of the real symmetric tridiagonal matrix

$$\tilde{T}_{n+1} = \begin{bmatrix} T_n & \sqrt{\beta_n} \mathbf{e}_n \\ \sqrt{\beta_n} \mathbf{e}_n^T & a_n \end{bmatrix}, \quad \beta_n = (2 + \gamma)b_n, \quad \mathbf{e}_n^T = [0, 0, \dots, 1] \in \mathbf{R}^n, \tag{19}$$

$\tilde{v}_{k,1}$ is the first component of the normalized eigenvector corresponding to λ_k .

From the relation (10) it follows that

$$\tilde{\mathcal{G}}_{n+1,\gamma} f = [(2 + \gamma)I - (1 + \gamma)\mathcal{G}_n] f, \quad \forall f \in \mathbf{P}_{2n+1}.$$

Therefore, $\tilde{\mathcal{G}}_{n+1,\gamma}$ is the $(n + 1)$ -point Gauss quadrature rule for the linear functional $L = (2 + \gamma)I - (1 + \gamma)\mathcal{G}_n$. Lemma 2.1 can easily be proved using this property (see for example [13] or [3]). The following result is a consequence of Lemma 2.1.

Corollary 2.2 *The nodes of the anti-Gauss rule $\tilde{\mathcal{G}}_{n+1,\gamma}$ for any $\gamma > -1$ are the roots of the polynomial q_{n+1} defined by*

$$q_{n+1} = p_{n+1} - (1 + \gamma) b_n p_{n-1}, \quad n \geq 1, \tag{20}$$

where p_k and b_k are given by the relations (16) and (17).

Proof: Let

$$p_{n+1}(x) = \det(x\mathcal{I}_{n+1} - T_{n+1}), \quad \tilde{p}_{n+1}(x) = \det(x\mathcal{I}_{n+1} - \tilde{T}_{n+1})$$

where T_{n+1} is the Jacobi matrix (15) of order $(n + 1)$, \tilde{T}_{n+1} is the matrix (19) for the modified anti-Gauss rule, and \mathcal{I}_{n+1} denotes the identity matrix of order $(n + 1)$. Expanding these determinants according to their last rows, and using the relations (16) and (17), we obtain

$$\begin{aligned} p_{n+1}(x) &= (x - a_n)p_n(x) - b_n p_{n-1}(x), \\ \tilde{p}_{n+1}(x) &= (x - a_n)p_n(x) - (2 + \gamma)b_n p_{n-1}(x). \end{aligned}$$

Thus if \tilde{x}_i is an eigenvalue of \tilde{T}_{n+1} , it is a root of \tilde{p}_{n+1} . Now the result follows from $p_{n+1}(\tilde{x}_i) - \tilde{p}_{n+1}(\tilde{x}_i) = p_{n+1}(\tilde{x}_i) = (1 + \gamma)b_n p_{n-1}(\tilde{x}_i)$. QED

The following lemma will be used in the next section.

Lemma 2.3 ([6]) *Let $\{p_m(x) = \sum_{i=0}^m c_{i,m} x^i\}$ be the monic orthogonal polynomials obtained by the relations (16) and (17), q_{n+1} be the polynomial defined as in (20), and let $M_k := x^k$. Then, for $n, k \in \mathbf{N}$ we have*

$$\begin{aligned} R_n^G [M_{2n+k}] &= \int_a^b \omega(x) p_n(x) M_{n+k} dx - \sum_{i=n-k}^{n-1} c_{i,n} R_n^G [M_{n+k+i}], \\ \tilde{R}_{n+1,\gamma} [M_{2n}] &= -(1 + \gamma)R_n^G [M_{2n}] = -(1 + \gamma)I[p_n^2], \\ \tilde{R}_{n+1,\gamma} [M_{2n+k}] &= \int_a^b \omega(x) q_{n+1}(x) M_{n+k-1} dx - c_{n,n+1} \tilde{R}_{n+1,\gamma} [M_{2n+k-1}] \\ &\quad - \sum_{i=n-k+1}^{n-1} \{c_{i,n+1} - (1 + \gamma) b_n c_{i,n-1}\} \tilde{R}_{n+1,\gamma} [M_{n+k+i-1}]. \end{aligned}$$

3 Degree optimal average quadrature rules for the generalized Hermite weight function

The monic generalized Hermite polynomials $H_k^\alpha := H_k^{(\alpha)}$ are defined by

$$\begin{aligned} H_{-1}^\alpha &= 0, \quad H_0^\alpha = 1, \\ H_{k+1}^\alpha &= x H_k^\alpha - b_k^H H_{k-1}^\alpha, \quad 2\alpha > -1, \quad k = 0, 1, \dots, \end{aligned} \tag{21}$$

$$b_0^H = \Gamma\left(\alpha + \frac{1}{2}\right), \quad b_k^H = \frac{k}{2} + \left(\frac{1 + (-1)^{k+1}}{2}\right)\alpha, \quad k = 1, 2, \dots \quad (22)$$

(see [4, Chapter 5] or [8, page 29]). These polynomials are orthogonal over the interval $[-\infty, \infty]$ with respect to the generalized Hermite weight function (8):

$$I_\alpha^H [H_i^\alpha H_j^\alpha] = h_i \delta_{ij}, \quad (23)$$

where

$$I_\alpha^H [fg] := \int_{-\infty}^\infty |x|^{2\alpha} \exp(-x^2) f(x) g(x) dx, \quad 2\alpha > -1, \quad (24)$$

$$h_k = \Gamma\left(\left\lfloor \frac{k+2}{2} \right\rfloor\right) \Gamma\left(\left\lfloor \frac{k+1}{2} \right\rfloor + \alpha + \frac{1}{2}\right), \quad b_{k+1}^H = \frac{h_{k+1}}{h_k}, \quad k \geq 0. \quad (25)$$

Here δ_{ij} is the Kronecker symbol, $\lfloor \cdot \rfloor$ and $\Gamma(\cdot)$ denote the greatest integer and Gamma functions, respectively.

Now we can state and prove the following theorem on the modified anti-Gauss and average rules for the generalized Hermite weight function.

Theorem 3.1 *Let \mathcal{G}_n^H and $\tilde{\mathcal{G}}_{n+1,\gamma}^H$ be the Gauss and anti-Gauss rules associated with the (monic) generalized Hermite polynomials $\{H_k^\alpha\}$, respectively. The nodes of the anti-Gauss rule $\tilde{\mathcal{G}}_{n+1,\gamma}^H$ are the zeros of the polynomial q_{n+1} ,*

$$q_{n+1} = H_{n+1}^\alpha - (1 + \gamma) \left(\frac{n}{2} + \frac{1 + (-1)^{n+1}}{2}\alpha\right) H_{n-1}^\alpha, \quad (26)$$

and are interlaced by the nodes of \mathcal{G}_n^H . For any $\gamma > -1$, all the weights of $\tilde{\mathcal{G}}_{n+1,\gamma}^H$ and $\mathcal{L}_{2n+1,\gamma}^H$ are positive, where $\mathcal{L}_{2n+1,\gamma}^H$ is the modified average rule

$$\mathcal{L}_{2n+1,\gamma}^H = \frac{1}{2 + \gamma} \left\{ (1 + \gamma) \mathcal{G}_n^H + \tilde{\mathcal{G}}_{n+1,\gamma}^H \right\}. \quad (27)$$

Proof: The result for the first part of the assertion follows from Corollary 2.2, taking $b_k = b_k^H$ and $p_k = H_k^\alpha$ in (20).

Consider the tridiagonal matrix \tilde{T}_{n+1} in (19). Since, by (25), all the subdiagonal elements of \tilde{T}_{n+1} for $\tilde{\mathcal{G}}_{n+1,\gamma}^H$ are positive for $2\alpha > -1$ and $\gamma > -1$, the interlacing property of the nodes follows from the Cauchy’s interlacing theorem for real symmetric tridiagonal matrices with positive subdiagonal elements (see Parlet [16]). The positivity of the subdiagonal elements of \tilde{T}_{n+1} also implies the positivity of $\tilde{\mathcal{G}}_{n+1,\gamma}^H$ and hence the positivity of the average rule (27). QED

In the remaining part of the paper, the errors of Gauss, anti-Gauss, and average rules for the generalized Hermite weight function will be denoted by

$$R_n^H, \quad \tilde{R}_{n+1,\gamma}^H, \quad R_{2n+1,\gamma}^H. \quad (28)$$

To prove our next result we need the following two lemmas.

Lemma 3.2 Let I_α^H be as in (24) and let $M_k(x) = x^k$. Then we have

$$I_\alpha^H [H_n^\alpha M_{n+2k}] = \frac{1}{k!} \Gamma \left(\left\lfloor \frac{n}{2} \right\rfloor + k + 1 \right) \Gamma \left(\left\lfloor \frac{n+1}{2} \right\rfloor + k + \alpha + \frac{1}{2} \right) \tag{29}$$

and $I_\alpha^H [H_n^\alpha M_{n+2k+1}] = 0$ for all $n, k \in \mathbf{N}$

Proof: The result can easily be obtained by using the properties of the generalized Hermite polynomials. QED

Lemma 3.3 Let $\{H_j^\alpha(x) = \sum_{i=0}^j A_{i,j} x^i\}$ be the monic generalized Hermite polynomials, and let $M_k(x) = x^k$. Then for $n, k \in \mathbf{N}$ and $\gamma > -1$ we have

$$R_n^H [M_{2n+k}] = \tilde{R}_{n+1,\gamma}^H [M_{2n+k}] = 0, \quad k = 1, 3, \dots, \tag{30}$$

and the following relations

$$\begin{aligned} R_n^H [M_{2n+2}] &= \Gamma \left(\left\lfloor \frac{n+4}{2} \right\rfloor \right) \Gamma \left(\left\lfloor \frac{n+3}{2} \right\rfloor + \alpha + \frac{1}{2} \right) \\ &\quad + \left\lfloor \frac{n}{2} \right\rfloor \left(\left\lfloor \frac{n+1}{2} \right\rfloor + \alpha - \frac{1}{2} \right) h_n, \\ \tilde{R}_{n+1,\gamma}^H [M_{2n+2}] &= \Gamma \left(\left\lfloor \frac{n+3}{2} \right\rfloor \right) \Gamma \left(\left\lfloor \frac{n+2}{2} \right\rfloor + \alpha + \frac{1}{2} \right) (1 - (1 + \gamma)b_n) \\ &\quad - (1 + \gamma) \left((1 + \gamma)b_n + \left\lfloor \frac{n+1}{2} \right\rfloor \left(\left\lfloor \frac{n}{2} \right\rfloor + \alpha + \frac{1}{2} \right) \right) h_n, \\ R_n^H [M_{2n+4}] &= \frac{1}{2} \Gamma \left(\left\lfloor \frac{n+6}{2} \right\rfloor \right) \Gamma \left(\left\lfloor \frac{n+5}{2} \right\rfloor + \alpha + \frac{1}{2} \right) \\ &\quad - A_{n-4,n} h_n - A_{n-2,n} R_n^H [M_{2n+2}], \\ \tilde{R}_{n+1,\gamma}^H [M_{2n+4}] &= \Gamma \left(\left\lfloor \frac{n+5}{2} \right\rfloor \right) \Gamma \left(\left\lfloor \frac{n+6}{2} \right\rfloor + \alpha \right) \\ &\quad - \Gamma \left(\left\lfloor \frac{n+5}{2} \right\rfloor \right) \Gamma \left(\left\lfloor \frac{n+4}{2} \right\rfloor + \alpha + \frac{1}{2} \right) (1 + \gamma)b_n \\ &\quad + (A_{n-3,n+1} - (1 + \gamma)b_n A_{n-3,n-1}) (1 + \gamma)h_n \\ &\quad - (A_{n-1,n+1} - (1 + \gamma)b_n A_{n-1,n-1}) \tilde{R}_{n+1,\gamma}^H [M_{2n+2}], \end{aligned}$$

where $b_k = b_k^H$ and h_k are given by (22) and (25).

Proof: Since $H_i^\alpha(-x) = (-1)^i H_i^\alpha(x)$ for all $i \in \mathbf{N}$, the polynomials $\{q_i\}$ defined by (26) satisfy

$$q_i(-x) = (-1)^i q_i(x), \quad i = 1, 2, \dots$$

Therefore, the nodes of \mathcal{G}_n^H and $\tilde{\mathcal{G}}_{n+1,\gamma}^H$ are symmetric with respect to the origin. On the other hand, from the relation

$$\tilde{w}_k = \int_{-\infty}^{\infty} \frac{q_{n+1}(x) \omega_\alpha^H(x)}{(x - \tilde{x}_k) q'_{n+1}(\tilde{x}_k)} dx = \int_{-\infty}^{\infty} \frac{q_{n+1}(x) \omega_\alpha^H(x)}{(x + \tilde{x}_k) q'_{n+1}(-\tilde{x}_k)} dx, \tag{31}$$

where \tilde{x}_i and \tilde{w}_i , $i = 1, 2, \dots, n+1$, are the nodes and weights of $\tilde{\mathcal{G}}_{n+1,\gamma}^H$, it follows that the weights corresponding to the nodes \tilde{x}_k and \tilde{x}_{n+1-k} are equal. This is also true for the Gauss rules for the generalized Hermite weight function; i.e., the weights corresponding to the nodes x_k and x_{n-k} are equal. Now, using these results, the relation (30) is easily obtained.

The remaining equations can be obtained using Lemma 2.3 and the results given by (23, 25, 26, 29). QED

Note that the coefficients of the polynomials H_n^α can also be obtained from the well known relations between the Laguerre and Hermite polynomials

$$H_{2k}^\alpha(x) = (-1)^k k! L_k^{(\alpha-1/2)}(x^2), \quad H_{2k+1}^\alpha(x) = (-1)^k k! x L_k^{(\alpha+1/2)}(x^2), \quad (32)$$

see [4, Chapter 5], where $L_k^{(\alpha)}(x)$ denotes the Laguerre polynomial

$$L_k^{(\alpha)}(x) = \sum_{j=0}^k \frac{\Gamma(k + \alpha + 1)}{\Gamma(j + \alpha + 1) j! (k - j)!} (-x)^j. \quad (33)$$

We now give the following theorem which states that there exists a unique value of γ such that the corresponding modified average rule associated with the generalized Hermite weight function has the highest possible degree.

Theorem 3.4 *Let $\mathcal{L}_{2n+1,\gamma}^H$ be the modified average rule (27) for the generalized Hermite weight function (8). The modified average rule of the highest possible degree for the Generalized Hermite weight function is unique and is obtained for*

$$\gamma = \gamma^* = \begin{cases} (2\alpha + 1)/n & \text{if } n \text{ is even,} \\ (1 - 2\alpha)/(2\alpha + n) & \text{if } n \text{ is odd.} \end{cases} \quad (34)$$

We have $\deg(\mathcal{L}_{2n+1,\gamma^*}^H) = 2n + 3$.

Proof: Letting again $M_k = x^k$ for the notational convenience and substituting the values given in Lemma 3.3 for the errors into

$$R_{2n+1,\gamma}^H[M_{2n+2}] = \frac{1}{2 + \gamma} \left\{ (1 + \gamma) R_n^H[M_{2n+2}] + \tilde{R}_{n+1,\gamma}^H[M_{2n+2}] \right\}$$

we obtain

$$R_{2n+1,\gamma}^H[M_{2n+2}] = \begin{cases} \left(\gamma - \frac{1+2\alpha}{n} \right) B_n & \text{if } n \text{ is even,} \\ \left(\gamma + \frac{2\alpha-1}{2\alpha+n} \right) C_n & \text{if } n \text{ is odd,} \end{cases}$$

where

$$B_n = - \binom{n}{2}^2 \Gamma\left(\frac{n}{2}\right) \Gamma\left(\frac{n+1}{2} + \alpha\right), \quad C_n = \left(\alpha + \frac{n}{2}\right)^2 \Gamma\left(\frac{n+1}{2}\right) \Gamma\left(\frac{n}{2} + \alpha\right),$$

which has the unique root (for $n \geq 1$, $2\alpha > -1$, $\gamma > -1$):

$$\gamma = \gamma^* = \begin{cases} (2\alpha + 1)/n & \text{if } n \text{ is even,} \\ (1 - 2\alpha)/(2\alpha + n) & \text{if } n \text{ is odd.} \end{cases}$$

From this result and the relations (10), (11) and (30) it follows that

$$R_{2n+1, \gamma^*}^H [M_k] = 0, \quad k = 0, 1, \dots, 2n + 3.$$

Now, taking $\gamma = \gamma^*$ in Lemma 3.3, a straightforward computation, using (10) and (11), shows that

$$R_{2n+1, \gamma^*}^H [M_{2n+4}] \neq 0, \quad n \geq 1.$$

Consequently, by definition (3), we have $\deg(\mathcal{L}_{2n+1, \gamma^*}^H) = 2n + 3$. QED

4 Numerical Examples

In this section we give some numerical results obtained by using the modified anti-Gauss and corresponding average rules for the generalized Hermite weight function. All results in the tables given below were generated by using Matlab 7.04 on a personal computer (with Intel Pentium IV processor and Windows XP system) with about 16 significant decimal digits. The results for the Gauss and anti-Gauss rules were generated by using the Matlab routine "gauss.m", included in the OPQ suit of W. Gautschi [8], which may be downloaded from the Web Site: <http://www.cs.purdue.edu/archives/2002/wxg/codes/>.

In the following examples, the errors of the Gauss, anti-Gauss, and average rules for the generalized Hermite weight function are denoted as in (28), and the following notations are used:

$$I_\alpha^H[f] = \int_{-\infty}^{\infty} |x|^{2\alpha} \exp(-x^2) f(x) dx, \quad (35)$$

$$a(b) := a \times 10^b, \quad \theta := (1 + \gamma)^{-1},$$

$$\mathcal{E}_{n, \gamma}^H := \mathcal{L}_{2n+1, \gamma}^H - \mathcal{G}_n^H, \quad \tilde{\mathcal{E}}_{n, \gamma}^H := \frac{1}{2 + \gamma} (\tilde{\mathcal{G}}_{n+1, \gamma}^H - \mathcal{G}_n^H). \quad (36)$$

Example 4.1 Consider the integral

$$I_{-1/4}^H[f_\beta], \quad f_\beta(x) = \left(\frac{x}{2}\right)^{22} \exp\left(\frac{\beta}{9}x\right). \quad (37)$$

The exact value of the integral for $\beta = 0$ is

$$I_{-1/4}^H[f_0] = \frac{\Gamma(45/4)}{4194304} = 1.5621505111433654 \dots$$

For $\beta = 1$ Mathematica 5.1 gives the exact value of the integral in terms of the modified Bessel functions. Evaluating the result using Mathematica we get

$$I_{-1/4}^H[f_1] = 1.6720078580613728476 \dots$$

Table 1 displays the errors of the Gauss, anti-Gauss and average rules for the given integral. It is seen that the theoretical and numerical results are in agreement. For example, the errors in the Gauss and anti-Gauss rules have opposite signs; the degree of the modified average rule with γ^* , when the rounding errors are taken into account, is $2n + 3$; and the absolute value of the error of the $(n + 1)$ -point anti-Gauss rule, multiplied by $\theta = (1 + \gamma)^{-1}$, is almost equal to the absolute value of the error of the n -point Gauss rule, etc. Note that the results obtained for $\tilde{\mathcal{E}}_{n,\gamma}^H$ were not displayed in this and the other tables given below, because the exponents and first two significant digits of $\mathcal{E}_{n,\gamma}^H$ and $\tilde{\mathcal{E}}_{n,\gamma}^H$ are the same.

Table 1: The errors of the quadrature rules for the integral (37)

β	n	$R_n^H[f_\beta]$	$\mathcal{E}_{n,\gamma^*}^H[f_\beta]$	$\theta \tilde{R}_{n+1,\gamma^*}^H[f_\beta]$	$R_{2n+1,0}^H[f_\beta]$	$R_{2n+1,\gamma^*}^H[f_\beta]$
0	9	2.3(-01)	2.3(-01)	-2.3(-01)	9.7(-03)	1.3(-03)
0	10	5.3(-02)	5.3(-02)	-5.3(-02)	2.5(-04)	1.1(-15)
0	11	5.3(-03)	5.3(-03)	-5.3(-03)	7.1(-15)	-4.4(-16)
1	10	6.4(-02)	6.4(-02)	-6.4(-02)	4.2(-04)	6.2(-05)
1	11	7.5(-03)	7.5(-03)	-7.5(-03)	2.7(-05)	2.6(-07)
1	12	2.1(-04)	2.1(-04)	-2.1(-04)	5.3(-08)	9.3(-10)
1	13	1.3(-06)	1.3(-06)	-1.3(-06)	4.0(-10)	1.0(-12)

Example 4.2 Let

$$I_\alpha^H[f], \quad f(x) = \cos^2 x, \quad \alpha = \pm 1/4. \tag{38}$$

The exact values can be obtained (for example using Mathematica 5.1) in terms of the Gamma, Bessel, and Hypergeometric functions. Their numerical values are

$$I_{-1/4}^H[f] = 3.00560219457205679 \dots, \quad I_{1/4}^H[f] = 0.68911817188406442 \dots$$

Table 2 shows the errors of the Gauss, anti-Gauss and average quadrature rules for the integral (38), for selected values of n .

Example 4.3 In this example we give an integral for which the Gauss quadrature rules converge slowly:

$$I_{1/4}^H[f], \quad f(x) = \frac{4 \exp(\arctan x)}{4 + x^2}. \tag{39}$$

Table 2: *The errors of the quadrature rules for the integral (38)*

α	n	$R_n^H[f]$	$\mathcal{E}_{n,\gamma^*}^H[f]$	$R_{2n+1,0}^H[f]$	$R_{2n+1,\gamma^*}^H[f]$
1/4	11	-6.1(-09)	-6.1(-09)	8.1(-11)	-2.7(-14)
1/4	12	2.7(-11)	2.7(-11)	-1.1(-14)	6.7(-16)
-1/4	10	5.8(-10)	5.8(-10)	-9.0(-13)	3.1(-13)
-1/4	12	1.1(-12)	1.1(-12)	-1.3(-15)	8.9(-16)

The exact value of the integral is not available, therefore the result obtained by using the 300-point Gauss rule with quadruple precision arithmetic was considered as the exact value of the integral in our calculation:

$$I_{1/4}^H[f] = 1.2627713585567107678 \dots$$

The numerical integrators of Mathematica 5.1 and Maple 9 give the same value (at least up to 20 significant digits) when 32-digit arithmetic is used. The results obtained by the Gauss, anti-Gauss, and average rules for the integral (39) are displayed in Table 3. Notice that, for the given integral, the 6-14-30-48-70-point average rules with γ^* yield more accurate results, in the given order, than the 14-30-48-70-96-point Gauss rules. Note that in this example the degree optimal average rules with even values of n give more accurate results.

Table 3: *The performance of the quadrature rules for the integral (39)*

n	$R_n^H[f]$	$\mathcal{E}_{n,\gamma^*}^H[f]$	$R_{2n+1,0}^H[f]$	$R_{2n+1,\gamma^*}^H[f]$
6	-3.5(-03)	-3.4(-03)	2.5(-04)	-3.7(-05)
14	-6.4(-05)	-6.4(-05)	2.9(-06)	2.3(-07)
30	-3.1(-07)	-3.1(-07)	9.6(-09)	3.0(-09)
48	-3.8(-09)	-3.9(-09)	9.5(-11)	4.1(-11)
70	-5.1(-11)	-5.1(-11)	1.1(-12)	5.5(-13)
96	-7.2(-13)	-7.3(-13)	1.3(-14)	7.1(-15)

For all integrals in the above examples, each of the differences given in (36) is almost equal to the error of \mathcal{G}_n^H , and hence anyone of them can be used to estimate the error of the n -point Gauss rule. Moreover, the exact value of each integral is bracketed by the values obtained by the Gauss and anti-Gauss rules. This behavior has also been observed for numerous other integrands. According to the results given in the tables, the degree optimal average rules, i.e., modified average rules with γ^* derived in this paper, give more accurate results, as expected, than the other average rules.

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