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ANTI-GAUSSIAN QUADRATURE FORMULAS

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ABSTRACT. An anti-Gaussian quadrature formula is an $(n+1)$-point formula of degree $2n-1$ which integrates polynomials of degree up to $2n+1$ with an error equal in magnitude but of opposite sign to that of the n-point Gaussian formula. Its intended application is to estimate the error incurred in Gaussian integration by halving the difference between the results obtained from the two formulas. We show that an anti-Gaussian formula has positive weights, and that its nodes are in the integration interval and are interlaced by those of the corresponding Gaussian formula. Similar results for Gaussian formulas with respect to a positive weight are given, except that for some weight functions, at most two of the nodes may be outside the integration interval. The anti-Gaussian formula has only interior nodes in many cases when the Kronrod extension does not, and is as easy to compute as the $(n+1)$-point Gaussian formula.

1. INTRODUCTION

Let w be a given weight function over an interval $[a,b]$ and let $G_w^{(n)}$ be the corresponding n-point Gauss-Christoffel quadrature formula

$$G_w^{(n)} f := \sum_{i=1}^{n} w_i^{(n)} f(x_i^{(n)}) \tag{1}$$

of degree $2n-1$ for the integral

$$If := \int_a^b f(x) w(x)\, \mathrm{d}x. \tag{2}$$

The defining property of $G_w^{(n)}$ is that

$$G_w^{(n)} p = Ip \quad \forall p \in \mathbb{P}^{2n-1}, \tag{3}$$

where $\mathbb{P}^m$ is the space of polynomials of degree not greater than m.

There are various questions of interest regarding the existence and other properties of quadrature formulas defined by a set of equations. To make the terminology precise, we shall say:

- The formula *exists* if the defining equations have a (possibly complex) solution.
- The formula is *real* if the points and weights are all real.
- A real formula is *internal* if all the points belong to the (closed) interval of integration. A node not belonging to the interval is called an *exterior node.*

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- The formula is *positive* if all the weights are positive.

The Gaussian formulas are known to be internal and positive.

In practice it is not easy to find an accurate estimate of the error $If - G_w^{(n)}f$ when f is some function that has not been subjected to very much analysis. The usual method is to use the difference $Af - G_w^{(n)}f$, where A is a quadrature formula of degree greater than $2n-1$. Any such quadrature formula A requires at least $n+1$ additional points. This is because, if we append n arbitrary points to $G_w^{(n)}$, the weights of the new points simply turn out to be 0 since the weights of a $(2n)$-point formula of degree at least $2n-1$ are unique. In fact, any set of $n+1$ points together with the original n points can be used to construct such a formula, because $Af - G_w^{(n)}f$ is a null rule [5] of degree $2n$, that is, a functional that maps polynomials of degree up to $2n$ to zero, but not polynomials of exact degree $2n+1$. It is known [12] that a null rule of degree $2n$ based on $2n+1$ points must be a multiple of the $(2n)$th divided difference on those points. One may therefore view the use of $Af - G_w^{(n)}f$ as a numerical approximation to the theoretical error of the Gaussian formula in terms of the $(2n)$th derivative obtained from the Peano kernel theorem [13].

Several possibilities for constructing a formula A with $n+1$ extra points have been singled out in the literature:

1. The $(n+1)$-point Gauss-Christoffel formula $G_w^{(n+1)}$ has degree $2n+1$ and can therefore serve as the formula A. It has been noted [3] that this procedure can be very unreliable.
2. For certain weight functions (including $w(x) = 1$) it is possible to find a $(2n+1)$-point formula containing the original n points, with degree at least $3n+1$. Such formulas were first computed for the case $w(x) = 1$ by Kronrod [11], and have found widespread acceptance as components of automatic quadrature algorithms [18]. Developments up to 1988 are surveyed by Gautschi [7]. The Kronrod formulas are of optimal degree, given that the points of $G_w^{(n)}$ are to be included, but often the weight function w is such that $G_w^{(n)}$ does not possess a real Kronrod extension, e.g. the Gauss-Laguerre and Gauss-Hermite cases [10].
3. In cases where no real Kronrod extension exists, Begumisa and Robinson [2] try to find a *suboptimal extension*, that is, a $(2n+1)$-point formula of degree greater than $2n$ but less than $3n+1$, by gradually reducing the degree aimed at until an extension is found to exist. Patterson [17] shows that such formulas can be found easily by his software package [16].

The idea of constructing two numerical methods with error terms of the same modulus but opposite signs has been used in the numerical solution of initial value problems in ordinary differential equations [4, 19, 20]. In this paper we consider the *anti-Gaussian* quadrature formula

$$H_w^{(n+1)}f := \sum_{i=1}^{n+1} \lambda_i^{(n+1)} f(\xi_i^{(n+1)}) \tag{4}$$

which is designed to have an error precisely opposite to the error in the Gauss-Christoffel formula $G_w^{(n)}$, that is,

$$Ip - H_w^{(n+1)}p = -(Ip - G_w^{(n)}p), \qquad p \in \mathbb{P}_{2n+1}. \tag{5}$$

The error $If - G_w^{(n)}f$ can then be estimated as $(H_w^{(n+1)}f - G_w^{(n)}f)/2$. In effect, we are using a $(2n+1)$-point formula $L_w^{(2n+1)} = (G_w^{(n)} + H_w^{(n+1)})/2$ of degree $2n+1$ to estimate the integral. We shall call this formula an *averaged Gaussian formula.* One can think of $\{G_w^{(n)}, L_w^{(2n+1)}\}$ as the first two terms in a stratified sequence [14] of quadrature formulas (each formula is a linear combination of the previous formula and a formula containing new points only).

The averaged Gaussian formula is of course also a suboptimal extension (and therefore subsumed in the theory of [16]), but we shall show that it has significant theoretical and practical properties. In particular, it always exists, it is an almost trivial task to construct it, it always has positive weights, its nodes are always real, and at worst two nodes may be exterior.

2. Construction of anti-Gaussian quadrature formulas

From (5) we see that

$$H_w^{(n+1)}p = 2Ip - G_w^{(n)}p, \qquad p \in \mathbb{P}_{2n+1}. \tag{6}$$

By comparing (6) with (3), we see that $H_w^{(n+1)}$ is the Gaussian formula for the linear functional $2I - G_w^{(n)}$. The points and weights of $H_w^{(n+1)}$ can therefore be found by the following (now classical) algorithm:

1. Find the coefficients $\{\alpha_j,\ j = 0, 1, \ldots, n\}$ and $\{\beta_j,\ j = 1, 2, \ldots, n\}$ which appear in the recurrence relation

$$\begin{aligned} \pi_{-1}(x) &= 0, \\ \pi_0(x) &= 1, \\ \pi_{j+1}(x) &= (x - \alpha_j)\pi_j(x) - \beta_j \pi_{j-1}(x), \quad j = 0, 1, \ldots, n, \end{aligned} \tag{7}$$

satisfied by the polynomials $\{\pi_j\}$ orthogonal with respect to the linear functional $2I - G_w^{(n)}$. The coefficient β_0 can be any finite number: following Gautschi [6], we put $\beta_0 = (2I - G_w^{(n)})\pi_0$, in other words, the functional applied to the constant polynomial π_0.

2. As shown by Golub and Welsch [9], the nodes of the quadrature formula are the eigenvalues, and the weights are proportional to the squares of the first components of the eigenvectors, of the symmetric tridiagonal matrix

$$\begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & \\ & \ddots & \ddots & \ddots \\ & & \sqrt{\beta_n} & \alpha_n \end{bmatrix}.$$

The coefficients $\{\alpha_j,\ j = 0, 1, \ldots, n\}$ and $\{\beta_j,\ j = 1, 2, \ldots, n\}$ are given by the well-known formulas of Stieltjes:

$$\alpha_j = \frac{(2I - G_w^{(n)})(x\pi_j^2)}{(2I - G_w^{(n)})(\pi_j^2)}, \qquad j = 0, 1, \ldots, n; \tag{8}$$

$$\beta_j = \frac{(2I - G_w^{(n)})(\pi_j^2)}{(2I - G_w^{(n)})(\pi_{j-1}^2)}, \qquad j = 1, 2, \ldots, n. \tag{9}$$

The proper use of (7) in conjunction with (8–9) is normally a task requiring great delicacy (thoroughly discussed by Gautschi in [6]), but in the present case the task is easy, since we shall show that the required coefficients may be obtained trivially from the corresponding coefficients for the original linear functional I. In the classical cases, the latter coefficients are known explicitly [1]; in others, the software (e.g. [8]) used to compute $G_w^{(n)}$ computes the recurrence coefficients as a preliminary step. The details are as follows:

Let $\{p_j\}$ be the sequence of polynomials orthogonal to the original weight function w, which satisfy the recurrence relation

$$\begin{aligned} p_{-1}(x) &= 0, \\ p_0(x) &= 1, \\ p_{j+1}(x) &= (x - a_j)p_j(x) - b_j p_{j-1}(x), \qquad j = 0, 1, \dots . \end{aligned}$$

As before, $b_0 = Ip_0$, and the other recurrence coefficients satisfy the relations

$$\begin{aligned} a_j &= \frac{I(xp_j^2)}{I(p_j^2)}, \qquad j = 0, 1, \dots ; \\ b_j &= \frac{I(p_j^2)}{I(p_{j-1}^2)}, \qquad j = 1, 2, \dots . \end{aligned} \tag{10}$$

The crucial observation is that because of the property (3), $(2I - G_w^{(n)})p = Ip$ for $p \in \mathbb{P}^{2n-1}$, and therefore

$$\alpha_j = a_j, \qquad j = 0, 1, \dots, n-1; \tag{11}$$

$$\beta_j = b_j, \qquad j = 0, 1, \dots, n-1; \tag{12}$$

$$\pi_j = p_j, \qquad j = 0, 1, \dots, n. \tag{13}$$

We need only compute α_n and β_n. Since the points $x_i,\ i = 1, 2, \dots, n$, in (1) are the zeros of π_n, the result of applying $G_w^{(n)}$ to any expression which contains π_n as a factor is 0. Using this observation, as well as the fact that the degree of π_{n-1}^2 is less than $2n - 1$, we find that

$$\alpha_n = \frac{2I(x\pi_n^2)}{2I(\pi_n^2)} \tag{14}$$

$$= a_n; \tag{15}$$

$$\beta_n = \frac{2I(\pi_n^2)}{I(\pi_{n-1}^2)} \tag{16}$$

$$= 2b_n. \tag{17}$$

In other words, we take precisely the same set of recurrence coefficients as when computing the Gauss-Christoffel formula $G_w^{(n+1)}$, except that the last coefficient β_n is doubled. The rest of the computation proceeds exactly as usual.

3. Theoretical properties

Theorem 1. *The anti-Gaussian formula $H_w^{(n+1)}$ has the following properties.*

1. *The weights $\lambda_i > 0,\ i = 1, 2, \dots, n + 1$.*
2. *The nodes $\xi_i,\ i = 1, 2, \dots, n + 1$, are all real, and are interlaced by those of the Gaussian formula $G_w^{(n)}$, i.e.,*

$$\xi_1 < x_1 < \xi_2 < x_2 < \cdots < x_n < \xi_{n+1}.$$

3. *The inner nodes are in the integration interval, i.e.*

$$\xi_2, \xi_3, \dots, \xi_n \in [a, b].$$

4. $\xi_1 \in [a, b]$ *if and only if* $\frac{p_{n+1}(a)}{p_{n-1}(a)} \geq b_n$, *and* $\xi_{n+1} \in [a, b]$ *if and only if* $\frac{p_{n+1}(b)}{p_{n-1}(b)} \geq b_n$, *where* p_j, $j = 0, 1, \dots, n+1$, *are the orthogonal polynomials and* b_j, $j = 1, 2, \dots, n$, *the recurrence coefficients corresponding to the original weight function as in* (10).

Proof. Since $b_n > 0$, $\sqrt{2b_n}$ is real, and the nodes are therefore eigenvalues of a real symmetric matrix, thus real. The weights are trivially positive since they are formed as squares of real quantities in the Golub-Welsch algorithm. The interlacing property of the nodes follows from the fact that the recurrence coefficients for $G_w^{(n)}$ are equal to the first n recurrence coefficients for $H_w^{(n+1)}$. Therefore the Gaussian nodes x_i are the eigenvalues of the $n \times n$ leading submatrix of the symmetric tridiagonal matrix with eigenvalues ξ_i, and Cauchy's interlace theorem (see e.g. [15, p.186]) can be applied.

From the interlacing property it follows that all the inner nodes are in the interval $[a, b]$. We derive the condition for x_{n+1} to be in $[a, b]$: the derivation for x_1 is similar.

Any real polynomial with leading coefficient 1 and having at most one zero to the right of b is negative, zero, or positive at b according to whether it has one zero greater than b, a zero at b, or no zeros greater than or equal to b. Therefore, $p_{n-1}(b)$ and $p_{n+1}(b)$ are both positive; and $\pi_{n+1}(b)$ is positive if and only if it has no zeros $\geq b$. (π_{n+1} cannot have more than one zero $\geq b$ because of the interlacing property.) From the equations (obtained by using (7), (10), (13), (15) and (17))

$$p_{n+1}(x) = (x - a_n)p_n(x) - b_n p_{j-1}(x),$$
$$\pi_{n+1}(x) = (x - a_n)p_n(x) - 2b_n p_{j-1}(x),$$

we note that $\pi_{n+1} = p_{n+1} - b_n p_{n-1}$. Therefore, $\pi_{n+1}(b) > 0$ if and only if $\frac{p_{n+1}(b)}{p_{n-1}(b)} > b_n$. □

For the classical weight functions, the recurrence coefficients and the values of the orthogonal polynomials at the end points are explicitly known. We thus obtain the following corollary of Theorem 1.

Theorem 2. *The anti-Gaussian formulas corresponding to the following weight functions are internal and positive:*

1. $w(x) = (1-x^2)^\alpha$ *over* $[-1, 1]$ *with* $\alpha \geq -\frac{1}{2}$ (*Gegenbauer*), *including the special cases*
   (a) $w(x) = 1$ *over* $[-1, 1]$ (*Legendre*),
   (b) $w(x) = (1 - x^2)^{-\frac{1}{2}}$ *over* $[-1, 1]$ (*Chebyshev*),
   (c) $w(x) = (1 - x^2)^{\frac{1}{2}}$ *over* $[-1, 1]$ (*Chebyshev, second kind*).
2. $w(x) = x^\alpha e^{-x}$ *over* $[0, \infty)$ *with* $\alpha > -1$ (*generalized Laguerre*).
3. $w(x) = |x|^\alpha e^{-x^2}$ *over* $(-\infty, \infty)$ *with* $\alpha > -1$ (*generalized Hermite*).

Proof. The Gegenbauer weight is a special case of the Jacobi weight, treated below. For the generalized Hermite weight, the result is trivial, since the integration interval contains all real numbers. For the generalized Laguerre weight, we use Tables 22.3 (leading coefficients), 22.4 (special values), and 22.7 (recurrence relations) from [1], to obtain

$$b_n = n(n+\alpha),$$
$$p_n(0) = (-1)^n n! \binom{n+\alpha}{n},$$

and hence

$$\frac{p_{n+1}(0)}{p_{n-1}(0)} = (n+\alpha)(n+\alpha+1) > b_n$$

since $\alpha > -1$. □

In the case of the Jacobi weight function, the characterization is not so simple.

Theorem 3. *The anti-Gaussian formula $H_w^{(n+1)}$ with $n \geq 1$ corresponding to $w(x) = (1-x)^\alpha(1+x)^\beta$ with $\alpha, \beta > -1$ is internal if and only if*

$$(2\alpha+1)n^2+(2\alpha+1)(\alpha+\beta+1)n+\tfrac{1}{2}(\alpha+1)(\alpha+\beta)(\alpha+\beta+1) \geq 0 \tag{18}$$

and

$$(2\beta+1)n^2+(2\beta+1)(\alpha+\beta+1)n+\tfrac{1}{2}(\beta+1)(\alpha+\beta)(\alpha+\beta+1) \geq 0. \tag{19}$$

Proof. Using the same tables from [1], we obtain

$$b_n = \frac{4n(n+\alpha)(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta-1)(2n+\alpha+\beta)^2(2n+\alpha+\beta+1)},$$
$$p_n(1) = \frac{2^n \binom{n+\alpha}{n}}{\binom{2n+\alpha+\beta}{n}},$$

and hence

$$\frac{p_{n+1}(1)}{b_n p_{n-1}(1)} = \frac{(n+\alpha+1)(n+\alpha+\beta+1)(n+\frac{\alpha+\beta}{2})}{n(n+\beta)(n+\frac{\alpha+\beta}{2}+1)}$$
$$= 1 + \frac{(2\alpha+1)n(n+\alpha+\beta+1)+\frac{1}{2}(\alpha+1)(\alpha+\beta)(\alpha+\beta+1)}{n(n+\beta)(n+\frac{\alpha+\beta}{2}+1)}.$$

Since the denominator in the last fraction and b_n are both positive, by Theorem 1 the largest node of $H_w^{(n+1)}$ is in the interval if and only if the numerator is positive. The proof for the leftmost node is similar. □

Theorem 3, while precise, is not very enlightening. We therefore offer a weaker corollary.

Theorem 4. *The anti-Gaussian formulas $H_w^{(n+1)}$, $n = 1, 2, \ldots$, for the Jacobi weight $w(x) = (1-x)^\alpha(1+x)^\beta$ are internal and positive when α and β satisfy the following four inequalities:*

$$\alpha \geq -\tfrac{1}{2}, \tag{20}$$

$$\beta \geq -\tfrac{1}{2}, \tag{21}$$

$$(2\alpha+1)(\alpha+\beta+2)+\frac{1}{2}(\alpha+1)(\alpha+\beta)(\alpha+\beta+1) \geq 0, \tag{22}$$

$$(2\beta+1)(\alpha+\beta+2)+\frac{1}{2}(\beta+1)(\alpha+\beta)(\alpha+\beta+1) \geq 0. \tag{23}$$

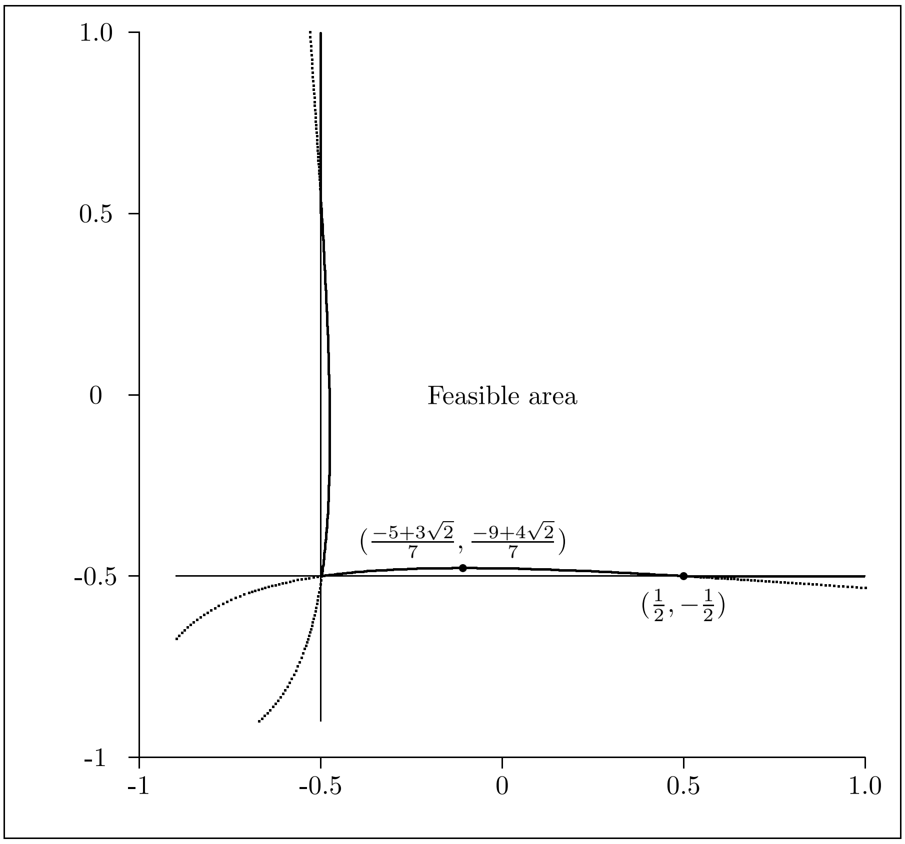

FIGURE 1. Anti-Gaussian formulas for the Jacobi weight are internal for all n when α and β are within the unbounded region to the north-east of the heavy lines

Proof. When (20–21) are satisfied, the coefficients of n^2 and n in the quadratic polynomials are positive. These polynomials are therefore increasing functions of n, and we need merely test whether they are positive when $n = 1$. Inequalities (22–23) are obtained by putting $n = 1$ in (18–19). $\square$

When $\alpha = \beta$, inequality (22) reduces to $(\alpha+1)(2\alpha+1)(2+\alpha) \geq 0$, which is satisfied when $\alpha \geq -\frac{1}{2}$, thus proving Case 1 of Theorem 2.

Figure 1 shows the region in the (α, β) plane in which the conditions of Theorem 4 are satisfied. Outside that region, the anti-Gaussian formula for at least one value of n has an exterior node.

Some sufficient conditions for an anti-Gaussian formula for the Jacobi weight to require exterior nodes can be deduced from Theorem 3. We mention only cases with $\alpha < \beta$: other cases can be obtained by interchanging α and β. Denote the left-hand side of (18) by $f(n, \alpha, \beta)$; we have:

1. For $\alpha < -\frac{1}{2}$, the formulas for sufficiently large n require an exterior node, because the coefficient of n^2 is negative.
2. For $\alpha = -\frac{1}{2}$ and $\beta = 0$, the formulas require an exterior node for all n, because $f(n, -\frac{1}{2}, 0) = -\frac{1}{8}$.

3. For $\beta^2 < \frac{1}{4}$ and α close enough to $-\frac{1}{2}$, the formulas require an exterior node for n small enough, because $f(n, -\frac{1}{2}+\epsilon, \beta)$ has zeros at
$$n = \tfrac{1}{2}(-\tfrac{1}{2} - \beta - \epsilon \pm \sqrt{\Delta}),$$
where
$$\Delta = \tfrac{1}{2}(1 + \epsilon + (\tfrac{1}{4} - \beta^2)/\epsilon).$$
The positive zero is therefore $O(\epsilon^{-1/2})$.

We conclude with the remark that when $|\alpha| = |\beta| = \frac{1}{2}$, the averaged Gaussian formula $L_w^{(2n+1)} = (G_w^{(n)} + H_w^{(n+1)})/2$ actually is the same as the Kronrod formula $K_w^{(2n+1)}$. This property follows from the facts that the Kronrod formula in its turn is the same as a formula of higher degree, that is, a $(2n+1)$-point Gaussian, Lobatto or Radau formula, as the case may be [7], and that in those cases the weights of the old points are precisely half of their previous values.

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