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Gauss and anti-Gauss quadrature formulae

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Abstract

The present thesis is about Gauss and anti-Gauss quadrature formulas. It is well known that many properties of Gauss formula arise from orthogonal polynomials, therefore, the first chapter is devoted to orthogonal polynomials along with their properties from both the computational and theoretical point of view. The second chapter is dedicated to the Gauss quadrature formula, focusing on its construction and most important properties, which demonstrate its superiority compared to other quadrature formulas. The third chapter is devoted to the anti-Gauss quadrature formula, a highly efficient method, presented by Laurie in order to practically estimate the error of the Gauss formula. After describing the formula and its most important properties, we focus on its behaviour for some of the classical weight functions. In the fourth and final chapter, the thesis concludes with some numerical examples, for the Legendre and Jacobi weight functions, which demonstrate the efficiency of anti-Gauss formula in estimating the error of the Gauss formula.

Chapter 1

Orthogonal Polynomials

The purpose of this chapter is to give the reader a brief introduction to orthogonal polynomials, along with their properties, and especially their use in numerical integration. For the relevant theory and a well rounded study, Szegö (1975) [11] is still the best source.

1.1 Introduction and Basic Theory

Let $\lambda(t)$ be a real non-decreasing function such that both $\lim_{t\to-\infty}\lambda(t)$ and $\lim_{t\to+\infty}\lambda(t)$ exist and be finite.

The r-order moment of the induced positive measure $\mathrm{d}\lambda$ is

$$\mu_r = \mu_r(\mathrm{d}\lambda) = \int_{\mathbb{R}} t^r \mathrm{d}\lambda(t), \tag{1.1}$$

and we assume that $\mu_r < +\infty$ for $r = 0, 1, 2, \ldots$, with $\mu_0 > 0$.

Now, if $\mathbb{P}$ is the space of real polynomials and $\mathbb{P}_d \subset \mathbb{P}$ is the space of polynomials with degree $\leq d$, we can define the following inner product $\forall u, v \in \mathbb{P}$ (with respect to the measure $\mathrm{d}\lambda$)

$$(u,v)_{\mathrm{d}\lambda} = \int_{\mathbb{R}} u(t)v(t)\mathrm{d}\lambda(t), \tag{1.2}$$

satisfying

(a) $(u,u)_{\mathrm{d}\lambda} = \int_{\mathbb{R}} u(t)u(t)\mathrm{d}\lambda(t) \geq 0 \;\; \forall u \in \mathbb{P}$ and
$(u,u)_{\mathrm{d}\lambda} = 0 \Leftrightarrow \int_{\mathbb{R}} u(t)u(t)\mathrm{d}\lambda(t) = 0 \Leftrightarrow u(t) = 0 \;\; \forall t \in \mathbb{R} \Leftrightarrow u = 0$, since $\mathrm{d}\lambda(t) > 0$.

(b) $(u,v)_{\mathrm{d}\lambda} = \int_{\mathbb{R}} u(t)v(t)\mathrm{d}\lambda(t) = \int_{\mathbb{R}} v(t)u(t)\mathrm{d}\lambda(t) = (v,u)_{\mathrm{d}\lambda}\ \forall u,v \in \mathbb{P}$.

(c) $(\lambda u + \mu v, w)_{\mathrm{d}\lambda} = \int_{\mathbb{R}}[\lambda u(t) + \mu v(t)]w(t)\mathrm{d}\lambda(t)$
$= \int_{\mathbb{R}}[\lambda u(t)w(t) + \mu v(t)w(t)]\mathrm{d}\lambda(t)$
$= \lambda \int_{\mathbb{R}} u(t)w(t)\mathrm{d}\lambda(t) + \mu \int_{\mathbb{R}} v(t)w(t)\mathrm{d}\lambda(t)$
$= \lambda(u,w)_{\mathrm{d}\lambda} + \mu(v,w)_{\mathrm{d}\lambda}\ \forall u,v,w \in \mathbb{P}$ and $\lambda, \mu \in \mathbb{R}$.

Hence, (1.2) satisfies the properties of inner product.

Note that if $v = u$, by (1.2), we get the norm of u (with respect to the measure $\mathrm{d}\lambda$),

$$\|u\|_{\mathrm{d}\lambda} = \sqrt{(u,u)_{\mathrm{d}\lambda}} = \left(\int_{\mathbb{R}} u^2(t)\mathrm{d}\lambda(t) \right)^{1/2}. \tag{1.3}$$

Definition 1.1. Let u, v be the elements of a vector space with an inner product $(\cdot,\cdot)$. Then u is said to be orthogonal to v if $(u,v) = 0$.

Definition 1.2. (Monic orthogonal polynomials)
The polynomials $\pi_k(t) = t^k + \dots,\ k = 0,1,2,\dots$ are called monic orthogonal polynomials, with respect to the measure $\mathrm{d}\lambda$, if

$$\begin{aligned} (\pi_k, \pi_\ell)_{\mathrm{d}\lambda} = 0 \quad \text{for } k \neq \ell, \quad k, \ell = 0, 1, 2, \ldots, \\ \|\pi_k\|_{\mathrm{d}\lambda} > 0 \quad \text{for } k = 0, 1, 2, \ldots. \end{aligned} \tag{1.4}$$

Remark 1.3. If the index k is unbounded then there are infinite many orthogonal polynomials and finitely many otherwise.

Definition 1.4. The polynomials $\tilde{\pi}_k(t)$ satisfying

$$\tilde{\pi}_k = \frac{\pi_k}{\|\pi_k\|_{\mathrm{d}\lambda}}, \; k = 0, 1, \ldots,$$

are called orthonormal polynomials. These polynomials have the following property

$$(\tilde{\pi}_k, \tilde{\pi}_\ell)_{\mathrm{d}\lambda} = \begin{cases} 0 & \text{if } k \neq \ell, \\ 1 & \text{if } k = \ell. \end{cases} \tag{1.5}$$

Definition 1.5. The inner product $(\cdot, \cdot)$ is said to be positive definite if $(u, u)_{\mathrm{d}\lambda} > 0 \; \forall u \in \mathbb{P}, \; u \neq 0$.

For the rest of the chapter $(\cdot, \cdot)_{\mathrm{d}\lambda}$ will be denoted as $(\cdot, \cdot)$, because the only inner product that we use is the one with respect to the measure $\mathrm{d}\lambda$.

1.2 Properties of Orthogonal Polynomials

1.2.1 General Properties

For our next theorem, we will use the following Lemma.

Lemma 1.6. *([6], Lemma 1.4) If π_k, $k = 0, 1, \ldots, n$, are monic orthogonal polynomials and $p \in \mathbb{P}_n$ satisfies $(p, \pi_k) = 0$, $k = 0, 1, 2, \ldots, n$, then $p = 0$.*

Proof. Let $p \in \mathbb{P}$ so $p = \alpha_0 + \alpha_1 t, \ldots + \alpha_n t^n$. From hypothesis we know that

$$0 = (p, \pi_k) = (\alpha_0 + \alpha_1 t + \ldots + \alpha_n t^n, \pi_k) = (\alpha_k t^k, \pi_k) = \alpha_k (t^k, \pi_k) = \alpha_k (\pi_k, \pi_k).$$

As $(\pi_k, \pi_k) > 0$, we get $\alpha_k = 0$ for $k = 0, 1, \ldots, n$, thus $p = 0$. □

Theorem 1.7. *([6], Lemma 1.5) The set $\{\pi_0, \pi_1, \ldots, \pi_n\}$ forms a basis of $\mathbb{P}_n$. In particular, every $p \in \mathbb{P}_n$ can be uniquely represented in the form*

$$p = \sum_{k=0}^{n} c_k \pi_k. \tag{1.6}$$

Proof. We will first prove that π_i, for $i = 0, 1, \ldots, n$, are linearly independent. Lets assume that

$$\sum_{k=0}^{n} e_k \pi_k = 0,$$

then, by orthogonality,

$$0 = \left(\sum_{k=0}^{n} e_k \pi_k, \pi_j \right) = e_0(\pi_0, \pi_j) + e_1(\pi_1, \pi_j) + \ldots + e_n(\pi_n, \pi_j) = e_j(\pi_j, \pi_j),$$

and as $(\pi_j, \pi_j) > 0$,

$$e_j = 0 \text{ for } j = 0, 1, \ldots, n.$$

Now if

$$p = \sum_{k=0}^{n} c_k \pi_k,$$

then, by orthogonality,

$$(p, \pi_j) = \left(\sum_{k=0}^{n} c_k \pi_k, \pi_j \right) = \sum_{k=0}^{n} c_k \left(\pi_k, \pi_j \right) = c_k(\pi_j, \pi_j),$$

and, consequently,

$$c_j = \frac{(p, \pi_j)}{(\pi_j, \pi_j)}.$$

If c_j is chosen as above, then

$$\left(p - \sum_{k=0}^{n} c_k \pi_k, \pi_j\right) = 0,$$

and using Lemma 1.6, we get

$$p - \sum_{k=0}^{n} c_k \pi_k = 0,$$

thus,

$$p = \sum_{k=0}^{n} c_k \pi_k.$$

□

Theorem 1.8. *([6], Theorem 1.6) For every positive definite measure* $\mathrm{d}\lambda$ *there exists a unique set of monic orthogonal polynomials* $\{\pi_n\}$.

Proof. Lets assume that $\{\pi_n\}$ and $\{q_n\}$ are two sets of monic orthogonal polynomials with respect to the measure $\mathrm{d}\lambda$.

If $n = 0$, then $\pi_0(t) = q_0(t) = 1$, hence monic orthogonal polynomials are unique for $n = 0$. Now, if $n \geq 1$, then

$$deg(\pi_n - q_n) \leq n - 1,$$

and by the orthogonality of π_n and q_n, we get

$$(\pi_n, \pi_n - q_n) = (q_n, \pi_n - q_n) = 0.$$

Therefore,

$$0 = (\pi_n, \pi_n - q_n) - (q_n, \pi_n - q_n) = (\pi_n - q_n, \pi_n - q_n),$$

and from the properties of inner product (1.2), we have

$$\pi_n - q_n = 0,$$

that is,

$$\pi_n = q_n.$$

□

1.2.2 The Three Term Recurrence Relation

The three term recurrence relation is arguably the most important property satisfied by a set of orthogonal polynomials. It is useful from both the theoretical and computational point of view, and it would be particularly useful for what it follows.

Theorem 1.9. *([6], Theorem 1.27) Let* $\pi_k(\cdot) = \pi_k(\,\cdot\,; \mathrm{d}\lambda)$, $k = 0, 1, 2, \ldots,$ *be the monic orthogonal polynomials with respect to the measure* $\mathrm{d}\lambda$*. Then*

$$\begin{gathered} \pi_{k+1}(t) = (t - \alpha_k)\,\pi_k(t) - \beta_k \pi_{k-1}(t), \quad k = 0, 1, 2, \ldots, \\ \pi_{-1}(t) = 0, \quad \pi_0(t) = 1, \end{gathered} \tag{1.7}$$

where

$$\alpha_k = \frac{(t\pi_k, \pi_k)_{\mathrm{d}\lambda}}{(\pi_k, \pi_k)_{\mathrm{d}\lambda}}, \quad k = 0, 1, 2, \ldots, \tag{1.8}$$

$$\beta_k = \frac{(\pi_k, \pi_k)_{\mathrm{d}\lambda}}{(\pi_{k-1}, \pi_{k-1})_{\mathrm{d}\lambda}}, \quad k = 1, 2, \ldots. \tag{1.9}$$

Proof. As π_k are monic, the degree of $\pi_{k+1} - t\pi_k$ is $\leq k$. Using formula (1.6), we have

$$\pi_{k+1}(t) - t\pi_k(t) = -\alpha_k \pi_k(t) - \beta_k \pi_{k-1}(t) + \sum_{j=0}^{k-2} c_{kj} \pi_j(t), \tag{1.10}$$

where $\alpha_k, \beta_k, c_{kj}$ are certain constants and $\pi_{-1}(t) = 0$ and $\pi_0(t) = 1$. Taking the inner product of both sides of (1.10) with π_k, we get

$$(\pi_{k+1} - t\pi_k, \pi_k) = \left(-\alpha_k\pi_k - \beta_k\pi_{k-1} + \sum_{j=0}^{k-2} c_{kj}\pi_j, \pi_k \right),$$

and using properties of the inner product and orthogonality,

$$(\pi_{k+1}, \pi_k) - (t\pi_k, \pi_k) = -\alpha_k (\pi_k, \pi_k) - \beta_k (\pi_{k-1}, \pi_k) + \sum_{j=0}^{k-2} c_{kj} (\pi_j, \pi_k),$$

that is,

$$-(t\pi_k, \pi_k) = -\alpha_k(\pi_k, \pi_k),$$

which leads to (1.8).

Similarly, taking the inner product of (1.10) with π_{k-1} yields

$$-(t\pi_k, \pi_{k-1}) = -\beta_k (\pi_{k-1}, \pi_{k-1}). \tag{1.11}$$

Now using the commutativity of inner product (1.2), we have

$$-(t\pi_k, \pi_{k-1}) = -(\pi_k, t\pi_{k-1}), \tag{1.12}$$

and since $t\pi_{k-1} \in \mathbb{P}_k$ we can write $t\pi_{k-1}$ in the following form

$$t\pi_{k-1}(t) = \pi_k(t) + \gamma_{k-1}\pi_{k-1}(t) + \cdots + \gamma_0\pi_0(t),$$

then,

$$\begin{aligned} -(\pi_k, t\pi_{k-1}) &= -(\pi_k, \pi_k + \gamma_{k-1}\pi_{k-1} + \cdots + \gamma_0\pi_0) \\ &= -(\pi_k, \pi_k) - \gamma_{k-1}(\pi_k, \pi_{k-1}) - \cdots - \gamma_0(\pi_k, \pi_0) \\ &= -(\pi_k, \pi_k). \end{aligned}$$

Combining (1.11) and (1.12) with the above relation we get

$$-\left(\pi_k, \pi_k\right) = -\beta_k\left(\pi_{k-1}, \pi_{k-1}\right),$$

which leads to (1.9).

Finally, taking the inner product of both sides of (1.10), successively, with π_i, $i = 0, 1, 2, \ldots, k-2$, gives

$$(\pi_{k+1}, \pi_i) - (t\pi_k, \pi_i) = (-\alpha_k \pi_k, \pi_i) - (\beta_k \pi_{k-1}, \pi_i) + \left(\sum_{j=0}^{k-2} c_{kj}\pi_j, \pi_i\right),$$

and using properties of inner product and orthogonality,

$$(c_{ki}\pi_i, \pi_i) = -(t\pi_k, \pi_i) = -(\pi_k, t\pi_i) = 0,$$

that is,

$$c_{ki}(\pi_i, \pi_i) = (c_{ki}\pi_i, \pi_i) = 0.$$

Hence, $c_{ki} = 0$ for $i = 0, 1, \ldots, k-2$. □

Remark 1.10. Only if $(\cdot, \cdot)$ is positive definite, (1.8) and (1.9) are well defined.

Definition 1.11. The nth-order Jacobi matrix associated with the measure $\mathrm{d}\lambda$ is the $n \times n$, symmetric, tridiagonal matrix

$$J_n = J_n(\mathrm{d}\lambda) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & 0 & \ldots & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & \alpha_{n-1} \end{bmatrix}. \tag{1.13}$$

Theorem 1.12. *([6], Theorem 1.31) The zeros $\tau_\nu^{(n)}$ of $\pi_n(\,\cdot\,; \mathrm{d}\lambda)$ are the eigenvalues of the Jacobi matrix $J_n(\mathrm{d}\lambda)$, while $\tilde{\pi}(\tau_\nu^{(n)})$ are the corresponding eigenvectors, where*

$$\tilde{\pi}(t) = [\tilde{\pi}_0(t), \tilde{\pi}_1(t), \ldots, \tilde{\pi}_{n-1}(t)]^T. \tag{1.14}$$

Proof. We will first prove that the orthonormal polynomials $\tilde{\pi}(\,\cdot\,;\mathrm{d}\lambda)$ satisfy the three term recurrence relation

$$\begin{gathered}\sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(t) = (t-\alpha_k)\tilde{\pi}_k(t) - \sqrt{\beta_k}\tilde{\pi}_{k-1}(t), \quad k = 0,1,2,\ldots, \\ \tilde{\pi}_{-1}(t) = 0, \quad \tilde{\pi}_0(t) = \frac{1}{\sqrt{\beta_0}}\ .\end{gathered} \tag{1.15}$$

We know that

$$\pi_{k+1}(t) = (t-\alpha_k)\,\pi_k(t) - \beta_k\pi_{k-1}(t).$$

Replacing now $\pi_k(t)$ by $\|\pi_k\|\tilde{\pi}_k(t)$, dividing with $\|\pi_{k+1}\|$, multiplying both sides by $\frac{\|\pi_{k+1}\|}{\|\pi_k\|} = \sqrt{\beta_{k+1}}$ and using (1.9), we get

$$\frac{\pi_{k+1}(t)}{\|\pi_{k+1}\|} = (t-\alpha_k)\frac{\|\pi_k\|\tilde{\pi}_k(t)}{\|\pi_{k+1}\|} - \beta_k\frac{1}{\|\pi_{k+1}\|}\pi_{k-1}(t),$$

that is,

$$\sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(t) = (t-\alpha_k)\tilde{\pi}_k(t) - \frac{\|\pi_k\|^2}{\|\pi_{k-1}\|^2}\frac{\|\pi_{k+1}\|}{\|\pi_k\|}\frac{1}{\|\pi_{k+1}\|}\pi_{k-1}(t),$$

so, finally,

$$\sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(t) = (t-\alpha_k)\tilde{\pi}_k(t) - \sqrt{\beta_k}\tilde{\pi}_{k-1}(t).$$

Equivalently,

$$t\tilde{\pi}_k(t) = \sqrt{\beta_k}\tilde{\pi}_{k-1}(t) + \alpha_k\tilde{\pi}_k(t) + \sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(t),\ k = 0,1,\ldots,n-1,$$

and in vector form, by means of (1.13) and (1.14),

$$t\tilde{\pi}(t) = J_n\tilde{\pi}(t) + \sqrt{\beta_n}\tilde{\pi}_n(t)e_n,$$

where $e_n = [0,0,\ldots,1]^{\mathrm{T}}$ is the *nth* coordinate vector in $\mathbb{R}^n$. Finally, if we set $t = \tau_\nu^{(n)}$, we obtain

$$J_n\tilde{\pi}(\tau_\nu^{(n)}) = \tau_\nu^{(n)}\tilde{\pi}(\tau_\nu^{(n)}), \tag{1.16}$$

which proves our assertions. $\square$

Remark 1.13. The result of Theorem 1.12 is particularly important for Gaussian integration, where we have to find the nodes τ_k, which are the zeros of $\pi_k(t\,;\mathrm{d}\lambda)$, and the weights w_k, which can be expressed in terms of the eigenvector $\tilde{\pi}(\tau_k)$.

Remark 1.14. If $\lambda(t)$ is absolutely continuous, then

$$\mathrm{d}\lambda(t) = w(t)\mathrm{d}t, \tag{1.17}$$

where $w(t)$ is a nonnegative integrable function on $\mathbb{R}$ called weight function.

Gauss type quadrature formulas are characterized by the weight function that is used. For example, the Gauss-Legendre quadrature formula is the Gauss formula using the weight function $w(t) = 1$, which is the Legendre weight function.

Remark 1.15. Monic orthogonal polynomials can also be constructed by applying Gramm-Schmidt orthogonalization to the sequence $e_k(t) = t^k$, starting with $\pi_0 = e_0 = 1$, we get

$$\pi_k = e_k - \sum_{\ell=0}^{k-1} c_\ell \pi_\ell, \;\; c_\ell = \frac{(e_k, \pi_\ell)}{(\pi_\ell, \pi_\ell)}, \tag{1.18}$$

with $c_\ell \pi_\ell$ being the projection of e_k with respect to π_ℓ. It is noteworthy that the proof by the Gram-Schmidt process has the benefit of being constructive.

1.2.3 Symmetry

Definition 1.16. An absolute continuous measure $\mathrm{d}\lambda(t) = w(t)\mathrm{d}t$ is symmetric (with respect to the origin) if its support interval is $[-\alpha, \alpha]$, $0 < \alpha \leq \infty$, and $w(t) = w(-t)\ \forall t \in \mathbb{R}$.

Theorem 1.17. *([6], Theorem 1.17) If* $\mathrm{d}\lambda$ *is symmetric, then*

$$\pi_k(-t;\mathrm{d}\lambda) = (-1)^k \pi_k(t;\mathrm{d}\lambda),\ \ k = 0, 1, 2, \ldots. \tag{1.19}$$

Hence, π_k *is even or odd depending on the parity of* k.

Proof. Define $\hat{\pi}_k(t) = (-1)^k \pi_k(-t;\mathrm{d}\lambda)$. For $k \neq \ell$, we have

$$\begin{aligned}(\hat{\pi}_k, \hat{\pi}_\ell)_{\mathrm{d}\lambda} &= \int_{-a}^{a} (-1)^k \pi_k(-t)(-1)^\ell \pi_\ell(-t)\mathrm{d}\lambda(t) \\ &= (-1)^{k+\ell} \int_{-a}^{a} \pi_k(-t)\pi_\ell(-t)w(t)\mathrm{d}t.\end{aligned}$$

Setting $-t = \tau$, we have, in view of $w(-\tau) = w(\tau)$,

$$\begin{aligned}(\hat{\pi}_k, \hat{\pi}_\ell)_{\mathrm{d}\lambda} &= (-1)^{k+\ell} \int_{a}^{-a} \pi_k(\tau)\pi_\ell(\tau)w(-\tau)(-\mathrm{d}\tau) \\ &= (-1)^{k+\ell} \int_{-a}^{a} \pi_k(\tau)\pi_\ell(\tau)w(\tau)\mathrm{d}\tau \\ &= (-1)^{k+\ell} (\pi_k, \pi_\ell)_{\mathrm{d}\lambda} \\ &= 0.\end{aligned}$$

Since all $\hat{\pi}_k$ are monic, from Theorem 1.8, we obtain $\hat{\pi}_k(t) = \pi_k(t;\mathrm{d}\lambda)$, which is equivalent to (1.19). □

1.2.4 Zeros

Theorem 1.18. *([6], Theorem 1.19) All zeros of* $\pi_n(\cdot) = \pi_n(\,\cdot\,;\mathrm{d}\lambda)$, $n \geq 1$ *are real, simple and located in the interior of the support interval* $[a, b]$ *of* $\mathrm{d}\lambda$.

Proof. Let t_i, $i = 1, 2, \ldots, n$, be the zeros of π_n. Then at least one of them must be in (a, b), because, if π_n keeps constant sign on (a, b), we have

$$(\pi_n, 1) = \int_a^b [\pi_n(t) \cdot 1]\mathrm{d}\lambda(t) \neq 0,$$

which contradicts that π_n is orthogonal to all polynomials of lower degree.

Now, if we assume that there is a double zero t_s, we define the polynomial

$$r(t) = \frac{\pi_n(t)}{(t-t_s)^2}, \ r \in \mathbb{P}_{n-2},$$

and considering the inner product of π_n with r, we get

$$(\pi_n, r) = \int_a^b \pi_n(t)\frac{\pi_n(t)}{(t-t_s)^2}\mathrm{d}\lambda(t) = \int_a^b \left[\frac{\pi_n(t)}{(t-t_s)}\right]^2 \mathrm{d}\lambda(t) > 0,$$

which again contradicts the orthogonality of π_n to all polynomials of lower degree.

Finally, lets assume that there are ℓ zeros in (a, b) with $\ell < n$. We define $q_{n-\ell} \in \mathbb{P}_{n-\ell}$ such as

$$\pi_n(t)(t-t_1)(t-t_2)\dots(t-t_\ell) = q_{n-\ell}(t)(t-t_1)^2(t-t_2)^2\dots(t-t_\ell)^2,$$

where $q_{n-\ell}$ has no zeros in (a, b). Then

$$(\pi_n, (t-t_1)\dots(t-t_\ell)) = \int_a^b q_{n-\ell}(t)(t-t_1)^2\dots(t-t_\ell)^2\mathrm{d}\lambda(t) \neq 0,$$

which again contradicts the orthogonality of π_n to all polynomials of lower degree. Therefore, we must have that $\ell = n$. □

Before we go to another property of the zeros, we present the Christoffel-Darboux formula.

Theorem 1.19. *([6], Theorem 1.32) Let* $\tilde{\pi}_k(\cdot) = \tilde{\pi}_k(\,\cdot\,; \mathrm{d}\lambda)$ *denote the orthonormal polynomials with respect to the measure* $\mathrm{d}\lambda$*. Then*

$$\sum_{k=0}^{n} \tilde{\pi}_k(x)\tilde{\pi}_k(t) = \sqrt{\beta_{n+1}}\frac{\tilde{\pi}_{n+1}(x)\tilde{\pi}_n(t) - \tilde{\pi}_n(x)\tilde{\pi}_{n+1}(t)}{x-t} \tag{1.20}$$

and

$$\sum_{k=0}^{n} [\tilde{\pi}_k(t)]^2 = \sqrt{\beta_{n+1}}\left[\tilde{\pi}'_{n+1}(t)\tilde{\pi}_n(t) - \tilde{\pi}'_n(t)\tilde{\pi}_{n+1}(t)\right]. \tag{1.21}$$

Proof. From (1.15), we have

$$\sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(t) = (t-\alpha_k)\,\tilde{\pi}_k(t) - \sqrt{\beta_k}\tilde{\pi}_{k-1}(t),$$

that is,

$$(t-\alpha_k)\tilde{\pi}_k(t) = \sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(t) + \sqrt{\beta_k}\tilde{\pi}_{k-1}(t),$$

and multiplying both sides by $\tilde{\pi}_k(x)$, we get

$$(t-\alpha_k)\tilde{\pi}_k(t)\tilde{\pi}_k(x) = \sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(t)\tilde{\pi}_k(x) + \sqrt{\beta_k}\tilde{\pi}_{k-1}(t)\tilde{\pi}_k(x). \tag{1.22}$$

Interchanging x and t in (1.22), we obtain

$$(x-\alpha_k)\tilde{\pi}_k(x)\tilde{\pi}_k(t) = \sqrt{\beta_{k+1}}\tilde{\pi}_{k+1}(x)\tilde{\pi}_k(t) + \sqrt{\beta_k}\tilde{\pi}_{k-1}(x)\tilde{\pi}_k(t). \tag{1.23}$$

Subtracting (1.22) from (1.23), we have

$$\begin{aligned}(x-t)\tilde{\pi}_k(x)\tilde{\pi}_k(t) =& \sqrt{\beta_{k+1}}\left[\tilde{\pi}_{k+1}(x)\tilde{\pi}_k(t) - \tilde{\pi}_k(x)\tilde{\pi}_{k+1}(t)\right] - \\ &- \sqrt{\beta_k}\left[\tilde{\pi}_k(x)\tilde{\pi}_{k-1}(t) - \tilde{\pi}_{k-1}(x)\tilde{\pi}_k(t)\right].\end{aligned}$$

Dividing both sides by $x-t$ and then summing from $k=0$ to $k=n$, gives, as $\pi_{-1}=0$, (1.20). On the other hand, by means of (1.20), we have

$$\begin{aligned}&\sum_{k=0}^{n}\tilde{\pi}_k(x)\tilde{\pi}_k(t) = \sqrt{\beta_{n+1}}\frac{\tilde{\pi}_{n+1}(x)\tilde{\pi}_n(t) - \tilde{\pi}_n(x)\tilde{\pi}_{n+1}(t)}{x-t} \\ &= \sqrt{\beta_{n+1}}\frac{\tilde{\pi}_{n+1}(x)\tilde{\pi}_n(t) - \tilde{\pi}_n(x)\tilde{\pi}_{n+1}(t) + \tilde{\pi}_{n+1}(t)\tilde{\pi}_n(t) - \tilde{\pi}_{n+1}(t)\tilde{\pi}_n(t)}{x-t} \\ &= \sqrt{\beta_{n+1}}\frac{\tilde{\pi}_{n+1}(x)\tilde{\pi}_n(t) - \tilde{\pi}_{n+1}(t)\tilde{\pi}_n(t) - \tilde{\pi}_n(x)\tilde{\pi}_{n+1}(t) + \tilde{\pi}_{n+1}(t)\tilde{\pi}_n(t)}{x-t} \\ &= \sqrt{\beta_{n+1}}\left[\frac{\tilde{\pi}_{n+1}(x)\tilde{\pi}_n(t) - \tilde{\pi}_{n+1}(t)\tilde{\pi}_n(t)}{x-t} - \frac{\tilde{\pi}_n(x)\tilde{\pi}_{n+1}(t) - \tilde{\pi}_{n+1}(t)\tilde{\pi}_n(t)}{x-t}\right],\end{aligned}$$

thus,

$$\begin{aligned}\sum_{k=0}^{n}\tilde{\pi}_k(x)\tilde{\pi}_k(t) =& \sqrt{\beta_{n+1}}\frac{\tilde{\pi}_{n+1}(x)\tilde{\pi}_n(t) - \tilde{\pi}_{n+1}(t)\tilde{\pi}_n(t)}{x-t} \\ &- \sqrt{\beta_{n+1}}\frac{\tilde{\pi}_n(x)\tilde{\pi}_{n+1}(t) - \tilde{\pi}_{n+1}(t)\tilde{\pi}_n(t)}{x-t},\end{aligned}$$

that is,

$$\sum_{k=0}^{n} \tilde{\pi}_k(x)\tilde{\pi}_k(t) = \sqrt{\beta_{n+1}} \left[\frac{\tilde{\pi}_{n+1}(x) - \tilde{\pi}_{n+1}(t)}{x-t} \tilde{\pi}_n(t) - \frac{\tilde{\pi}_n(x) - \tilde{\pi}_n(t)}{x-t} \tilde{\pi}_{n+1}(t) \right].$$

Finally, by taking the limit $x \to t$, we get (1.21). □

Theorem 1.20. *([6], Theorem 1.20) The zeros of $\pi_{n+1}(\cdot)$ alternate with those of $\pi_n(\cdot)$, more specifically,*

$$\tau_{n+1}^{(n+1)} < \tau_n^{(n)} < \tau_n^{(n+1)} < \cdots < \tau_1^{(n)} < \tau_1^{(n+1)}. \tag{1.24}$$

Proof. From (1.21), we obtain

$$\tilde{\pi}'_{n+1}(t)\tilde{\pi}_n(t) - \tilde{\pi}'_n(t)\tilde{\pi}_{n+1}(t) > 0. \tag{1.25}$$

Now lets assume that $\tau_k^{(n+1)}$ and $\tau_{k+1}^{(n+1)}$ are two consecutive zeros of $\tilde{\pi}_{n+1}(t)$. As $\tilde{\pi}_k = \frac{\pi_k}{\|\pi_k\|}$, the zeros of $\tilde{\pi}_k(t)$ and $\pi_k(t)$ are the same. Since all $n+1$ zeros of $\tilde{\pi}_{n+1}(t)$ are real and simple, $\tilde{\pi}'_{n+1}(\tau_k^{(n+1)})$ and $\tilde{\pi}'_{n+1}(\tau_{k+1}^{(n+1)})$ have opposite signs. Hence,

$$\tilde{\pi}'_{n+1}(\tau_k^{(n+1)})\tilde{\pi}'_{n+1}(\tau_{k+1}^{(n+1)}) < 0.$$

Setting in (1.25), $t = \tau_k^{(n+1)}$ and $t = \tau_{k+1}^{(n+1)}$, we get

$$\tilde{\pi}'_{n+1}(\tau_k^{(n+1)})\tilde{\pi}_n(\tau_k^{(n+1)}) > 0 \tag{1.26}$$

and

$$\tilde{\pi}'_{n+1}(\tau_{k+1}^{(n+1)})\tilde{\pi}_n(\tau_{k+1}^{(n+1)}) > 0, \tag{1.27}$$

respectively. By (1.26) and (1.27), we have

$$[\tilde{\pi}'_{n+1}(\tau_k^{(n+1)})\tilde{\pi}_n(\tau_k^{(n+1)})][\tilde{\pi}'_{n+1}(\tau_{k+1}^{(n+1)})\tilde{\pi}_n(\tau_{k+1}^{(n+1)})] > 0,$$

that is,

$$[\tilde{\pi}'_{n+1}(\tau_k^{(n+1)})\tilde{\pi}'_{n+1}(\tau_{k+1}^{(n+1)})][\tilde{\pi}_n(\tau_k^{(n+1)})\tilde{\pi}_n(\tau_{k+1}^{(n+1)})] > 0.$$

As mentioned before, $\tilde{\pi}'_{n+1}(\tau_k^{(n+1)})\tilde{\pi}'_{n+1}(\tau_{k+1}^{(n+1)}) < 0$, hence, we obtain

$$\tilde{\pi}_n(\tau_k^{(n+1)})\tilde{\pi}_n(\tau_{k+1}^{(n+1)}) < 0,$$

which shows that between $\tau_k^{(n+1)}$ and $\tau_{k+1}^{(n+1)}$ there is one zero of $\tilde{\pi}_n$. Given that there n pairs of consecutive zeros of $\tilde{\pi}_{n+1}$ our result is proved. □

1.3 Classical Orthogonal Polynomials

This section contains information from Gautschi [6], Abramowitz and Stegun [1], Szegö [11] and Askey [3].

There is not general accepted definition of classical orthogonal polynomials. In bibliography, classical are considered those satisfying a linear ordinary differential or difference equation and possessing a Rodrigues-type formula,

$$P_n(x) = \frac{c_n}{w(x)} \frac{\mathrm{d}^n}{\mathrm{d}x^n} B(x)^n w(x), \tag{1.28}$$

where $w(x)$ is the weight function, c_n is a real sequence, $B(x)$ satisfies the following relation

$$\lim_{x\to a} B(x)w(x) = \lim_{x\to b} B(x)w(x) = 0,$$

and a, b are such that

$$\int_a^b P_m(x)P_n(x)w(x)\mathrm{d}x = K_{m,n}\delta_{m,n},$$

with $K_{m,n}$ being constants and $\delta_{m,n}$ the Kronecker's delta. Legendre, Chebyshev, Gegenbauer, Jacobi, Laguerre and Hermite polynomials are probably the most widely used and studied classical orthogonal polynomials.

Orthogonal polynomials are used for several reasons in mathematics, and one of their major contribution is in approximation theory. Chebyshev polynomials of the first two kinds are widely used in numerical analysis.

We will now present some of the most commonly used classical orthogonal polynomials, providing their three term recursion relation, the corresponding weight function $w(t)$, the coefficient k_n of the nth degree polynomial leading term, i.e.,

$$p_n(t) = k_n t^n + \dots,$$

as well as the polynomial's L_2 norm,

$$h_n = \|p_n\|_{2,w}^2 = \|p_n\|^2.$$

Legendre Polynomials

The Legendre polynomials are usually denoted as P_n and have the normalization $P(1) = 1$. Polynomials P_n are bounded by 1 in $[-1, 1]$, $k_n = \frac{(2n)!}{2^n(n!)^2}$, $h_n = \frac{1}{n+\frac{1}{2}}$, their weight function is $w(t) = 1$ on the interval $[-1, 1]$ and their recurrence relation is

$$(k+1)P_{k+1}(t) = (2k+1)tP_k(t) - kP_{k-1}(t),$$
$$P_0(t) = 1,\ P_1(t) = t.$$

Chebyshev Polynomials

The notation for the nth-degree Chebyshev polynomials of first kind is T_n. These polynomials are defined by

$$T_n(\cos\theta) = \cos n\theta,\ 0 \le \theta \le \pi, \tag{1.29}$$

so that $T_n(1) = 1,\ k_0 = 1,\ k_n = 2^{n-1},\ n \geq 1,\ h_0 = \pi,\ h_n = \frac{1}{2}\pi,\ n \geq 1$, and their weight function $w(t) = (1-t^2)^{-\frac{1}{2}}$ on the interval $[-1,1]$. Now, note that $|T_n| \leq 1$ on $[-1,1]$, and it is easy to obtain the zeros of T_n, since we need to solve the trigonometric equation

$$T_n(x) = 0,$$

that is,

$$T_n(\cos\theta) = 0,$$

so

$$\theta = \frac{2k-1}{2n}\pi,$$

which leads to

$$x_k^{(n)} = \cos\frac{2k-1}{2n}\pi \text{ for } k = 1, 2, \ldots, n.$$

The importance of Chebyshev polynomials in approximation stems from the following property

$$\|p_n^\circ\|_\infty \geq \|T_n^\circ\|_\infty = \frac{1}{2^{n-1}},\ n \geq 1,\ \forall p_n^\circ \in \mathbb{P}_n^\circ, \tag{1.30}$$

where $\|\cdot\|_\infty$ is the uniform norm $\|u\|_\infty = \max_{-1\leq t\leq 1}|u(t)|$, and $\mathbb{P}_n^\circ$ is the class of monic polynomials of degree n. Evidently, equality stands for $p_n^\circ = T_n^\circ$, where $T_n^\circ = 2^{1-n}T_n,\ n \geq 1$.

The Chebyshev polynomials of the second kind U_n are defined by

$$U_n(\cos\theta) = \frac{\sin(n+1)\theta}{\sin\theta},\ 0 \leq \theta \leq \pi, \tag{1.31}$$

so that $U_n(1) = n+1,\ k_0 = 1,\ k_n = 2^n,\ n \geq 1,\ h_n = \frac{\pi}{2},\ n \geq 0$, and their weight function $w(t) = (1-t^2)^{\frac{1}{2}}$ on the interval $[-1,1]$. Now, replacing the uniform norm with the L_1 norm, we also get an extremal property

$$\|p_n^\circ\|_1 \geq \|U_n^\circ\|_1, \quad n \geq 1, \quad \forall p_n^\circ \in \mathbb{P}_n^\circ,$$

and equality stands for $p_n^\circ = U_n^\circ$, where $U_n^\circ = 2^{-n}U_n$.

Finally, the Chebyshev polynomials of the third and fourth kinds, respectively, are defined by

$$V_n(\cos\theta) = \frac{\cos\left(n+\frac{1}{2}\right)\theta}{\cos\frac{1}{2}\theta}, \quad W_n(\cos\theta) = \frac{\sin\left(n+\frac{1}{2}\right)\theta}{\sin\frac{1}{2}\theta}, \quad 0 \le \theta \le \pi, \tag{1.32}$$

so that $V_n(1) = 1$, $W_n(1) = 2n+1$.

All four Chebyshev polynomials satisfy the same recurrence relation

$$y_{k+1} = 2ty_k - y_{k-1}, \quad k = 1, 2, \ldots. \tag{1.33}$$

Polynomials y_0, y_1, weight functions $w(t)$, leading terms k_n, $n \ge 0$, and norms h_n, $n \ge 0$, of all four Chebyshev polynomials are provided in Table 1.1.

Table 1.1: Chebyshev polynomials

Kind	y_0	y_1	k_0	k_n	h_0	h_n	$w(t)$
T_n	1	t	1	2^{n-1}	π	$\frac{1}{2}\pi$	$(1-t^2)^{-\frac{1}{2}}$
U_n	1	$2t$	1	2^n	$\frac{1}{2}\pi$	$\frac{1}{2}\pi$	$(1-t^2)^{\frac{1}{2}}$
V_n	1	$2t-1$	1	2^n	π	π	$(1-t)^{-\frac{1}{2}}(1+t)^{\frac{1}{2}}$
W_n	1	$2t+1$	1	2^n	π	π	$(1-t)^{\frac{1}{2}}(1+t)^{-\frac{1}{2}}$

Gegenbauer Polynomials

The Gegenbauer polynomials are denoted by $P_n^{(\lambda)}$ and are defined by

$$P_n^{(\lambda)}(t) = \frac{\Gamma\left(\lambda+\frac{1}{2}\right)}{\Gamma(2\lambda)} \frac{\Gamma(n+2\lambda)}{\Gamma\left(n+\lambda+\frac{1}{2}\right)} P_n^{\left(\lambda-\frac{1}{2},\lambda-\frac{1}{2}\right)}(t) \quad \text{if } \lambda \ne 0, \tag{1.34}$$

where $P_n^{(\alpha,\beta)}$ is the Jacobi polynomial which is defined further down and Γ is the Gamma function

$$\Gamma(z) = \int_0^\infty x^{z-1}e^{-x}\mathrm{d}t,$$

defined for $z \in \mathbb{C}$ with positive real part. Special cases are $P_n^{(\frac{1}{2})} = P_n$ and $P_n^{(1)} = U_n$. Note that $P_0^{(\lambda)} = 1$ and

$$\lim_{\lambda\to 0} P_n^{(\lambda)}(t) = 0,$$

but,

$$\lim_{\lambda\to 0} \frac{P_n^{(\lambda)}(t)}{\lambda} = \frac{2}{n}T_n(t),\ n \geq 1.$$

For $\lambda \neq 0$, one has

$$P_n^{(\lambda)}(1) = \binom{n+2\lambda-1}{n},\ n \geq 1,$$

$$k_n = \frac{2^n}{n!}\frac{\Gamma(n+\lambda)}{\Gamma(\lambda)},$$

$$h_n = \frac{2^{1-2\lambda}\Gamma(n+2\lambda)}{n!(n+\lambda)\Gamma^2(\lambda)}\pi,$$

and the weight function is $w(t) = (1-t^2)^{\lambda-\frac{1}{2}}$, where $\lambda > \frac{1}{2}$, on the interval $[-1, 1]$. The three term recurrence relation is

$$(k+1)P_{k+1}^{(\lambda)}(t) = 2(k+\lambda)tP_k^{(\lambda)}(t) - (k+2\lambda-1)P_{k-1}^{(\lambda)}(t),\quad k = 1, 2, \ldots,$$
$$P_0^{(\lambda)}(t) = 1,\ P_1^{(\lambda)}(t) = 2\lambda t.$$

Note again that dividing the above recurrence relation with λ and then taking the $\lim_{\lambda\to 0}$ we will have the three term recurrence relation for the Chebyschev polynomials of first kind.

Jacobi Polynomials

The standard notation for Jacobi polynomials of degree n is $P_n^{(\alpha,\beta)}$. It is normalized by $P_n^{(\alpha,\beta)}(1) = \binom{n+a}{n}$ giving

$$k_n = \frac{1}{2^n}\binom{2n+\alpha+\beta}{n}, \tag{1.35}$$

$$h_n = \frac{2^{\alpha+\beta+1}}{2n+\alpha+\beta+1}\frac{\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{n!\Gamma(n+\alpha+\beta+1)},$$

and the weight function is $w(t) = (1-t)^\alpha(1+t)^\beta$, $\alpha \geq -1$, $\beta \geq -1$, on the interval $[-1,1]$. The three term recurrence relation is

$$\begin{aligned}
&2(k+1)(k+\alpha+\beta+1)(2k+\alpha+\beta)P_{k+1}^{(\alpha,\beta)}(t)\\
&= (2k+\alpha+\beta+1)\left[(2k+\alpha+\beta+2)(2k+\alpha+\beta)t+\alpha^2-\beta^2\right]P_k^{(\alpha,\beta)}(t)\\
&-2(k+\alpha)(k+\beta)(2k+\alpha+\beta+2)P_{k-1}^{(\alpha,\beta)}(t),\ k=1,2,\ldots,\\
&P_0^{(\alpha,\beta)}(t)=1,\ P_1^{(\alpha,\beta)}(t)=\frac{1}{2}(\alpha+\beta+2)t+\frac{1}{2}(\alpha-\beta).
\end{aligned}$$

Note that interchanging the parameters α and β has the following effect

$$P_n^{(\beta,\alpha)}(t) = (-1)^n P_n^{(\alpha,\beta)}(-t). \tag{1.36}$$

Laguerre Polynomials

The Laguerre and generalized Laguerre polynomials are usually denoted by $L_n = L_n^{(0)}$ and $L_n^{(\alpha)}$. They are normalized by

$$L_n^{(\alpha)}(0) = \binom{n+\alpha}{n}, \tag{1.37}$$

and satisfy

$$k_n = \frac{(-1)^n}{n!}, \tag{1.38}$$

$$h_n = \frac{\Gamma(\alpha + n + 1)}{n!}.$$

Their weight functions are $w(t) = e^{-t}$ and $w(t) = t^{\alpha}\mathrm{e}^{-t},\ \alpha > -1$, on the interval $[0, \infty]$ and their three term recurrence relation is

$$\begin{aligned}(k+1)L_{k+1}^{(\alpha)}(t) =&(2k + \alpha + 1 - t)L_k^{(\alpha)}(t) - (k+\alpha)L_{k-1}^{(\alpha)}(t),\ k = 1, 2, \dots, \\ L_0^{(\alpha)}(t) = 1,&\ L_1^{(\alpha)}(t) = \alpha + 1 - t.\end{aligned}$$

Hermite Polynomials

The Hermite polynomials are denoted by H_n and satisfy

$$k_n = 2^n,$$

$$h_n = \sqrt{\pi} 2^n n!,$$

with their weight function to be $w(t) = \mathrm{e}^{-t^2}$ on the interval $[-\infty, \infty]$. The three term recurrence relation is

$$\begin{aligned} H_{k+1}(t) =& 2tH_k(t) - 2kH_{k-1}(t),\ k = 1, 2, \dots, \\ H_0(t) = 1,&\ H_1(t) = 2t. \end{aligned}$$

The following extremal property holds

$$|H_n(t)| \le \mathrm{e}^{t^2/2} \sqrt{2^n n!},\ t \in \mathbb{R}.$$

Finally, the generalized Hermite polynomials are denoted by $H_n^{(\mu)}$ with

$$k_n = 2^n,$$

$$h_n = 2^{2n} \Gamma\left(\left\lfloor \frac{n+2}{2} \right\rfloor\right) \left(\Gamma\left(\left\lfloor \frac{n+1}{2} \right\rfloor\right) + \mu + \frac{1}{2}\right),$$

and the weight function $w(t) = |t|^{2\mu} \mathrm{e}^{-t^2},\ \mu > -\frac{1}{2}$, on the interval $[-\infty, \infty]$.

Remark 1.21. Legendre, Chebyshev and Gegenbauer polynomials are actually special cases of Jacobi polynomials defined for specific values of the coefficients α and β. For example, from (1.34), we can see that Gegenbauer polynomials can be expressed in terms of Jacobi polynomials $P_n^{(\alpha,\beta)}$. This is also shown by the corresponding weight function, that is, the Gegenbauer's weight function can be written as

$$w(t) = (1-t^2)^{\lambda - \frac{1}{2}} = [(1-t)(1+t)]^{\lambda - \frac{1}{2}} = (1-t)^{\lambda - \frac{1}{2}} (1+t)^{\lambda - \frac{1}{2}},$$

which is exactly Jacobi's weight function with $\alpha = \beta = \lambda - \frac{1}{2}$.

We conclude this chapter with the table 1.2, which contains the most widely used weight functions, along with their corresponding recurrence coefficients and their support interval.

Table 1.2: Weight functions and recurrence coefficients for classical orthogonal polynomials.

Name	$w(t)$	Support	α_k	β_0	$\beta_k,\ k \geq 1$
Legendre	1	$[-1,1]$	0	2	$1/\left(4-k^{-2}\right)$
1st Chebyshev	$(1-t^2)^{-1/2}$	$[-1,1]$	0	π	$\frac{1}{2}(k=1), \frac{1}{4}(k \geq 2)$
2nd Chebyshev	$(1-t^2)^{1/2}$	$[-1,1]$	0	$\frac{1}{2}\pi$	$\frac{1}{4}$
3rd Chebyshev	$(1-t)^{-1/2}(1+t)^{1/2}$	$[-1,1]$	$\frac{1}{2}(k=0)$, $0(k>0)$	π	$\frac{1}{4}$
4th Chebyshev	$(1-t)^{1/2}(1+t)^{-1/2}$	$[-1,1]$	$-\frac{1}{2}(k=0)$, $0(k>0)$	π	$\frac{1}{4}$
Gegenbauer	$(1-t^2)^{\lambda-1/2}, \lambda > -\frac{1}{2}$	$[-1,1]$	0	$\sqrt{\pi}\frac{\Gamma\left(\lambda+\frac{1}{2}\right)}{\Gamma(\lambda+1)}$	$\frac{k(k+2\lambda-1)}{4(k+\lambda)(k+\lambda-1)}$
Jacobi	$(1-t)^{\alpha}(1+t)^{\beta},\ \alpha,\beta > -1$	$[-1,1]$	α_k^J	β_0^J	β_k^J
Laguerre	e^{-t}	$[0,\infty]$	$2k+1$	1	k^2
Generalized Laguerre	$t^{\alpha}\mathrm{e}^{-t}, \alpha > -1$	$[0,\infty]$	$2k+\alpha+1$	$\Gamma(1+\alpha)$	$k(k+\alpha)$
Hermite	e^{-t^2}	$[-\infty,\infty]$	0	$\sqrt{\pi}$	$\frac{1}{2}k$
Generalized Hermite	$\lvert t\rvert^{2\mu}\mathrm{e}^{-t^2}, \mu > -\frac{1}{2}$	$[-\infty,\infty]$	0	$\Gamma(\mu+\frac{1}{2})$	$\frac{1}{2}k(k \text{ even })$, $\frac{1}{2}k+\mu(k \text{ odd })$

$$\alpha_k^J = \frac{\beta^2-\alpha^2}{(2k+\alpha+\beta)(2k+\alpha+\beta+2)}^{*},\quad \beta_0^J = \frac{2^{\alpha+\beta+1}\Gamma(\alpha+1)\Gamma(\beta+1)}{\Gamma(\alpha+\beta+1)},\quad \beta_k^J = \frac{4k(k+\alpha)(k+\beta)(k+\alpha+\beta)}{(2k+\alpha+\beta)^2(2k+\alpha+\beta+1)(2k+\alpha+\beta-1)}^{+}.$$

* If $k=1$, the last factors in the numerator and denominator of β_1^J should be (must be, if $\alpha+\beta+1=0$) cancelled.

+ If $k=0$, the common factor $\alpha+\beta$ in the numerator and denominator of α_0^J should be (must be,(if $\alpha+\beta=0$) cancelled.

Chapter 2

Gauss Quadrature Formula

This chapter is dedicated to Gauss quadrature formula, which is an optimal formula with very interesting and useful properties.

2.1 Numerical Integration

Finding the value of a definite integral is not always an easy task and some times it is not even possible. This leads us to numerical integration, which allows to find approximately the value of an integral. A classical way for constructing a numerical integration formula is by means of interpolation. The idea is to interpolate the function to be integrated with a polynomial and then calculate the integral of the interpolating polynomial.

Lets assume that we want to approximate the integral

$$\int_a^b f(t)\mathrm{d}t.$$

We interpolate f with a polynomial $p \in \mathbb{P}_n$ at the $n+1$ distinct points

$t_0 < t_1 < \cdots < t_n$. Considering Lagrange's polynomials,

$$\ell_k(t) = \prod_{\substack{\ell=0 \\ \ell \neq k}}^{n} \frac{t - t_\ell}{t_k - t_\ell},$$

where

$$\ell_k(t_i) = \delta_{ki} = \begin{cases} 0 & \text{if } k \neq i, \\ 1 & \text{if } k = i, \end{cases}$$

we have

$$p_n(f;t) = \sum_{k=0}^{n} \ell_k(t) f\left(t_k\right),$$

with interpolation error

$$r_{n+1}(f;t) = \prod_{k=0}^{n} \left(t - t_k\right) \frac{f^{(n+1)}(\xi)}{(n+1)!}, \; a < \xi = \xi(t) < b,$$

under the assumption that $f \in C^{n+1}[a,b]$. Hence,

$$f(t) = p_n(f;t) + r_{n+1}(f;t),$$

and by integrating both sides we obtain

$$\begin{aligned} \int_a^b f(t)\mathrm{d}t &= \int_a^b p_n(f;t)\mathrm{d}t + \int_a^b r_{n+1}(f;t)\mathrm{d}t \\ &= \int_a^b \sum_{k=0}^{n} \ell_k(t) f\left(t_k\right) \mathrm{d}t + \int_a^b r_{n+1}(f;t)\mathrm{d}t \\ &= \sum_{k=0}^{n} \left[\int_a^b \ell_k(t)\mathrm{d}t\right] f(t_k) + \int_a^b r_{n+1}(f;t)\mathrm{d}t \\ &= \sum_{k=0}^{n} A_k f(t_k) + E_{n+1}(f), \end{aligned}$$

where

$$A_k = \int_a^b \ell_k(t)\mathrm{d}t$$

and

$$E_{n+1}(f) = \int_a^b \prod_{k=0}^{n} (t - t_k)\, \frac{f^{(n+1)}(\xi)}{(n+1)!} \mathrm{d}t.$$

For example, applying the simplest kind of interpolation, for $n = 1$, we have $t_0 = a$, $t_1 = b$, with

$$\ell_0(t) = \frac{t - t_1}{t_0 - t_1} = \frac{t - b}{a - b} = \frac{b - t}{b - a}$$

and

$$\ell_1(t) = \frac{t - t_0}{t_1 - t_0} = \frac{t - a}{b - a},$$

thus,

$$A_0 = \int_a^b \ell_0(t)\mathrm{d}t = \int_a^b \frac{b - t}{b - a}\mathrm{d}t = \frac{b - a}{2}$$

and

$$A_1 = \int_a^b \ell_1(t)\mathrm{d}t = \int_a^b \frac{t - a}{b - a}\mathrm{d}t = \frac{b - a}{2}.$$

Hence,

$$\begin{aligned}\int_a^b f(t)\mathrm{d}t &= \int_a^b p_1(t)\mathrm{d}t + E_2(f) \\ &= \sum_{k=0}^{1} A_k f(t_k) + E_2(f),\end{aligned}$$

that is,

$$\int_a^b f(t)\mathrm{d}t = \frac{b - a}{2}[f(a) + f(b)] + E_2(f). \tag{2.1}$$

Formula (2.1) is the well-known Trapezoidal rule. For the error term, we have

$$E_2(f) = \int_a^b (t - a)(b - t)\frac{f''(\xi(t))}{2}\mathrm{d}t.$$

From the Mean Value Theorem for integrals, we recall that since $(t-a)(b-t)$ has constant sign on the interval $[a, b]$,

$$E_2(f) = \int_a^b (t - a)(b - t)\frac{f''(\xi(t))}{2}\mathrm{d}t = -\frac{f''(\xi)}{12}(b - a)^3,\ \xi \in [a, b].$$

Since the length of $[a, b]$ is not always small, we apply formula (2.1) on each of the subintervals of the decomposition

$$a = x_0 < x_1 < \ldots < x_{n-1} < x_n = b,\ h = \frac{b-a}{n},\ x_k = a + kh,\ k = 0, 1, \ldots, n,$$

and we obtain

$$\int_{x_k}^{x_{k+1}} f(t)\mathrm{d}t = \frac{h}{2}[f(x_k) + f(x_{k+1})] - \frac{1}{12}h^3 f''(\xi_k),\ x_k < \xi_k < x_{k+1},$$

which added, for $k = 0, 1, \ldots, n-1$, gives

$$\int_a^b f(t)\mathrm{d}t = h\left[\frac{1}{2}f(x_0) + f(x_1) + \ldots + f(x_{n-1}) + \frac{1}{2}f(x_n)\right] - \frac{1}{12}h^3 \sum_{k=0}^{n-1} f''(\xi_k). \tag{2.2}$$

Formula (2.2) is called the composite Trapezoidal rule.

If f is smooth enough and the interval $[a, b]$ is finite, a simple integration rule such as the composite Trapezoidal rule is sufficient in order to approximate the integral. Complications arise if f has an integrable singularity on $[a, b]$, in which case we write the integral in the form

$$\int_a^b f(t)w(t)\mathrm{d}t,$$

where w is a positive or at least nonnegative weight function, assumed integrable over (a, b), and including the singularity. The interval (a, b) may be finite or infinite and if (a, b) is infinite it is required that all moments of the weight function

$$\mu_r = \int_a^b t^r w(t)\mathrm{d}t,\ r = 0, 1, \ldots,$$

exist and are finite. We assume that f is integrable with respect to the weight function w, that is,

$$\int_a^b f(t)w(t)\mathrm{d}t < \infty.$$

Again, the idea is to integrate the polynomial interpolating $f(t)$. Let

$$a = \tau_1 < \tau_2 < \cdots < \tau_{n-1} < \tau_n = b$$

be a decomposition of $[a, b]$ and $p_{n-1}(f; \tau_1, \tau_2, \ldots, \tau_n, t)$ the polynomial interpolating $f(t)$ at these points, thus,

$$f(t) = p_{n-1}(f; t) + r_n(f; t).$$

Using Lagrange polynomials, we obtain

$$p_{n-1}(f; t) = \sum_{k=1}^{n} \ell_k(t) f\left(\tau_k\right),$$

where

$$\ell_k(t) = \prod_{\substack{\ell=1 \\ \ell \neq k}}^{n} \frac{t - \tau_\ell}{\tau_k - \tau_\ell}$$

and

$$r_n(f; t) = \prod_{k=1}^{n} \left(t - \tau_k\right) \frac{f^{(n)}(\xi)}{n!}, \; a < \xi = \xi(t) < b,$$

assuming that $f \in C^n[a, b]$. Hence,

$$f(t) = p_{n-1}(f; t) + r_n(f; t).$$

Multiplying both sides of the above relation with $w(t)$ and then integrating, we have

$$\begin{aligned}
\int_a^b f(t) w(t) \mathrm{d}t &= \int_a^b p_{n-1}(f; t) w(t) \mathrm{d}t + \int_a^b r_n(f; t) w(t) \mathrm{d}t \\
&= \int_a^b \sum_{k=1}^{n} \ell_k(t) f\left(\tau_k\right) w(t) \mathrm{d}t + \int_a^b r_n(f; t) w(t) \mathrm{d}t \\
&= \sum_{k=1}^{n} \left[\int_a^b \ell_k(t) w(t) \mathrm{d}t\right] f\left(\tau_k\right) + \int_a^b r_n(f; t) w(t) \mathrm{d}t,
\end{aligned}$$

which leads to the formula

$$\int_a^b f(t)w(t)\mathrm{d}t = \sum_{k=1}^{n} w_k f(\tau_k) + R_n(f), \tag{2.3}$$

where

$$w_k = \int_a^b \ell_k(t)w(t)\mathrm{d}t = \int_a^b \prod_{\substack{\ell=1 \\ \ell\neq k}}^{n} \frac{t-\tau_\ell}{\tau_k-\tau_\ell} w(t)\mathrm{d}t \tag{2.4}$$

and

$$R_n(f) = \int_a^b r_n(f;t)w(t)\mathrm{d}t. \tag{2.5}$$

Formula (2.3) is called an interpolatory formula with a weight function, τ_k are the nodes and w_k the weights of the formula.

From the theory of interpolation we know that if $f \in \mathbb{P}_{n-1}$, then

$$p_{n-1}(f;t) = f(t),\ t \in [a,b],$$

therefore,

$$r_n(f;t) = 0 \ \ \forall f \in \mathbb{P}_{n-1},$$

and as a result

$$R_n(f) = 0 \ \ \forall f \in \mathbb{P}_{n-1}.$$

Definition 2.1. A quadrature formula has degree of exactness d if and only if the quadrature error is zero for every polynomial of degree $\leq d$, and there is a polynomial of degree $d+1$ for which the error is different than zero.

Hence, formula (2.3) has degree of exactness, at least, $n-1$.

Remark 2.2. The case $w(t) = 1$ on $[-1,1]$, with the τ_k being equally spaced in $[-1,1]$, was alluded to by Newton in 1687, and a few years later Cotes constructed it. By extension, formula (2.3) is sometimes called generalized Newton-Cotes formula with a weight function.

Remark 2.3. Trapezoidal rule (2.1) is a special case of formula (2.3) with $w(t) = 1$.

Definition 2.4. A n-point quadrature formula is called interpollatory if it has degree of exactness $d = n - 1$.

2.2 Gauss Quadrature Formula

As already mentioned, given a set of n distinct points, it is always possible to construct a quadrature formula of type (2.3) with degree of exactness $d = n - 1$. The question that naturally arises is if there is an n-point quadrature formula of type (2.3) with degree of exactness greater than $n-1$. The answer to this question will be given by Jacobi's theorem. Let

$$\omega_n(t) = \prod_{k=1}^{n}(t - \tau_k), \tag{2.6}$$

be the so-called node polynomial.

Theorem 2.5. *([5], Theorem 3.2.1) Given an integer k with $0 \leq k \leq n$, the quadrature formula* (2.3) *has degree of exactness $d = n - 1 + k$ if and only if both of the following conditions are satisfied.*

(a) The formula (2.3) *is interpolatory.*

(b) The node polynomial ω_n satisfies

$$\int_a^b \omega_n(t)p(t)w(t)\mathrm{d}t = 0 \quad \forall p \in \mathbb{P}_{k-1}.$$

Before we proceed with the proof of Theorem 2.5, it is interesting to note that condition (b) imposes that ω_n is orthogonal to all polynomials of degree $\leq k-1$ relative to the weight function w. Since $w(t) \geq 0$, we necessarily have $k \leq n$, otherwise ω_n would be orthogonal to itself. Thus, $k = n$ is the maximum value that k can take and this leads to maximum degree of exactness $d_{\max} = 2n-1$, in other words, $\omega_n = \pi_n(\,\cdot\,; w)$, that is, ω_n is the nth-degree orthogonal polynomial relative to the weight function w. This optimal formula is called Gauss quadrature formula associated with the weight function w.

Remark 2.6. The nodes τ_k of Gauss quadrature formula are the zeros of $\pi_n(\,\cdot\,; w)$ and the weights are given by (2.4).

Remark 2.7. The optimal formula was first presented by Gauss in 1814, for the special case $w(t) = 1$ on $[-1, 1]$, and it was extended to more general weight functions by Christoffel in 1877. It is, therefore, also referred to as the Gauss-Christoffel quadrature formula.

Proof. Initially, taking into account that formula (2.3) has degree of exactness $n-1+k,\ k \geq 0$, we conclude that it has degree of exactness at least $n-1$, that is, formula (2.3) is interpolatory and (a) is true. Moreover, under this assumption, formula (2.3) will integrate exactly polynomials of degree $n-1+k,\ k = 0, 1, \ldots, n$, and since $\omega_n \in \mathbb{P}_n$ and $p \in \mathbb{P}_{k-1}$, we have $\omega_n p \in \mathbb{P}_{n-1+k}$, hence,

$$\int_a^b \omega_n(t) p(t) w(t) \mathrm{d}t = \sum_{k=1}^{n} \omega_n(\tau_k) p(\tau_k) w_k.$$

As the $\tau_k,\ k = 1, 2, \ldots, n$, are zeros of ω_n, we have

$$\int_a^b \omega_n(t) p(t) w(t) \mathrm{d}t = \sum_{k=1}^{n} \omega_n(\tau_k) p(\tau_k) w_k = 0,$$

that is, (b) is true.

On the other hand, if (a) and (b) hold true, we need to show that for every $p \in \mathbb{P}_{n-1+k}$, we have $E_n(p) = 0$, that is, formula (2.3) has degree of exactness $n - 1 + k$. Indeed, considering $p \in \mathbb{P}_{n-1+k}$, and dividing p by ω_n, we get

$$p = \omega_n q + r, \;\; q \in \mathbb{P}_{k-1}, \;\; r \in \mathbb{P}_{n-1}, \tag{2.7}$$

hence,

$$\begin{aligned}\int_a^b p(t)w(t)\mathrm{d}t &= \int_a^b [\omega_n(t)q(t) + r(t)]w(t)\mathrm{d}t \\ &= \int_a^b \omega_n(t)q(t)w(t)\mathrm{d}t + \int_a^b r(t)w(t)\mathrm{d}t.\end{aligned}$$

Now, using (b) and the fact that $q \in \mathbb{P}_{n-1}$, we obtain

$$\int_a^b \omega_n(t)q(t)w(t)\mathrm{d}t = 0.$$

Since $r \in \mathbb{P}_{n-1}$, by means of (a), we have $E_n(r) = 0$, thus,

$$\int_a^b p(t)w(t)\mathrm{d}t = \int_a^b r(t)w(t)\mathrm{d}t = \sum_{k=1}^n r(\tau_k)w_k,$$

and as $r = p - \omega_n q$,

$$\begin{aligned}\int_a^b p(t)w(t)\mathrm{d}t &= \sum_{k=1}^n [p(\tau_k) - \omega_n(\tau_k)q(\tau_k)]w_k \\ &= \sum_{k=1}^n p(\tau_k)w_k - \sum_{k=1}^n \omega_n(\tau_k)q(\tau_k)w_k.\end{aligned}$$

As $\omega_n(\tau_k) = 0$, we finally obtain

$$\int_a^b p(t)w(t)\mathrm{d}t = \sum_{k=1}^n p(\tau_k)w_k,$$

that is, $E_n(p) = 0$. □

In order to denote the superiority of Gauss quadrature formula, we present a simple but interesting example ([5], Example pp. 172-174).

We consider the case of $n = 2$ and the weight function $w(t) = t^{-1/2}$ on the interval $[0, 1]$. Initially, we consider the Newton-Cotes formula. Nodes will be at the end points of $[0, 1]$ and the formula is

$$\int_0^1 f(t)t^{-1/2}\mathrm{d}t = w_1^{\mathrm{NC}} f(0) + w_2^{\mathrm{NC}} f(1).$$

From Lagrange's polynomials we obtain

$$\ell_1(t) = \frac{t-1}{0-1} = 1-t,\ \ell_2(t) = \frac{t-0}{1-0} = t,$$

and using (2.4), we compute the weights

$$\begin{aligned} w_1^{\mathrm{NC}} &= \int_0^1 \ell_1(t)t^{-1/2}\mathrm{d}t = \int_0^1 (1-t)t^{-1/2}\mathrm{d}t = \int_0^1 \left(t^{-1/2} - t^{1/2}\right)\mathrm{d}t \\ &= \left(2t^{1/2} - \frac{2}{3}t^{3/2}\right)\Big|_0^1 = \frac{4}{3}, \end{aligned}$$

and

$$w_2^{\mathrm{NC}} = \int_0^1 \ell_2(t)t^{-1/2}\mathrm{d}t = \int_0^1 tt^{-1/2}\mathrm{d}t = \int_0^1 t^{1/2}\mathrm{d}t = \frac{2}{3}\ t^{3/2}\big|_0^1 = \frac{2}{3},$$

thus,

$$\int_0^1 f(t)t^{-1/2}\mathrm{d}t = \frac{2}{3}(2f(0) + f(1)) + R_2^{\mathrm{NC}}(f). \tag{2.8}$$

In order to construct the Gauss formula, we need to find the nodes and the weights. Considering

$$\pi_2(t) = t^2 - c_1 t + c_2,$$

to be the orthogonal polynomial of degree two, relative to the weight function $w(t) = t^{-1/2}$, the nodes can be obtained by its roots. We will first define constants c_1 and c_2, using the fact that π_2 is orthogonal to $1 \in \mathbb{P}_0$ and $t \in \mathbb{P}_1$. Indeed,

$$\begin{aligned}
0 &= \int_0^1 \pi_2(t)t^{-1/2}\mathrm{d}t = \int_0^1 (t^2 - c_1 t + c_2)t^{-1/2}\mathrm{d}t \\
&= \int_0^1 \left(t^{3/2} - c_1 t^{1/2} + c_2 t^{-1/2}\right)\mathrm{d}t = \left(\frac{2}{5}t^{5/2} - \frac{2}{3}c_1 t^{3/2} + 2c_2 t^{1/2}\right)\Big|_0^1 \\
&= \frac{2}{5} - \frac{2}{3}c_1 + 2c_2,
\end{aligned}$$

and

$$\begin{aligned}
0 &= \int_0^1 \pi_2(t)tt^{-1/2}\mathrm{d}t = \int_0^1 (t^2 - c_1 t + c_2)t^{1/2}\mathrm{d}t \\
&= \int_0^1 \left(t^{5/2} - c_1 t^{3/2} + c_2 t^{1/2}\right)\mathrm{d}t = \left(\frac{2}{7}t^{7/2} - \frac{2}{5}c_1 t^{5/2} + \frac{2}{3}c_2 t^{3/2}\right)\Big|_0^1 \\
&= \frac{2}{7} - \frac{2}{5}c_1 + \frac{2}{3}c_2,
\end{aligned}$$

which leads to the linear system

$$\begin{aligned}
\frac{1}{3}c_1 - c_2 &= \frac{1}{5}, \\
\frac{1}{5}c_1 - \frac{1}{3}c_2 &= \frac{1}{7}.
\end{aligned}$$

Multiplying the first relation by $\frac{1}{3}$ and subtracting the second from the product, we find

$$\frac{1}{3}\left(\frac{1}{3}c_1 - c_2\right) - \frac{1}{5}c_1 + \frac{1}{3}c_2 = \frac{1}{15} - \frac{1}{7},$$

that is,

$$\left(\frac{1}{9} - \frac{1}{5}\right)c_1 = \frac{7-15}{105}$$

and

$$-\frac{4}{45}c_1 = -\frac{8}{105},$$

so, finally, $c_1 = \frac{6}{7}$, and using this, we have $c_2 = \frac{3}{35}$. Hence,

$$\pi_2(t) = t^2 - \frac{6}{7}t + \frac{3}{35}.$$

Therefore,

$$\tau_1 = \frac{1}{7}\left(3 - 2\sqrt{\frac{6}{5}}\right) = 0.1155871100,$$
$$\tau_2 = \frac{1}{7}\left(3 + 2\sqrt{\frac{6}{5}}\right) = 0.7415557471.$$

In order to find w_1^{G} and w_2^{G}, instead of (2.4), we will use the fact that the 2-point Gauss formula has degree of exactness $d^G = 3$, hence, the formula will be exact for $f(t) = 1$ and $f(t) = t$, which yields

$$\int_0^1 t^{-1/2}\mathrm{d}t = w_1^{\mathrm{G}} + w_2^{\mathrm{G}},$$
$$\int_0^1 tt^{-1/2}\mathrm{d}t = \tau_1 w_1^{\mathrm{G}} + \tau_2 w_2^{\mathrm{G}},$$

thus,

$$w_1^{\mathrm{G}} + w_2^{\mathrm{G}} = 2,$$
$$\tau_1 w_1^{\mathrm{G}} + \tau_2 w_2^{\mathrm{G}} = \frac{2}{3}.$$

Multiplying the first relation by τ_1 and subtracting the second from the product, we find

$$\tau_1(w_1^{\mathrm{G}} + w_2^{\mathrm{G}}) - \tau_1 w_1^{\mathrm{G}} - \tau_2 w_2^{\mathrm{G}} = 2\tau_1 - \frac{2}{3},$$

which leads to

$$(\tau_1 - \tau_2)w_2^{\mathrm{G}} = 2\tau_1 - \frac{2}{3},$$

that is,

$$w_2^{\mathrm{G}} = \frac{2\tau_1 - \frac{2}{3}}{\tau_1 - \tau_2}.$$

Similarly, multiplying the first relation by τ_2 and subtracting the second from the product, gives

$$w_1^{\mathrm{G}} = \frac{2\tau_2 - \frac{2}{3}}{\tau_2 - \tau_1}.$$

Substituting now the value of τ_1 and τ_2, we obtain

$$w_1^{\mathrm{G}} = 1 + \frac{1}{3}\sqrt{\frac{5}{6}} = 1.3042903097,$$
$$w_2^{\mathrm{G}} = 1 - \frac{1}{3}\sqrt{\frac{5}{6}} = 0.6957096903,$$

thus, the Gauss formula takes the form

$$\begin{aligned}\int_0^1 f(t)t^{-1/2}\mathrm{d}t = &\left(1 + \frac{1}{3}\sqrt{\frac{5}{6}}\right) f\left(\frac{1}{7}\left(3 - 2\sqrt{\frac{6}{5}}\right)\right) \\ &+ \left(1 - \frac{1}{3}\sqrt{\frac{5}{6}}\right) f\left(\frac{1}{7}\left(3 + 2\sqrt{\frac{6}{5}}\right)\right) + R_2^{\mathrm{G}}(f).\end{aligned} \tag{2.9}$$

Now, lets try to approximate the integral

$$I = \int_0^1 \cos\left(\frac{1}{2}\pi t\right) t^{-1/2}\mathrm{d}t.$$

For its exact value, we consider the Fresnel integral (cf. [1], Section 7),

$$C(z) = \int_0^z \cos\left(\frac{\pi}{2}s^2\right)\mathrm{d}s = \sum_{n=0}^{\infty} \frac{(-1)^n(\pi/2)^{2n}}{(2n)!(4n+1)} z^{4n+1}.$$

Using the change of variables $s = t^{1/2}$, $\mathrm{d}s = \frac{1}{2}t^{-1/2}\mathrm{d}t$, we have

$$C(z) = \frac{1}{2}\int_0^z \cos\left(\frac{\pi}{2}t\right) t^{-1/2}\mathrm{d}t,$$

and setting $z = 1$,

$$C(1) = \frac{1}{2}\int_0^1 \cos\left(\frac{\pi}{2}t\right) t^{-1/2}\mathrm{d}t = \frac{1}{2}I,$$

thus,

$$I = 2C(1) = 1.5597868008\ldots.$$

Using first the Newton-Cotes formula (2.8), we obtain

$$I^{\mathrm{NC}} = \frac{4}{3} = 1.333\ldots,$$

while using the Gauss formula (2.9), we get

$$I^{\mathrm{G}} = 1.2828510665 + 0.2747384931 = 1.5575895596,$$

with respective errors

$$R_2^{\mathrm{NC}} = 0.2264534674\ldots,$$

$$R_2^{\mathrm{G}} = 0.0021972412\ldots,$$

showing indeed the superiority of Gauss formula.

2.3 Properties of Gauss quadrature formula

Considering the n-point Gauss formula (2.3), in this section we present the most important of its properties (cf. [2], [5] and [7]).

(i) All nodes τ_k, are real, distinct and contained in (a, b). This is a classical property of orthogonal polynomials, and its proof is given in Theorem 1.18.

(ii) All weights w_k are positive. Considering ℓ_j to be the Lagrange polynomial, Stieltjes observed that formula (2.3) is exact for $\ell_j^2 \in \mathbb{P}_{2n-2}$. Since $w(t)$ and $\ell_j^2(t)$ are positive, we have

$$\int_a^b \ell_j^2(t) w(t) \mathrm{d}t > 0.$$

Then,

$$\int_a^b \ell_j^2(t)w(t)\mathrm{d}t = \sum_{k=1}^{n} w_k \ell_j^2(\tau_k) = \sum_{k=1}^{n} w_k \delta_{jk}^2,\ j = 1, 2, \ldots, n,$$

where δ_{jk} is the Kronecker's delta. Therefore, $w_k > 0$.

(iii) Gauss formula converges for continuous functions in $[a, b]$, that is, if $f \in C[a, b]$, then $R_n(f) \to 0$ as $n \to \infty$. For the proof, we use Weierstrass approximation theorem, which implies that if $\hat{p}_{2n-1}$ is the best approximation of f in $[a, b]$ from space $\mathbb{P}_{2n-1}$, then

$$\lim_{n\to\infty} \|f - \hat{p}_{2n-1}\|_\infty = 0.$$

Since $\hat{p}_{2n-1} \in \mathbb{P}_{2n-1}$, we know that $R_n(\hat{p}_{2n-1}) = 0$, thus, given that $w(t)$ and w_k, $k = 1, 2, \ldots, n$, are positive

$$\begin{aligned}
|R_n(f)| &= |R_n(f) - R_n(\hat{p}_{2n-1})| = |R_n(f - \hat{p}_{2n-1})| \\
&= \left| \int_a^b [f(t) - \hat{p}_{2n-1}(t)]\, w(t)\mathrm{d}t - \sum_{k=1}^{n} w_k [f(\tau_k) - \hat{p}_{2n-1}(\tau_k)] \right| \\
&\le \int_a^b |f(t) - \hat{p}_{2n-1}(t)|\, w(t)\mathrm{d}t + \sum_{k=1}^{n} w_k |f(\tau_k) - \hat{p}_{2n-1}(\tau_k)| \\
&\le \|f - \hat{p}_{2n-1}\|_\infty \left[\int_a^b w(t)\mathrm{d}t + \sum_{k=1}^{n} w_k \right].
\end{aligned}$$

Because $1 = t^0 \in \mathbb{P}_0$, Gauss formula will be exact for $f(t) = 1$, hence,

$$\int_a^b w(t)\mathrm{d}t = \int_a^b t^0 w(t)\mathrm{d}t = \sum_{k=1}^{n} w_k,$$

thus,

$$\begin{aligned}
|R_n(f)| &\le 2 \left(\int_a^b w(t)\mathrm{d}t \right) \|f - \hat{p}_{2n-1}\|_\infty \\
&= 2\mu_0 \|f - \hat{p}_{2n-1}\|_\infty,
\end{aligned}$$

where μ_0 is given by (1.1). From Weierstrass approximation theorem, we have

$$|R_n(f)| \leq 2\mu_0 \left\| f - \hat{p}_{2n-1} \right\|_\infty \to 0, \text{ as } n \to \infty.$$

(iv) The nodes of the $(n+1)$-point formula alternate with those of the n-point formula, more specifically,

$$\tau_{n+1}^{(n+1)} < \tau_n^{(n)} < \tau_n^{(n+1)} < \cdots < \tau_1^{(n)} < \tau_1^{(n+1)}.$$

This is another well-known property of orthogonal polynomials, and its proof is given in Theorem 1.20.

(v) The next property arises, once again, from orthogonal polynomials, in particular, from their three term recurrence relation, Theorem 1.9. Considering $\pi_k(\cdot) = \pi_k(\,\cdot\,; w)$ to be the kth degree orthogonal polynomial, with respect to the weight function $w(t)$, there are coefficients α_k and β_k such that

$$\begin{aligned} \pi_{k+1}(t) &= (t - \alpha_k)\, \pi_k(t) - \beta_k \pi_{k-1}(t), \;\; k = 0, 1, 2 \ldots, \\ \pi_0(t) &= 1, \quad \pi_{-1}(t) = 0, \end{aligned}$$

where α_k and β_k are defined in (1.8) and (1.9), respectively, and $\beta_0 = \int_a^b w(t)\mathrm{d}t = \mu_0$. Let now $J_n(w)$ be the nth-order Jacobi matrix defined in Definition 1.11, that is,

$$J_n = J_n(w) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & 0 & \ldots & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \ldots & \alpha_{n-1} \end{bmatrix}.$$

In Theorem 1.12, we proved that the eigenvalues of J_n are the zeros of $\tilde{\pi}_n$, i.e., the nodes of n-point Gauss formula. We will now prove that we can express the weights of the Gauss formula in terms of J_n's normalized eigenvectors. In Theorem 1.12, we saw that

$$\tilde{\pi}(\tau_k^{(n)}) = \left[\tilde{\pi}_0(\tau_k^{(n)}), \tilde{\pi}_1(\tau_k^{(n)}), \ldots, \tilde{\pi}_{n-1}(\tau_k^{(n)})\right]^T$$

is the k-eigenvector of J_n. Thus,

$$v_k = \frac{\tilde{\pi}(\tau_k^{(n)})}{\left\|\tilde{\pi}(\tau_k^{(n)})\right\|_2} = \frac{\tilde{\pi}(\tau_k^{(n)})}{\left(\sum_{j=0}^{n-1}\left[\tilde{\pi}_j(\tau_k^{(n)})\right]^2\right)^{1/2}}, \tag{2.10}$$

is the corresponding normalized eigenvector and $\|\cdot\|_2$ is the euclidean norm on $\mathbb{R}^n$. Considering now (2.10) in vector form

$$\begin{bmatrix} v_{k,1} \\ v_{k,2} \\ \vdots \\ v_{k,n-1} \end{bmatrix} = \frac{1}{\left(\sum_{j=0}^{n-1}\left[\tilde{\pi}_j(\tau_k^{(n)})\right]^2\right)^{1/2}} \begin{bmatrix} \tilde{\pi}_0(\tau_k^{(n)}) \\ \tilde{\pi}_1(\tau_k^{(n)}) \\ \vdots \\ \tilde{\pi}_{n-1}(\tau_k^{(n)}) \end{bmatrix},$$

and comparing the first component on each side, we obtain

$$v_{k,1} = \frac{\tilde{\pi}_0(\tau_k^{(n)})}{\left(\sum_{j=0}^{n-1}\left[\tilde{\pi}_j(\tau_k^{(n)})\right]^2\right)^{1/2}}.$$

Thus,

$$\frac{1}{\tilde{\pi}_0(\tau_k^{(n)})} v_{k,1} = \frac{1}{\left(\sum_{j=0}^{n-1}\left[\tilde{\pi}_j(\tau_k^{(n)})\right]^2\right)^{1/2}},$$

and since, from (1.15), $\tilde{\pi}_0\,(t) = \frac{1}{\sqrt{\beta_0}}$, after squaring the above relation, we get

$$\beta_0 v_{k,1}^2 = \frac{1}{\sum_{j=0}^{n-1}\left[\tilde{\pi}_j(\tau_k^{(n)})\right]^2}. \tag{2.11}$$

On the other hand, since $\tilde{\pi}_i\tilde{\pi}_j \in \mathbb{P}_{2n-2},\ i,j = 0,1,\ldots,n-1$, the n-point Gauss formula will integrate exactly $\tilde{\pi}_i\tilde{\pi}_j$. Thus,

$$\int_a^b \tilde{\pi}_i(t)\tilde{\pi}_j(t)w(t)\mathrm{d}t = \sum_{k=1}^{n} w_k\tilde{\pi}_i(\tau_k)\tilde{\pi}_j(\tau_k), \quad i,j = 0,1,\ldots,n-1. \tag{2.12}$$

By definition, $\tilde{\pi}_i, \tilde{\pi}_j$ are orthonormal, with respect to the weight function $w(t)$, hence,

$$\int_a^b \tilde{\pi}_i(t)\tilde{\pi}_j(t)w(t)\mathrm{d}t = (\tilde{\pi}_i, \tilde{\pi}_j) = \delta_{ij}, \quad i,j = 0,1,\ldots,n-1, \tag{2.13}$$

therefore, from (2.12) and (2.13), we have

$$\sum_{k=1}^{n} w_k\tilde{\pi}_i(\tau_k)\tilde{\pi}_j(\tau_k) = \delta_{ij}, \quad i,j = 0,1,\ldots,n-1,$$

and in matrix form

$$P^T W P = I, \tag{2.14}$$

where

$$W = \begin{bmatrix} w_1 & 0 & \cdots & 0 \\ 0 & w_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & w_n \end{bmatrix}$$

and

$$P = \begin{bmatrix} \tilde{\pi}_0(\tau_1^{(n)}) & \tilde{\pi}_1(\tau_1^{(n)}) & \cdots & \tilde{\pi}_{n-1}(\tau_1^{(n)}) \\ \tilde{\pi}_0(\tau_2^{(n)}) & \tilde{\pi}_1(\tau_2^{(n)}) & \cdots & \tilde{\pi}_{n-1}(\tau_2^{(n)}) \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{\pi}_0(\tau_n^{(n)}) & \tilde{\pi}_1(\tau_n^{(n)}) & \cdots & \tilde{\pi}_{n-1}(\tau_n^{(n)}) \end{bmatrix}.$$

In (ii), we proved that the w_k are positive, therefore, W is invertible and from (2.14),

$$\det(P^T W P) = \det(I) = 1,$$

thus,

$$\det(P^T)\det(W)\det(P) = 1,$$

hence,

$$\det(P) \neq 0,\ \det(P^T) \neq 0,$$

and this yields that P and P^T are also invertible. From (2.14) we have

$$WP = \left(P^T\right)^{-1},$$

therefore,

$$W = (P^T)^{-1}P^{-1} = (PP^T)^{-1},$$

which is equivalent to

$$W^{-1} = PP^T,$$

and since

$$W^{-1} = \begin{bmatrix} \frac{1}{w_1} & 0 & \cdots & 0 \\ 0 & \frac{1}{w_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{w_n} \end{bmatrix},$$

we have

$$\frac{1}{w_k} = \sum_{j=0}^{n-1} \left[\tilde{\pi}_j(\tau_k^{(n)})\right]^2,$$

which leads to

$$w_k = \frac{1}{\sum_{j=0}^{n-1} \left[\tilde{\pi}_j(\tau_k^{(n)})\right]^2}. \tag{2.15}$$

Finally, from (2.11) and (2.15), we get

$$w_k = \beta_0 v_{k,1}^2,\ k = 1, 2, \ldots, n. \tag{2.16}$$

Therefore, by means of (1.16) and (2.16), the problem of constructing the Gauss formula, i.e., computing its nodes and weights comes down to finding the eigenvalues and eigenvectors of a symmetric tridiagonal matrix. The most commonly used method is the Golub-Welsch algorithm, which solves the eigenvalue problem by means of the QR algorithm.

(vi) In this last property, we will use Hermite interpolation in order to give an error estimate for the n-point Gauss formula. In Hermite interpolation, we use values of the function and its derivatives. In its simplest form, let p the polynomial which satisfies

$$p(t_i) = f(t_i),\ i = 1, 2, \ldots, n,$$
$$p'(t_i) = f'(t_i),\ i = 1, 2, \ldots, n.$$

The above $2n$ conditions guarantee the existence of a polynomial $p \in \mathbb{P}_{2n-1}$, denoted by p_{2n-1}, and given by the formula

$$p_{2n-1}(t) = \sum_{i=1}^{n} f(t_i)H_i(t) + \sum_{i=1}^{n} f'(t_i)K_i(t), \tag{2.17}$$

where H_i and K_i are defined by

$$\begin{aligned} H_i(t) &= [1 - 2\,(t - t_i)\,\ell_i'(t_i)]\,\ell_i^2(t), \\ K_i(t) &= (t - t_i)\,\ell_i^2(t), \end{aligned} \tag{2.18}$$

and satisfy

$$\begin{aligned} H_i(t_j) &= \delta_{ij},\ H_i'(t_j) = 0 \text{ for all } j, \\ K_i(t_j) &= 0 \text{ for all } j,\ K_i'(t_j) = \delta_{ij}. \end{aligned} \tag{2.19}$$

We shall show that

$$f(t) = p_{2n-1}(t) + r_{2n-1}(t), \tag{2.20}$$

where

$$r_{2n-1}(t) = \prod_{i=1}^{n}(t - t_i)^2 \frac{f^{(2n)}(\xi(t))}{(2n)!}, \ a < \xi(t) < b, \tag{2.21}$$

is the Hermite interpolation error, assuming that $f \in C^{2n}[a, b]$.

Indeed, if $t \in \{t_1, \ldots, t_n\}$, then

$$\prod_{i=1}^{n}(t - t_i)^2 = 0,$$

thus,

$$r_{2n-1}(t) = 0,$$

and (2.20) is true. Assume now that $t \in [a, b]$ with $t \neq t_i$, $i = 1, 2, \ldots, n$, and, without loss of generality, $t_1 < t_2 < \ldots < t_n$. We define the functions

$$\phi(x) = \prod_{i=1}^{n}(x - t_i)^2 \tag{2.22}$$

and

$$\psi(x) = f(x) - p_{2n-1}(x) - \frac{f(t) - p_{2n-1}(t)}{\phi(t)}\phi(x), \ x \in [a, b]. \tag{2.23}$$

It is easy to see that $\psi \in C^{2n}[a, b]$, and setting $x = t_i$, $i = 1, 2, \ldots, n$, or $x = t$ in (2.23), we get

$$\psi(t_i) = 0, \ i = 1, 2, \ldots, n, \ \psi(t) = 0.$$

Therefore, from Rolle's theorem, there exist $\xi_1, \ldots, \xi_n$,

$$t_1 < \xi_1 < t_2 < \ldots < t_j < \xi_j < t < \xi_{j+1} < t_{j+1} < \ldots < \xi_n < t_n,$$

such that $\psi'(\xi_i) = 0$, $i = 1, 2, \ldots, n$. Given that $p'(t_i) = p'_{2n-1}(t_i) = f'(t_i)$, $i = 1, 2, \ldots, n$, and the t_i's are the zeros of ϕ of multiplicity 2, it easy to see that $\psi'(t_i) = 0,\ i = 1, 2, \ldots, n$. Hence, ψ' has, at least, $2n$ distinct zeros, therefore, by Rolle's theorem ψ'' will have, at least, $2n-1$ distinct zeros. Proceeding that way, we finally get that $\psi^{(2n)}$ has, at least, one zero $\xi(t) \in (a, b)$. Since

$$\psi^{(2n)}(x) = f^{(2n)}(x) - \frac{f(t) - p_{2n-1}(t)}{\phi(t)}(2n)!,$$

we have

$$0 = \psi^{(2n)}(\xi(t)) = f^{(2n)}(\xi(t)) - \frac{f(t) - p_{2n-1}(t)}{\phi(t)}(2n)!,$$

which, solved for $f(t) - p_{2n-1}(t)$, yields (2.20)-(2.21).

In 1885, Markov observed that the n-point Gauss formula can be constructed by means of Hermite interpolation. Given that

$$\pi_n(t) = \pi_n(t; w) = \prod_{i=1}^{n}(t - \tau_i),$$

we have

$$\pi_n'(t) = \sum_{k=1}^{n}\prod_{\substack{\ell=1\\ \ell\neq k}}^{n}(t - \tau_\ell),$$

hence,

$$\pi_n'(\tau_k) = \prod_{\substack{\ell=1\\ \ell\neq k}}^{n}(\tau_k - \tau_\ell).$$

Therefore,

$$\ell_k(t) = \prod_{\substack{\ell=1\\ \ell\neq k}}^{n}\frac{t - \tau_\ell}{\tau_k - \tau_\ell} = \frac{\pi_n(t)}{(t - \tau_k)\pi_n'(\tau_k)}. \tag{2.24}$$

Multiplying both sides of (2.20) by $w(t)$, and then taking the integral, we have

$$\int_a^b f(t)w(t)\mathrm{d}t = \int_a^b p_{2n-1}(t)w(t)\mathrm{d}t + \int_a^b r_{2n-1}(t)w(t)\mathrm{d}t.$$

First,

$$\begin{aligned}\int_a^b p_{2n-1}(t)w(t)\mathrm{d}t &= \int_a^b \left[\sum_{i=1}^n f(\tau_i)H_i(t) + \sum_{i=1}^n f'(\tau_i)K_i(t)\right] w(t)\mathrm{d}t \\ &= \sum_{i=1}^n f(\tau_i)\int_a^b H_i(t)w(t)\mathrm{d}t + \sum_{i=1}^n f'(\tau_i)\int_a^b K_i(t)w(t)\mathrm{d}t.\end{aligned}$$

From (2.18) and (2.24), we have

$$\begin{aligned}\int_a^b H_i(t)w(t)\mathrm{d}t &= \int_a^b \left[1-2\left(t-t_i\right)\ell_i'(t_i)\right]\ell_i^2(t)w(t)\mathrm{d}t \\ &= \int_a^b \ell_i^2(t)w(t)\mathrm{d}t - 2\ell_i'(t_i)\int_a^b \left(t-t_i\right)\ell_i^2(t)w(t)\mathrm{d}t \\ &= \int_a^b \ell_i^2(t)w(t)\mathrm{d}t - \frac{2\ell_i'(t_i)}{\pi_n'(\tau_i)}\int_a^b \pi_n(t)\ell_i(t)w(t)\mathrm{d}t,\end{aligned}$$

and since $\pi_n(t)$ is orthogonal, with respect to the weight function $w(t)$, to polynomials of lower degree and $\ell_i \in \mathbb{P}_{n-1}$,

$$\int_a^b \pi_n(t)\ell_i(t)w(t)\mathrm{d}t = 0.$$

Therefore, by means of Stieltjes observation in property (ii), we obtain

$$\int_a^b H_i(t)w(t)\mathrm{d}t = \int_a^b \ell_i^2(t)w(t)\mathrm{d}t = w_i.$$

Similarly,

$$\begin{aligned}\int_a^b K_i(t)w(t)\mathrm{d}t &= \int_a^b (t-\tau_i)\ell_i^2(t)w(t)\mathrm{d}t \\ &= \frac{1}{\pi_n'(\tau_i)}\int_a^b \pi_n(t)\ell_i(t)w(t)\mathrm{d}t = 0.\end{aligned}$$

Hence,

$$\int_a^b p_{2n-1}(t)w(t)\mathrm{d}t = \sum_{i=0}^n w_i f(\tau_i), \tag{2.25}$$

which proves our assertion. By constructing the n-point Gauss formula via Hermite interpolation, we are able to obtain, as a biproduct, an expression for the error term. We have

$$\begin{aligned}
R_n(f) &= \int_a^b r_{2n-1}(t)w(t)\mathrm{d}t \\
&= \int_a^b \prod_{i=1}^{n}(t-\tau_i)^2 \frac{f^{(2n)}(\xi(t))}{(2n)!}w(t)\mathrm{d}t \\
&= \int_a^b [\pi_n(t;w)]^2 \frac{f^{(2n)}(\xi(t))}{(2n)!}w(t)\mathrm{d}t, \ a < \xi(t) < b.
\end{aligned}$$

Assuming that $f \in C^{2n}[a,b]$,

$$m \le f^{(2n)}(\xi(t)) \le M,$$

and since $[\pi_n(t;w)]^2$ and $w(t)$ are positive for $t \in [a,b]$, we have

$$m \int_a^b [\pi_n(t;w)]^2 w(t)\mathrm{d}t \le (2n)! R_n(f) \le M \int_a^b [\pi_n(t;w)]^2 w(t)\mathrm{d}t,$$

thus,

$$m \le \frac{(2n)! R_n(f)}{\int_a^b [\pi_n(t;w)]^2 w(t)\mathrm{d}t} \le M.$$

As $f \in C^{2n}[a,b]$, we can apply the Intermediate Value Theorem, which imposes that there is $\xi \in (a,b)$ such that

$$\frac{(2n)! R_n(f)}{\int_a^b [\pi_n(t;w)]^2 w(t)\mathrm{d}t} = f^{(2n)}(\xi),$$

that is,

$$R_n(f) = \frac{f^{(2n)}(\xi)}{(2n)!} \int_a^b [\pi_n(t;w)]^2 w(t)\mathrm{d}t, \ a < \xi < b. \tag{2.26}$$

Chapter 3

Anti-Gauss Quadrature Formula

This chapter is about the anti-Gauss quadrature formula, an efficient method constructed by Laurie (cf. [8]) in order to estimate the error of the Gauss formula.

3.1 Introduction

The remainder term of the Gauss formula contains $f^{(2n)}(\xi)$, therefore, its practical value is limited, since high order derivatives are difficult to estimate. In practice, if we set $I(f) = \int_a^b f(t)w(t)\mathrm{d}t$ and $Q_n^G(f) = \sum_{k=1}^n w_k f(\tau_k)$, we can estimate the error term

$$|R_n(f)| = \left|I(f) - Q_n^G(f)\right|,$$

by means of

$$|R_n(f)| \cong \left|Q_m(f) - Q_n^G(f)\right|,$$

where $Q_m(f)$ is the quadrature sum of a formula with $m > n$ points and degree of exactness $d_m > 2n-1$, i.e., $Q_m(f)$ plays the role of the true value of the integral.

One idea is to start with the n Gauss points and add some more in order to obtain the new formula. It is noteworthy that in order to improve on the degree of exactness of the Gauss formula we need to add, at least, $n+1$ more points. This is because if we start with the n Gauss points and add up to n new ones, the resulting quadrature formula is the Gauss formula itself. Indeed, let $Q_{2n}(f)$ be the $2n$-point quadrature formula

$$Q_{2n}(f) = \sum_{i=1}^{n} w_i f(\tau_i) + \sum_{i=1}^{n} w_i^\star f(\tau_i^\star).$$

By means of (2.4), we have

$$\begin{aligned} w_k^\star &= \int_a^b \frac{(t-\tau_1)\dots(t-\tau_n)(t-\tau_1^\star)\dots(t-\tau_{k-1}^\star)(t-\tau_{k+1}^\star)\dots(t-\tau_n^\star)}{\prod_{\ell=1}^n(\tau_k^\star-\tau_\ell)\prod_{\substack{\ell=1\\ \ell\neq k}}^n(\tau_k^\star-\tau_\ell^\star)} w(t)\mathrm{d}t \\ &= \int_a^b \pi_n(t)\frac{(t-\tau_1^\star)\dots(t-\tau_{k-1}^\star)(t-\tau_{k+1}^\star)\dots(t-\tau_n^\star)}{\prod_{\ell=1}^n(\tau_k^\star-\tau_\ell)\prod_{\substack{\ell=1\\ \ell\neq k}}^n(\tau_k^\star-\tau_\ell^\star)} w(t)\mathrm{d}t, \end{aligned}$$

and since $(t-\tau_1^\star)\dots(t-\tau_{k-1}^\star)(t-\tau_{k+1}^\star)\dots(t-\tau_n^\star) \in \mathbb{P}_{n-1}$, by orthogonality, $w_k^\star = 0,\ k = 1, 2, \dots, n$, hence

$$Q_{2n}(f) = \sum_{i=1}^{n} w_i f(\tau_i) = Q_n^G(f).$$

Therefore, we are seeking a $(2n+1)$-point formula, containing the Gauss nodes $\tau_i,\ i = 1, 2, \dots, n$, with degree higher than $2n-1$. Kronrod, in 1964, constructed an optimal extension of $Q_n^G(f)$ for $w(t) = 1$ on $[-1, 1]$, having degree of exactness, at least, $3n+1$, which is now called Gauss-Kronrod quadrature formula. Unfortunately, for many classical weight functions, among which the Gegenbauer and Jacobi, for certain values of the parameters λ and α, β, respectively, as well as the Laguerre and Hermite weight functions, the Gauss-Kronrod formula fails to exist with real nodes, all contained in the interval of integration, and positive weights.

Hence, the quadrature formula $Q_m(f)$ should satisfy the following properties:

(i) Its $n+1$ nodes are real and contained on the interval of integration.

(ii) Its weights are positive.

(iii) $Q_m(f)$ should be easily constructed.

(iv) $Q_m(f)$ must have degree of exactness higher than $2n-1$.

Despite the fact that $Q_{n+1}^{G}(f)$ fulfills these properties, it has been noted that using it in place of $Q_m(f)$ can be very unreliable (cf. [4]).

In 1996, Laurie constructed the anti-Gauss formula

$$Q_{n+1}^{AG}(f) = \sum_{i=1}^{n+1} \lambda_i f(\xi_i), \tag{3.1}$$

defined by the property

$$I(p) - Q_{n+1}^{AG}(p) = -\left[I(p) - Q_n^{G}(p)\right] \quad \forall p \in \mathbb{P}_{2n+1}, \tag{3.2}$$

that is, the anti-Gauss formula has an error exactly opposite to that of the n-point Gauss formula $\forall p \in \mathbb{P}_{2n+1}$. Then

$$I(p) - Q_n^{G}(p) = I(p) - Q_{n+1}^{AG}(p) + Q_{n+1}^{AG}(p) - Q_n^{G}(p) \quad \forall p \in \mathbb{P}_{2n+1},$$

thus,

$$I(p) - Q_n^{G}(p) - \left[I(p) - Q_{n+1}^{AG}(p)\right] = Q_{n+1}^{AG}(p) - Q_n^{G}(p) \quad \forall p \in \mathbb{P}_{2n+1}. \tag{3.3}$$

Now, inserting (3.2) into (3.3), we have

$$2\left[I(p) - Q_n^G(p)\right] = Q_{n+1}^{AG}(p) - Q_n^G(p)\ \forall p \in \mathbb{P}_{2n+1},$$

hence,

$$I(p) - Q_n^G(p) = \frac{Q_{n+1}^{AG}(p) - Q_n^G(p)}{2} \quad \forall p \in \mathbb{P}_{2n+1}, \tag{3.4}$$

that is, the error of the n-point Gauss formula can be estimated by

$$|R_n(f)| \cong \frac{\left|Q_{n+1}^{AG}(f) - Q_n^G(f)\right|}{2}.$$

Also, from (3.2), we have

$$I(p) - Q_{n+1}^{AG}(p) = -I(p) + Q_n^G(p) \quad \forall p \in \mathbb{P}_{2n+1},$$

thus,

$$I(p) = \frac{Q_{n+1}^{AG}(p) + Q_n^G(p)}{2} \quad \forall p \in \mathbb{P}_{2n+1}.$$

This leads to the $(2n+1)$-point formula

$$Q_{2n+1}^{AvG}(f) = \frac{1}{2}\left[Q_n^G(f) + Q_{n+1}^{AG}(f)\right], \tag{3.5}$$

which is called averaged Gauss quadrature formula, and as, by (3.2),

$$Q_{n+1}^{AG}(p) + Q_n^G(p) = 2I(p) \quad \forall p \in \mathbb{P}_{2n+1},$$

that is,

$$Q_{2n+1}^{AvG}(p) = I(p) \quad \forall p \in \mathbb{P}_{2n+1},$$

formula (3.5) has degree of exactness $2n+1$.

3.2 Construction of the anti-Gauss quadrature formula

In this section we will show that the construction of the anti-Gauss formula can be done in a like manner as the construction of the Gauss formula.

Initially, from (3.2), we have

$$Q_{n+1}^{AG}(p) = 2I(p) - Q_n^G(p) \quad \forall p \in \mathbb{P}_{2n+1}. \tag{3.6}$$

Defining now the Gauss formula by

$$Q_n^G(p) = I(p) \quad \forall p \in \mathbb{P}_{2n-1}, \tag{3.7}$$

we can consider I to be the linear functional

$$I(f) = \int_a^b f(t)w(t)\mathrm{d}t.$$

In that sense, from (3.6), the anti-Gauss formula is a $(n+1)$-point Gauss formula with respect to the linear functional $2I - Q_n^G$. Hence, we can find its nodes and weights the same way we did in the case of the Gauss formula. From (1.8) and (1.9), we have

$$\alpha_k = \frac{(t\pi_k, \pi_k)}{(\pi_k, \pi_k)} = \frac{\int_a^b t\,[\pi_k(t)]^2\, w(t)\mathrm{d}t}{\int_a^b [\pi_k(t)]^2\, w(t)\mathrm{d}t} = \frac{I(t\pi_k^2)}{I(\pi_k^2)}, \ k = 0, 1, \ldots, n, \tag{3.8}$$

and similarly

$$\beta_0 = I(\pi_0), \ \beta_k = \frac{I(\pi_k^2)}{I(\pi_{k-1}^2)}, \ k = 1, 2, \ldots, n, \tag{3.9}$$

with π_n to be the orthogonal polynomial, of degree n, with respect to the linear functional I, that is, π_n is defined by the property

$$\int_a^b \pi_n(t)p(t)w(t)\mathrm{d}t = I(\pi_n p) = 0 \quad \forall p \in \mathbb{P}_{n-1}. \tag{3.10}$$

Let now $\hat{\alpha}_k$ and $\hat{\beta}_k$, $k = 0, 1, \ldots, n$, be the coefficients that satisfy the recurrence relation

$$\begin{aligned} \hat{\pi}_{k+1}(t) &= (t - \hat{\alpha}_k)\,\hat{\pi}_k(t) - \hat{\beta}_k \hat{\pi}_{k-1}(t),\ k = 0, 1, 2 \ldots, \\ \hat{\pi}_0(t) &= 1,\ \hat{\pi}_{-1}(t) = 0, \end{aligned} \tag{3.11}$$

where $\hat{\pi}_n$ is the orthogonal polynomial, of degree n, with respect to the linear functional $2I - Q_n^G$. Interchanging I with $2I - Q_n^G$ in (3.8) and (3.9), gives

$$\hat{\alpha}_k = \frac{(2I - Q_n^G)(t\hat{\pi}_k^2)}{(2I - Q_n^G)(\hat{\pi}_k^2)},\ k = 0, 1, \ldots, n, \tag{3.12}$$

and

$$\hat{\beta}_0 = (2I - Q_n^G)(\hat{\pi}_0),\ \hat{\beta}_k = \frac{(2I - Q_n^G)(\hat{\pi}_k^2))}{(2I - Q_n^G)(\hat{\pi}_{k-1}^2)},\ k = 1, 2, \ldots, n. \tag{3.13}$$

Considering now the corresponding $(n+1) \times (n+1)$ Jacobi matrix

$$\hat{J}_{n+1} = \begin{bmatrix} \hat{\alpha}_0 & \sqrt{\hat{\beta}_1} & 0 & \ldots & 0 & 0 \\ \sqrt{\hat{\beta}_1} & \hat{\alpha}_1 & \sqrt{\hat{\beta}_2} & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & \sqrt{\hat{\beta}_n} & \hat{\alpha}_n \end{bmatrix}, \tag{3.14}$$

as we shall prove in the next section, the nodes and weights of the anti-Gauss formula can be expressed in terms of the eigenvalues and eigenvectors of $\hat{J}_{n+1}$, just as we discussed in property (v) for the Gauss formula. Therefore, in order to construct formula (3.1), we only need to find the coefficients $\hat{\alpha}_k$ and $\hat{\beta}_k$.

From (3.7), we have

$$(2I - Q_n^G)(p) = 2I(p) - Q_n^G(p) = 2I(p) - I(p) = I(p) \quad \forall p \in \mathbb{P}_{2n-1}. \tag{3.15}$$

Considering now that $t\hat{\pi}_k^2 \in \mathbb{P}_{2n-1}$, $\hat{\pi}_k^2 \in \mathbb{P}_{2n-2}$ and $\hat{\pi}_{k-1}^2 \in \mathbb{P}_{2n-4}$ for $k = 0, 1, \ldots, n-1$, from (3.12), (3.13) and (3.15), we obtain

$$\hat{\alpha}_k = \frac{(2I - Q_n^G)(t\hat{\pi}_k^2)}{(2I - Q_n^G)(\hat{\pi}_k^2)} = \frac{I(t\hat{\pi}_k^2)}{I(\hat{\pi}_k^2)},\ k = 0, 1, \ldots, n-1, \tag{3.16}$$

and, similarly,

$$\hat{\beta}_k = \frac{(2I - Q_n^G)(\hat{\pi}_k^2)}{(2I - Q_n^G)(\hat{\pi}_{k-1}^2)} = \frac{I(\hat{\pi}_k^2)}{I(\hat{\pi}_{k-1}^2)},\ k = 0, 1, \ldots, n-1. \tag{3.17}$$

Since $\hat{\pi}_0 = \pi_0$ and $\hat{\pi}_1 = \pi_1$, then $\hat{\alpha}_0 = \alpha_0$, $\hat{\beta}_0 = \beta_0$, and by means of (3.16) and (3.17), we get

$$\begin{aligned} \hat{\alpha}_k &= \alpha_k,\ k = 0, 1, \ldots, n-1, \\ \hat{\beta}_k &= \beta_k,\ k = 0, 1, \ldots, n-1, \\ \hat{\pi}_k &= \pi_k,\ k = 0, 1, \ldots, n. \end{aligned} \tag{3.18}$$

What remains is to compute $\hat{\alpha}_n$ and $\hat{\beta}_n$. From (3.12) and (3.18), we have

$$\hat{\alpha}_n = \frac{(2I - Q_n^G)(t\pi_n^2)}{(2I - Q_n^G)(\pi_n^2)} = \frac{2I(t\pi_n^2) - Q_n^G(t\pi_n^2)}{2I(\pi_n^2) - Q_n^G(\pi_n^2)},$$

that is,

$$\hat{\alpha}_n = \frac{2I(t\pi_n^2) - \sum_{i=1}^n w_i \left(\tau_i \left[\pi_n(\tau_i)\right]^2\right)}{2I(\pi_n^2) - \sum_{i=1}^n w_i \left(\left[\pi_n(\tau_i)\right]^2\right)}.$$

By definition τ_i are the zeros of the polynomial π_n, therefore, the factor $[\pi_n(\tau_i)]^2$ will vanish and, from (3.8), we obtain

$$\hat{\alpha}_n = \frac{2I(t\pi_n^2)}{2I(\pi_n^2)} = \frac{I(t\pi_n^2)}{I(\pi_n^2)} = \alpha_n.$$

Now, from (3.13) and (3.18), we have

$$\hat{\beta}_n = \frac{(2I - Q_n^G)(\pi_n^2)}{(2I - Q_n^G)(\pi_{n-1}^2)} = \frac{2I(\pi_n^2) - Q_n^G(\pi_n^2)}{2I(\pi_{n-1}^2) - Q_n^G(\pi_{n-1}^2)}.$$

Similarly, since $Q_n^G(\pi_n^2) = 0$ and $\pi_{n-1}^2 \in \mathbb{P}_{2n-2}$, hence, by (3.9), $Q_n^G(\pi_{n-1}^2) = I(\pi_{n-1}^2)$, we get

$$\hat{\beta}_n = \frac{2I(\pi_n^2)}{I(\pi_{n-1}^2)} = 2\beta_n.$$

Finally, we have

$$\begin{aligned}
&\hat{\alpha}_k = \alpha_k,\ \ k = 0, 1, \ldots, n, \\
&\hat{\beta}_k = \beta_k,\ \ k = 0, 1, \ldots, n-1,\ \ \hat{\beta}_n = 2\beta_n, \\
&\hat{\pi}_k = \pi_k,\ \ k = 0, 1, \ldots, n.
\end{aligned} \tag{3.19}$$

3.3 Properties of the anti-Gauss formula

Anti-Gauss formula has almost all of the properties we discussed in the first section. Considering Q_{n+1}^{AG} to be the $(n+1)$-point anti-Gauss formula defined in (3.1), in this section we present these properties (cf. [8], Theorem 1, [9], Theorem 2.1).

(i) The nodes ξ_i, $i = 1, 2, \ldots, n+1$, are real and the weights λ_i, $i = 1, 2, \ldots, n+1$, are positive. Considering Q_{n+1}^{AG} to be the $(n+1)$-point anti-Gauss formula for the linear functional $2I - Q_n^G$, we will express ξ_i and λ_i in terms of $\hat{J}_{n+1}$ eigenvalues and eigenvectors. From (3.14) and

(3.19), we have

$$
\begin{aligned}
\hat{J}_{n+1} &= \begin{bmatrix} \hat{\alpha}_0 & \sqrt{\hat{\beta}_1} & 0 & \dots & 0 & 0 \\ \sqrt{\hat{\beta}_1} & \hat{\alpha}_1 & \sqrt{\hat{\beta}_2} & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \sqrt{\hat{\beta}_n} & \hat{\alpha}_n \end{bmatrix} \\
&= \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & 0 & \dots & 0 & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \sqrt{2\beta_n} & \alpha_n \end{bmatrix}.
\end{aligned} \tag{3.20}
$$

Precisely as in the proof of Theorem 1.12, it is easy to show that the orthonormal polynomials $\hat{\tilde{\pi}}_k = \frac{\hat{\pi}_k}{\|\hat{\pi}_k\|}$ satisfy the three term recurrence relation

$$
\sqrt{\hat{\beta}_{k+1}}\hat{\tilde{\pi}}_{k+1}(t) = (t - \hat{\alpha}_k)\,\hat{\tilde{\pi}}_k(t) - \sqrt{\hat{\beta}_k}\hat{\tilde{\pi}}_{k-1}(t), \; k = 0, 1, 2, \dots
$$
$$
\hat{\tilde{\pi}}_{-1}(t) = 0, \; \hat{\tilde{\pi}}_0(t) = \tfrac{1}{\sqrt{\hat{\beta}_0}},
$$

that is,

$$
t\hat{\tilde{\pi}}_k(t) = \sqrt{\hat{\beta}_k}\hat{\tilde{\pi}}_{k-1}(t) + \hat{\alpha}_k\hat{\tilde{\pi}}_k(t) + \sqrt{\hat{\beta}_{k+1}}\hat{\tilde{\pi}}_{k+1}(t),
$$

and in vector form

$$
t\hat{\tilde{\pi}}(t) = \hat{J}_{n+1}\hat{\tilde{\pi}}(t) + \sqrt{\beta_{n+1}}\hat{\tilde{\pi}}_{n+1}(t)e_{n+1}, \tag{3.21}
$$

where $e_{n+1} = [0, 0, \dots, 1]^{\mathrm{T}}$ is the $(n+1)$th coordinate vector in $\mathbb{R}^{n+1}$ and $\hat{\tilde{\pi}}(t)$ is defined as

$$
\hat{\tilde{\pi}}(t) = \left[\hat{\tilde{\pi}}_0(t), \hat{\tilde{\pi}}_1(t), \dots, \hat{\tilde{\pi}}_n(t)\right]^T.
$$

Therefore, setting $t = \xi_i$ in (3.21), since ξ_i, $i = 1, 2, \ldots, n+1$, are the zeros of $\hat{\tilde{\pi}}_{n+1}(t)$, we obtain

$$\hat{J}_{n+1}\hat{\tilde{\pi}}\left(\xi_i\right) = \xi_i\hat{\tilde{\pi}}\left(\xi_i\right). \tag{3.22}$$

Equation (3.22) implies that ξ_i are the eigenvalues of $\hat{J}_{n+1}$ and $\hat{\tilde{\pi}}\left(\xi_i\right)$ are the corresponding eigenvectors.

Lemma 3.1. *Let A be real symmetric matrix of order $n+1$. Then its eigenvalues are real.*

Proof. Let λ be an eigenvalue of A and v the corresponding eigenvector. Since A is a real matrix we know that $A = \bar{A}$, where $\bar{A}$ is the conjugate matrix of A. Therefore if $Av = \lambda v$, then $\overline{Av} = \overline{\lambda v}$, that is $A\bar{v} = \bar{\lambda}\bar{v}$. Hence,

$$\bar{v}^T Av = \bar{v}^T(Av) = \bar{v}^T(\lambda v) = \lambda \bar{v}^T v \tag{3.23}$$

and

$$\bar{v}^T Av = (A\bar{v})^T v = (\bar{\lambda}\bar{v})^T v = \bar{\lambda}\bar{v}^T v. \tag{3.24}$$

From (3.23) and (3.24), we get $\lambda\bar{v}^T v = \bar{\lambda}\bar{v}^T v$, and as $v \neq 0$, $\bar{\lambda} = \lambda$, that is, λ is real. □

Since $\hat{J}_{n+1}$ is a real, symmetric matrix of order $n+1$, its eigenvalues, i.e., ξ_i will be real. Now, we can prove, precisely as we did in property (v) of the n-point Gauss formula, that

$$\lambda_k = \hat{\beta}_0 \hat{v}_{k,1}^2, \;\; k = 1, 2, \ldots, n+1, \tag{3.25}$$

where $\hat{v}_k$ is the normalized eigenvector

$$\hat{v}_k = \frac{\hat{\tilde{\pi}}\left(\xi_k\right)}{\|\hat{\tilde{\pi}}\left(\xi_k\right)\|_2},$$

and from (3.19),

$$\hat{v}_{k,1} = \frac{\hat{\tilde{\pi}}_0\left(\xi_k\right)}{\left(\sum_{j=0}^{n}\left[\hat{\tilde{\pi}}_k\left(\xi_k\right)\right]^2\right)^{1/2}} = \frac{\tilde{\pi}_0\left(\xi_k\right)}{\left(\sum_{j=0}^{n}\left[\tilde{\pi}_k\left(\xi_k\right)\right]^2\right)^{1/2}}.$$

Therefore the $\hat{v}_{k,1},\ k = 0, 1, \ldots, n+1$, are real, and, consequently, the $\lambda_k,\ k = 0, 1, \ldots, n+1$, are positive, since $\hat{\beta}_0 = \beta_0 > 0$ and $\hat{v}_{k,1}^2 > 0$.

(ii) The nodes $\xi_k,\ k = 1, 2, \ldots, n+1$, alternate with those of the n-point Gauss formula, that is,

$$\xi_{n+1} < \tau_n < \xi_n < \cdots < \tau_1 < \xi_1. \tag{3.26}$$

At first, $\hat{J}_{n+1}$ is a real symmetric matrix, since, from (3.20),

$$\hat{J}_{n+1} = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & 0 & \ldots & 0 & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & \sqrt{2\beta_n} & \alpha_n \end{bmatrix},$$

and by definition $\beta_k,\ k = 0, 1, \ldots, n$, and $\alpha_k,\ k = 0, 1, \ldots, n$, are all real. Then, also from (3.20), we have

$$\hat{J}_{n+1} = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & 0 & \ldots & 0 & 0 \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & \sqrt{2\beta_n} & \alpha_n \end{bmatrix} = \begin{bmatrix} J_n & SB \\ SB^T & \alpha_n \end{bmatrix},$$

where $SB^T = [0, \ldots, 0, \sqrt{2\beta_n}] \in \mathbb{R}^n$, that is, J_n is a principal submatrix of $\hat{J}_{n+1}$. Therefore we can apply the Cauchy's interlace Theorem (cf. [10], pp. 202), which states that the eigenvalues of a real Hermitian matrix of order n interlace with those of any principal submatrix of order $n-1$.

(iii) The inner nodes of the anti-Gauss formula are contained in the integration interval, that is, $\xi_2, \xi_3, \ldots, \xi_n \in (a, b)$. In the first property for the Gauss formula we showed that its nodes τ_i, $i = 1, 2, \ldots, n$, are all contained in the interval (a, b) and by (3.26),

$$\tau_n < \xi_n < \tau_{n-1} < \cdots < \xi_2 < \tau_1,$$

hence, $\xi_i \in (a, b)$, $i = 2, 3, \ldots, n$.

(iv) For the outer nodes ξ_1 and ξ_{n+1} we have

$$\xi_1 \in [a, b] \text{ if and only if } \frac{\pi_{n+1}(b)}{\pi_{n-1}(b)} \geq \beta_n. \tag{3.27}$$

and

$$\xi_{n+1} \in [a, b] \text{ if and only if } \frac{\pi_{n+1}(a)}{\pi_{n-1}(a)} \geq \beta_n \tag{3.28}$$

Initially, by means of (3.19), we have

$$\begin{aligned}
\hat{\pi}_{n+1}(t) &= (t - \hat{\alpha}_n)\hat{\pi}_n(t) - \hat{\beta}_n\hat{\pi}_{n-1}(t) \\
&= (t - \alpha_n)\pi_n(t) - 2\beta_n\pi_{n-1}(t) \\
&= (t - \alpha_n)\pi_n(t) - \beta_n\pi_{n-1}(t) - \beta_n\pi_{n-1}(t),
\end{aligned}$$

and from (1.7),

$$\hat{\pi}_{n+1}(t) = \pi_{n+1}(t) - \beta_n\pi_{n-1}(t). \tag{3.29}$$

As τ_k is a zero of π_n, we have, from (1.7),

$$\pi_{n+1}(\tau_k) = -\beta_n \pi_{n-1}(\tau_k),$$

which, inserted into (3.29), yields

$$\hat{\pi}_{n+1}(\tau_k) = 2\pi_{n+1}(\tau_k). \tag{3.30}$$

Now,

$$\pi_{n+1}(t) = \prod_{i=1}^{n+1}(t - \tau_i^{(n+1)}),$$

thus,

$$\pi_{n+1}(\tau_k) = \prod_{i=1}^{n+1}(\tau_k - \tau_i^{(n+1)}),\ k = 1, 2, \dots, n, \tag{3.31}$$

and from (1.24), we have

$$\begin{aligned} \tau_k - \tau_i^{(n+1)} &> 0,\ i \geq k+1, \\ \tau_k - \tau_i^{(n+1)} &< 0,\ i \leq k. \end{aligned} \tag{3.32}$$

The later, in view of (3.30), leads to

$$\text{sign } \hat{\pi}_{n+1}(\tau_k) = \text{sign } \pi_{n+1}(\tau_k) = (-1)^k, \quad k = 1, 2, \dots, n. \tag{3.33}$$

Now, it is clear that

$$\lim_{t\to\infty} \hat{\pi}_{n+1}(t) = \lim_{t\to\infty} \pi_{n+1}(t) = \lim_{t\to\infty} \pi_{n-1}(t) = \infty. \tag{3.34}$$

Therefore, Theorem 1.18, combined with (3.34), implies that $\pi_{n+1}(b) > 0$ and $\pi_{n-1}(b) > 0$, since all their roots are contained on (a, b). In addition, ξ_1 is real (see (i)) and, by (3.34) and (3.33), $\xi_1 \in [a, b]$ if and only if $\hat{\pi}_{n+1}(b) \geq 0$, which, in view of (3.29), leads to $\pi_{n+1}(b) - \beta_n \pi_{n-1}(b) \geq 0$, that is, condition (3.27).

For the leftmost node, if $n+1$ is even, we know that

$$\lim_{t\to-\infty}\hat{\pi}_{n+1}(t)=\lim_{t\to-\infty}\pi_{n+1}(t)=\lim_{t\to-\infty}\pi_{n-1}(t)=\infty, \tag{3.35}$$

then, from Theorem 1.18, we have that $\pi_{n+1}(a)>0$ and $\pi_{n-1}(a)>0$, while, by (3.35) and (3.33), ξ_{n+1}, which is real, belongs in $[a,b]$ if and only if $\hat{\pi}_{n+1}(a)\geq 0$, which, by means of (3.29), leads to (3.28). On the other hand, if $n+1$ is odd, we have

$$\lim_{t\to-\infty}\hat{\pi}_{n+1}(t)=\lim_{t\to-\infty}\pi_{n+1}(t)=\lim_{t\to-\infty}\pi_{n-1}(t)=-\infty. \tag{3.36}$$

The later, in view of Theorem 1.18, implies that $\pi_{n+1}(a)<0$ and $\pi_{n-1}(a)<0$, while, by (3.33), $\xi_{n+1}\in[a,b]$ if and only if $\hat{\pi}_{n+1}(a)\leq 0$, which again, by (3.29), leads to (3.28).

So far, we proved that the anti-Gauss formula always exists, with real nodes and positive weights, while at most two of its nodes are not contained in the integration interval.

3.4 Anti-Gauss Quadrature Formula on Classical Weight Functions

We will now examine whether, for some of the classical weight functions presented in the previous chapter, the anti-Gauss formula has all its nodes in the interval of integration.

Theorem 3.2. *([8], Theorem 2) The anti-Gauss formula* (3.1) *for the generalized Hermite weight function*

$$w(t)=|t|^{2\mu}\mathrm{e}^{-t^2},\ \mu>-\frac{1}{2},\ t\in(-\infty,\infty), \tag{3.37}$$

or the generalized Laguerre weight function

$$w(t) = t^{\alpha}\mathrm{e}^{-t},\ \ \alpha > -1,\ \ t \in [0, \infty), \tag{3.38}$$

has all its nodes contained in $(-\infty, \infty)$ *and* $[0, \infty)$*, respectively.*

Proof. For the generalized Hermite weight function, there is nothing to prove since the nodes of the formula are always real and therefore are always contained in $(-\infty, \infty)$. For the generalized Laguerre weight function, we need to check if the leftmost node belongs to the interval, that is, if $\xi_{n+1} \geq 0$, which, by (3.28), is true if and only if

$$\frac{\pi^L_{n+1}(0)}{\pi^L_{n-1}(0)} \geq \beta_n,$$

where π^L_m is the Laguerre orthogonal polynomial of degree m. From Table 1.2, $\beta_n = n(n+\alpha)$ and, by means of (1.37) and (1.38), we have

$$L_n^{(\alpha)}(0) = \binom{n+a}{n} = \frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)\Gamma(\alpha+1)}$$

and

$$k_n = \frac{(-1)^n}{n!},$$

thus,

$$\begin{aligned} \pi^L_n(0) = \frac{L_n^{(\alpha)}(0)}{k_n} &= \frac{\frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)\Gamma(\alpha+1)}}{\frac{(-1)^n}{n!}} = (-1)^n n! \frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)\Gamma(\alpha+1)} \\ &= (-1)^n n! \frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)} = (-1)^n \frac{\Gamma(n+\alpha+1)}{\Gamma(\alpha+1)}. \end{aligned} \tag{3.39}$$

Hence, we have

$$\begin{aligned} \frac{\pi^L_{n+1}(0)}{\pi^L_{n-1}(0)} &= \frac{(-1)^{n+1}\frac{\Gamma(n+1+\alpha+1)}{\Gamma(\alpha+1)}}{(-1)^{n-1}\frac{\Gamma(n-1+\alpha+1)}{\Gamma(\alpha+1)}} = (-1)^2 \frac{\Gamma(n+\alpha+2)}{\Gamma(n+\alpha)} \\ &= \frac{(n+\alpha+1)(n+\alpha)\Gamma(n+\alpha)}{\Gamma(n+\alpha)} \\ &= (n+\alpha+1)(n+\alpha) \end{aligned}$$

and since $\alpha > -1$, we have $(n+\alpha+1) > n$, which leads to

$$\frac{\pi_{n+1}^{L}(0)}{\pi_{n-1}^{L}(0)} = (n+a+1)(n+a) > n(n+a) = \beta_n,$$

based on which $\xi_{n+1} \in [0, \infty)$. □

Theorem 3.3. *([8], Theorem 3) The anti-Gauss formula* (3.1) *for the Jacobi weight function*

$$w(t) = (1-t)^{\alpha}(1+t)^{\beta}, \ \alpha, \beta > -1, \ t \in [-1, 1], \tag{3.40}$$

has all its nodes contained in $[-1, 1]$ *if and only if*

$$(2\alpha+1)n^2 + (2\alpha+1)(\alpha+\beta+1)n + \frac{1}{2}(\alpha+1)(\alpha+\beta)(\alpha+\beta+1) \geq 0 \tag{3.41}$$

and

$$(2\beta+1)n^2 + (2\beta+1)(\alpha+\beta+1)n + \frac{1}{2}(\beta+1)(\alpha+\beta)(\alpha+\beta+1) \geq 0. \tag{3.42}$$

Remark 3.4. Condition (3.41) comes from the requirement that ξ_1 is included in $[-1, 1]$, and condition (3.42) from the requirement that ξ_{n+1} is included in $[-1, 1]$.

Proof. From Table 1.2, we have

$$\beta_n^J = \frac{4n(n+\alpha)(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta)^2(2n+\alpha+\beta+1)(2n+\alpha+\beta-1)},$$

and, from (1.35), $k_n = \frac{1}{2^n}\binom{2n+\alpha+\beta}{n}$ and $P_n^{(\alpha,\beta)}(1) = \binom{n+a}{n}$. Hence,

$$\begin{aligned}\pi_n^{(\alpha,\beta)}(1) &= \frac{P_n^{(\alpha,\beta)}(1)}{k_n} = \frac{\binom{n+a}{n}}{\frac{1}{2^n}\binom{2n+\alpha+\beta}{n}} = 2^n \frac{\frac{\Gamma(n+\alpha+1)}{\Gamma(n+1)\Gamma(\alpha+1)}}{\frac{\Gamma(2n+\alpha+\beta+1)}{\Gamma(n+1)\Gamma(n+\alpha+\beta+1)}} \\ &= 2^n \frac{\Gamma(n+\alpha+1)\Gamma(n+\alpha+\beta+1)}{\Gamma(\alpha+1)\Gamma(2n+\alpha+\beta+1)}.\end{aligned}$$

We need to find a condition such that

$$\frac{\pi_{n+1}^{(\alpha,\beta)}(1)}{\pi_{n-1}^{(\alpha,\beta)}(1)} \geq \beta_n^J,$$

which is equivalent to

$$\frac{\frac{\pi_{n+1}^{(\alpha,\beta)}(1)}{\pi_{n-1}^{(\alpha,\beta)}(1)}}{\beta_n^J} \geq 1. \tag{3.43}$$

As

$$\begin{aligned}
\frac{\pi_{n+1}^{(\alpha,\beta)}(1)}{\pi_{n-1}^{(\alpha,\beta)}(1)} &= \frac{2^{n+1}\frac{\Gamma(n+1+\alpha+1)\Gamma(n+1+\alpha+\beta+1)}{\Gamma(\alpha+1)\Gamma(2n+2+\alpha+\beta+1)}}{2^{n-1}\frac{\Gamma(n-1+\alpha+1)\Gamma(n-1+\alpha+\beta+1)}{\Gamma(\alpha+1)\Gamma(2n-2+\alpha+\beta+1)}} \\
&= 4\frac{\frac{(n+\alpha+1)(n+\alpha)\Gamma(n+\alpha)(n+\alpha+\beta+1)(n+\alpha+\beta)\Gamma(n+\alpha+\beta)}{(2n+\alpha+\beta+2)(2n+\alpha+\beta+1)(2n+\alpha+\beta)(2n+\alpha+\beta-1)\Gamma(2n+\alpha+\beta-1)}}{\frac{\Gamma(n+\alpha)\Gamma(n+\alpha+\beta)}{\Gamma(2n+\alpha+\beta-1)}} \\
&= \frac{4(n+\alpha)(n+\alpha+1)(n+\alpha+\beta)(n+\alpha+\beta+1)}{(2n+\alpha+\beta-1)(2n+\alpha+\beta)(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)},
\end{aligned}$$

we have

$$\frac{\frac{\pi_{n+1}^{(\alpha,\beta)}(1)}{\pi_{n-1}^{(\alpha,\beta)}(1)}}{\beta_n^J} = \frac{\frac{4(n+\alpha)(n+\alpha+1)(n+\alpha+\beta)(n+\alpha+\beta+1)}{(2n+\alpha+\beta-1)(2n+\alpha+\beta)(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)}}{\frac{4n(n+\alpha)(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta)^2(2n+\alpha+\beta+1)(2n+\alpha+\beta-1)}},$$

that is,

$$\frac{\frac{\pi_{n+1}^{(\alpha,\beta)}(1)}{\pi_{n-1}^{(\alpha,\beta)}(1)}}{\beta_n^J} = \frac{(n+\alpha+1)(n+\alpha+\beta+1)(2n+\alpha+\beta)}{n(2n+\alpha+\beta+2)(n+\beta)}. \tag{3.44}$$

For the numerator, we have

$$
\begin{aligned}
&(n+\alpha+1)(n+\alpha+\beta+1)(2n+\alpha+\beta) \\
&= 2n^3 + (5\alpha+3\beta+4)n^2 + (4\alpha^2+\beta^2+5\alpha\beta+6\alpha+4\beta+2)n \\
&+ (\alpha^3+2\alpha^2\beta+\alpha\beta^2+2\alpha^2+\beta^2+3\alpha\beta+\alpha+\beta) \\
&= 2n^3+\alpha n^2+\beta n^2+2n^2+2\beta n^2+\alpha\beta n+\beta^2 n+2\beta n+4\alpha n^2 \\
&+ 4\alpha^2 n+4\alpha\beta n+4\alpha n+2n^2+2\alpha n+2\beta n+2n^2+\alpha^3+\alpha^2\beta \\
&+ \alpha^2+\alpha^2\beta+\alpha\beta^2+\alpha\beta+\alpha^2+\alpha\beta+\alpha+\alpha\beta+\beta^2+\beta \\
&= (n^2+\beta n)(2n+\alpha+\beta+2)+(4\alpha n+2n)(n+\alpha+\beta+1) \\
&+ (\alpha^2+\alpha\beta+\alpha+\beta)(\alpha+\beta+1) \\
&= n(2n+\alpha+\beta+2)(n+\beta)+2(2\alpha+1)n(n+\alpha+\beta+1) \\
&+ (\alpha+1)(\alpha+\beta)(\alpha+\beta+1).
\end{aligned}
$$

The later, combined with (3.44), gives

$$
\begin{aligned}
\frac{\frac{\pi_{n+1}^{(\alpha,\beta)}(1)}{\pi_{n-1}^{(\alpha,\beta)}(1)}}{\beta_n^J} &= 1 + \frac{(2\alpha+1)n(n+\alpha+\beta+1)+\frac{1}{2}(\alpha+1)(\alpha+\beta)(\alpha+\beta+1)}{n(n+\beta)\left(n+\frac{\alpha+\beta}{2}+1\right)} \\
&= 1 + \frac{(2\alpha+1)n^2+(2\alpha+1)(\alpha+\beta+1)n+\frac{1}{2}(\alpha+1)(\alpha+\beta)(\alpha+\beta+1)}{n(n+\beta)\left(n+\frac{\alpha+\beta}{2}+1\right)}.
\end{aligned}
$$

According to (3.43) the fraction on the left has to be greater or equal to 1. Since $\alpha > -1$ and $\beta > -1$, the denominator is positive, therefore it is necessary that

$$
(2\alpha+1)n^2+(2\alpha+1)(\alpha+\beta+1)n+\frac{1}{2}(\alpha+1)(\alpha+\beta)(\alpha+\beta+1) \geq 0,
$$

which leads to (3.41). For the leftmost node, from (1.36), we have

$$
P_n^{(\beta,\alpha)}(t) = (-1)^n P_n^{(\alpha,\beta)}(-t),
$$

that is,

$$P_n^{(\alpha,\beta)}(-1) = (-1)^n P_n^{(\beta,\alpha)}(1),$$

therefore,

$$\pi_n^{(\alpha,\beta)}(-1) = (-1)^n \pi_n^{(\beta,\alpha)}(1).$$

Thus,

$$\frac{\pi_{n+1}^{(\alpha,\beta)}(-1)}{\pi_{n-1}^{(\alpha,\beta)}(-1)} = \frac{(-1)^{n+1}\pi_{n+1}^{(\beta,\alpha)}(1)}{(-1)^{n-1}\pi_{n-1}^{(\beta,\alpha)}(1)} = \frac{(-1)^2\pi_{n+1}^{(\beta,\alpha)}(1)}{\pi_{n-1}^{(\beta,\alpha)}(1)} = \frac{\pi_{n+1}^{(\beta,\alpha)}(1)}{\pi_{n-1}^{(\beta,\alpha)}(1)},$$

and

$$\frac{\frac{\pi_{n+1}^{(\alpha,\beta)}(-1)}{\pi_{n-1}^{(\alpha,\beta)}(-1)}}{\beta_n^J} = \frac{\frac{\pi_{n+1}^{(\beta,\alpha)}(1)}{\pi_{n-1}^{(\beta,\alpha)}(1)}}{\beta_n^J},$$

which means that in order to have

$$\frac{\frac{\pi_{n+1}^{(\alpha,\beta)}(-1)}{\pi_{n-1}^{(\alpha,\beta)}(-1)}}{\beta_n^J} \geq 1,$$

we need

$$\frac{\frac{\pi_{n+1}^{(\beta,\alpha)}(1)}{\pi_{n-1}^{(\beta,\alpha)}(1)}}{\beta_n^J} \geq 1,$$

that is, all we have to do is to interchange α and β in (3.41), which leads immediately to (3.42). □

Conditions (3.41) and (3.42) contain the factors n^2 and n, therefore their practical value is limited. In an attempt to provide some more enlightening conditions for the Jacobi weight function, we present the following theorem.

Theorem 3.5. *([8], Theorem 4) The anti-Gauss formula* (3.1) *for the Jacobi weight function* (3.40) *has all its nodes contained in* $[-1, 1]$*, if* α *and* β *satisfy the following inequalities*

$$\alpha \geq -\frac{1}{2}, \tag{3.45}$$

$$\beta \geq -\frac{1}{2}, \tag{3.46}$$

$$(2\alpha+1)(\alpha+\beta+2)+\frac{1}{2}(\alpha+1)(\alpha+\beta)(\alpha+\beta+1) \geq 0, \tag{3.47}$$

$$(2\beta+1)(\alpha+\beta+2)+\frac{1}{2}(\beta+1)(\alpha+\beta)(\alpha+\beta+1) \geq 0. \tag{3.48}$$

Proof. Considering the polynomials on the left side of (3.41) and (3.42), note that, assuming (3.45) and (3.46), we get

$$2\alpha+1 \geq 0,\ \ 2\beta+1 \geq 0,\ \ \alpha+\beta+1 \geq 0,$$

that is, the coefficients of n^2 and n are positive, therefore their first derivative will be positive and they can be treated as increasing functions of n,

$$g(n) = (2\alpha+1)n^2+(2\alpha+1)(\alpha+\beta+1)n+\frac{1}{2}(\alpha+1)(\alpha+\beta)(\alpha+\beta+1) \tag{3.49}$$

and

$$h(n) = (2\beta+1)n^2+(2\beta+1)(\alpha+\beta+1)n+\frac{1}{2}(\beta+1)(\alpha+\beta)(\alpha+\beta+1). \tag{3.50}$$

Then, for $n \geq 1$, we have $g(n) \geq g(1)$ and $h(n) \geq h(1)$, that is,

$$g(n) \geq (2\alpha+1)(\alpha+\beta+2)+\frac{1}{2}(\alpha+1)(\alpha+\beta)(\alpha+\beta+1)$$

and

$$h(n) \geq (2\beta+1)(\alpha+\beta+2)+\frac{1}{2}(\beta+1)(\alpha+\beta)(\alpha+\beta+1),$$

which, by (3.47) and (3.48), show that $g(n) \geq 0$ and $h(n) \geq 0$, proving (3.41) and (3.42). □

Remark 3.6. In the special case that $\alpha = \beta$, the conditions of Theorem 3.5 read

$$\alpha \geq -\frac{1}{2} \tag{3.51}$$

and

$$(\alpha + 1)(\alpha + 2)(2\alpha + 1) \geq 0. \tag{3.52}$$

By means of Remark 1.21 and Table 1.2, Legendre, Chebyshev and Gegenbauer weight functions are special cases of the Jacobi weight function. Using Theorem 3.5 and Remark 3.6, we can now check which of them have all their nodes contained in $[-1, 1]$.

(i) The Legendre weight function,

$$w(t) = 1,$$

is the Jacobi weight function with $\alpha = \beta = 0$, hence (3.51) and (3.52) are obviously both true, thus, the anti-Gauss formula for the Legendre weight function has all its nodes contained in $[-1, 1]$.

(ii) For the Chebyshev weight functions of the first or second kind, we have $\alpha = \beta = -\frac{1}{2}$ and $\alpha = \beta = \frac{1}{2}$, respectively, hence, (3.51) and (3.52) are again true, thus, the anti-Gauss formula for the Chebyshev weight functions of the first or second kind have all their nodes contained in $[-1, 1]$.

(iii) The Gegenbauer weight function is

$$w(t) = \left(1 - t^2\right)^{\lambda - 1/2}, \ \lambda > -\frac{1}{2}. \tag{3.53}$$

This is the Jacobi weight function with $\alpha = \beta = \lambda - \frac{1}{2}$. Hence, (3.51) is true for $\lambda - \frac{1}{2} \geq -\frac{1}{2}$, that is, $\lambda \geq 0$. Also, setting $\alpha = \lambda - \frac{1}{2}$ in (3.52), we get

$$2\lambda \left(\lambda + \frac{1}{2}\right) \left(\lambda + \frac{3}{2}\right) \geq 0,$$

which is true as long as $\lambda \geq 0$, thus, the anti-Gauss formula for the Gegenbauer weight function with $\lambda \geq 0$ has all its nodes contained in $[-1, 1]$.

(iv) The Chebyshev weight function of the third kind is

$$w(t) = (1-t)^{-1/2}(1+t)^{1/2},$$

that is, it is the Jacobi weight function with $\alpha = -\frac{1}{2}$, $\beta = \frac{1}{2}$. Therefore (3.45) and (3.46) are satisfied, and the same is the case with (3.47) and (3.48), whose left-hand side gives 0 and 4, respectively, thus, the anti-Gauss formula for the Chebyshev weight function of the third kind has all its nodes contained in $[-1, 1]$. On the other hand, the Chebyshev weight function of the fourth kind comes from the one of the third kind by interchanging α and β, hence, (3.45)-(3.48) are true, and the anti-Gauss formula for the Chebyshev weight function of the fourth kind has all its nodes contained in $[-1, 1]$.

From what was said above, it is clear that the anti-Gauss formula is not useful in practice when exterior nodes appear, as the function under the integral is not always known outside of the interval of integration. A few such cases for the Jacobi weight function, where exterior nodes appear, are presented below, although the list is incomplete. As (3.42) arises from (3.41) by interchanging α and β, we only deal with (3.41).

(i) For $\alpha < -\frac{1}{2}$, the leading coefficient in (3.41) will be negative. Therefore, as n increases, the factor n^2 will eventually dominate over the factor n and $g(n)$ will eventually be negative. Thus, (3.41) will not be satisfied and an exterior node of the anti-Gauss formula will appear.

(ii) As $g(n)$ is a quadratic polynomial that has to be positive, we can come up with some conclusions by studying the behaviour of its leading coefficient. By means of (i), we saw that if the leading coefficient of $g(n)$ is negative, then $g(n)$ will eventually be negative, and an exterior node will appear. Now, considering the leading coefficient of $g(n)$ to be equal to zero, that is, $2\alpha+1 = 0$, we have $\alpha = -\frac{1}{2}$ and $g(n) = \frac{1}{2}\frac{1}{2}(\beta-\frac{1}{2})(\beta+\frac{1}{2})$. Thus, $g(n)$ is nonnegative if $\frac{1}{4}(\beta^2 - \frac{1}{4}) \geq 0$, that is, $|\beta| \geq \frac{1}{2}$, while in the opposite case, $|\beta| < \frac{1}{2}$, an exterior node appears.

Putting everything together, we conclude that an exterior node appears in the following cases:

(i) The leading coefficient of $g(n)$ is negative, that is, $\alpha < -\frac{1}{2}$.

(ii) The leading coefficient of $h(n)$ is negative, that is, $\beta < -\frac{1}{2}$.

(iii) The leading coefficient of $g(n)$ is equal to zero, that is, $\alpha = -\frac{1}{2}$ and at the same time $-\frac{1}{2} < \beta < \frac{1}{2}$.

(iv) The leading coefficient of $h(n)$ is equal to zero, that is, $\beta = -\frac{1}{2}$ and at the same time $-\frac{1}{2} < \alpha < \frac{1}{2}$.

Chapter 4

Numerical Experiments

This chapter contains some numerical experiments, in order to demonstrate the efficiency of the anti-Gauss quadrature formula. We will estimate the error of the Gauss quadrature formula, using the anti-Gauss quadrature formula and the averaged Gauss formula, for the Legendre and the Jacobi weight functions (cf. [9]).

As we already mentioned in Chapter 3, the idea is to estimate the error of the Gauss quadrature formula as $\left|R_n^G(f)\right| \cong \left|Q_n^G(f) - Q_m(f)\right|$ for $m \geq n+1$. Therefore, we consider the cases that the $(n+1)$-point anti-Gauss formula (3.1) and the $(2n+1)$-point averaged Gauss formula (3.5) serve as the formula Q_m. For the anti-Gauss formula, we have

$$\left|R_n^G(f)\right| \cong \left|Q_n^G(f) - Q_{n+1}^{AG}(f)\right|, \tag{4.1}$$

and for the averaged Gauss formula, we have

$$\begin{aligned}\left|R_n^G(f)\right| \cong \left|Q_n^G(f) - Q_{2n+1}^{AvG}(f)\right| &= \left|Q_n^G(f) - \frac{Q_n^G(f) + Q_{n+1}^{AG}(f)}{2}\right| \\ &= \left|\frac{2Q_n^G(f) - Q_n^G(f) - Q_{n+1}^{AG}(f)}{2}\right| = \left|\frac{Q_n^G(f) - Q_{n+1}^{AG}(f)}{2}\right|.\end{aligned} \tag{4.2}$$

4.1 Legendre

In this section, the weight function used in estimates (4.1) and (4.2) is the Legendre weight $w(t) = 1$, while all computations were performed using the Variable-Precision Arithmetic (VPA) environment in MATLAB, with precision up to 1000 digits.

Example 4.1.1. Initially, we estimate the error of the Gauss formula for the integral $I = \int_{-1}^{1} e^t \mathrm{d}t = e^1 - e^{-1}$. In Tables 4.1 and 4.2, we give the numerical results for estimates (4.1) and (4.2), respectively, together with the modulus of the actual error.

Table 4.1: Estimate (4.1) and actual error for $I = \int_{-1}^{1} e^t \mathrm{d}t$.

n	Estimate (4.1)	Actual error
5	1.649563569467706e-09	8.247769138932894e-10
10	2.432437283897074e-24	1.216218354823625e-24
20	6.960214019148526e-60	3.480106980173639e-60
40	7.239283310034370e-143	3.619641653991043e-143

Table 4.2: Estimate (4.2) and actual error for $I = \int_{-1}^{1} e^t \mathrm{d}t$.

n	Estimate (4.2)	Actual error
5	8.247817847338532e-10	8.247769138932894e-10
10	1.216218641948537e-24	1.216218354823625e-24
20	3.480107009574263e-60	3.480106980173639e-60
40	3.619641655017185e-143	3.619641653991043e-143

Example 4.1.2. We approximate the integral $I = \int_{-1}^{1} e^{-t^2} \mathrm{d}t$ using the Gauss formula. The true value of the integral is $I = \sqrt{\pi} erf(1)$, where erf is the Gauss error function (cf. [1], Chapter 7)

$$erf(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-t^2} \mathrm{d}t = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n z^{2n+1}}{n!(2n+1)} \text{ for } z \in \mathbb{C}, \tag{4.3}$$

which is an odd function, that is,

$$erf(z) = -erf(-z). \tag{4.4}$$

Indeed, from (4.3), we have

$$\sqrt{\pi} erf(1) = 2 \int_0^1 e^{-t^2} \mathrm{d}t, \tag{4.5}$$

while

$$I = \int_{-1}^{0} e^{-t^2} \mathrm{d}t + \int_0^1 e^{-t^2} \mathrm{d}t,$$

Using the change of variables $s = -t$, $\mathrm{d}s = -\mathrm{d}t$, for the first integral, we have

$$I = \int_0^1 e^{-s^2} \mathrm{d}s + \int_0^1 e^{-t^2} \mathrm{d}t = 2 \int_0^1 e^{-t^2} \mathrm{d}t,$$

which in view of (4.5) is equivalent to

$$I = \sqrt{\pi} erf(1).$$

Again, in Tables 4.3 and 4.4, we give the numerical results for estimates (4.1) and (4.2), respectively, together with the modulus of the actual error.

Table 4.3: Estimate (4.1) and actual error for $I = \int_{-1}^{1} e^{-t^2} \mathrm{d}t$.

n	Estimate (4.1)	Actual error
5	3.130672405186399e-05	1.565507777521841e-05
10	1.006966058883533e-12	5.034875969157381e-13
20	1.428790122547697e-30	7.143955336131804e-31
40	3.869382477999645e-72	1.934691325738109e-72
80	3.646184218119460e-167	1.823092114388136e-167

Table 4.4: Estimate (4.2) and actual error for $I = \int_{-1}^{1} e^{-t^2} \mathrm{d}t$.

n	Estimate (4.2)	Actual error
5	1.565336202593200e-05	1.565507777521841e-05
10	5.034830294417667e-13	5.034875969157381e-13
20	7.143950612738487e-31	7.143955336131804e-31
40	1.934691238999822e-72	1.934691325738109e-72
80	1.823092109059730e-167	1.823092114388136e-167

Example 4.1.3. We will now approximate the integral $I = \int_{-1}^{1} e^{-1/t^2} \mathrm{d}t$. For the true value of the integral we will use the Complementary error function $erfc$ (cf. [1], Chapter 7), defined as

$$erfc(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2} \mathrm{d}t = 1 - erf(x). \tag{4.6}$$

From (4.6), we have

$$\sqrt{\pi} erfc(z) = 2 \int_z^\infty e^{-t^2} \mathrm{d}t, \tag{4.7}$$

while

$$I = \int_{-1}^{0} e^{-1/t^2} \mathrm{d}t + \int_0^1 e^{-1/t^2} \mathrm{d}t.$$

Using the change of variables $s = -t$, $\mathrm{d}s = -\mathrm{d}t$, for the first integral above, we obtain

$$I = \int_0^1 e^{-1/s^2} \mathrm{d}s + \int_0^1 e^{-1/t^2} \mathrm{d}t = 2 \int_0^1 e^{-1/t^2} \mathrm{d}t = -2 \int_1^0 e^{-1/t^2} \mathrm{d}t.$$

Now, using the change of variables $t = \frac{1}{s}$, $\mathrm{d}t = -\frac{1}{s^2}\mathrm{d}s$, we get

$$\begin{aligned} I &= -2 \int_1^\infty e^{-s^2} \left(-\frac{1}{s^2}\right) \mathrm{d}s = -2 \int_1^\infty e^{-s^2} \left(\frac{1}{s}\right)' \mathrm{d}s \\ &= 2e^{-1} + 2 \int_1^\infty e^{-s^2} (-2s) \left(\frac{1}{s}\right) \mathrm{d}s = 2e^{-1} - 4 \int_1^\infty e^{-s^2} \mathrm{d}s, \end{aligned}$$

which in view of (4.6) and (4.7) is equivalent to

$$I = 2e^{-1} - 2\sqrt{\pi} erfc(1) = 2e^{-1} - 2\sqrt{\pi}(1 - erf(1)),$$

that is,

$$I = 2e^{-1} + 2\sqrt{\pi}(erf(1) - 1).$$

As in the previous examples, Tables 4.5 and 4.6 present estimates (4.1) and (4.2), respectively, together with the modulus of the actual error.

Table 4.5: Estimate (4.1) and actual error for $I = \int_{-1}^{1} e^{-1/t^2} \mathrm{d}t$.

n	Estimate (4.1)	Actual error
5	0.015228276095027	0.007519003085511
10	5.869166215796041e-04	2.949257632352353e-04
20	3.290885090567718e-07	1.683469013353369e-07
40	9.870541920653552e-09	4.935191767365378e-09
80	1.549614680022323e-13	7.748073696627641e-14

Table 4.6: Estimate (4.2) and actual error for $I = \int_{-1}^{1} e^{-1/t^2} \mathrm{d}t$.

n	Estimate (4.2)	Actual error
5	0.007614138047513	0.007519003085511
10	2.934583107898021e-04	2.949257632352353e-04
20	1.645442545283859e-07	1.683469013353369e-07
40	4.935270960326776e-09	4.935191767365378e-09
80	7.748073400111616e-14	7.748073696627641e-14

Example 4.1.4. Finally, we approximate the integral $I = \int_{-1}^{1} \frac{1}{1+16t^2} \mathrm{d}t$. For the true value of the integral, we have

$$I = \int_{-1}^{1} \frac{1}{1+(4t)^2} \mathrm{d}t.$$

Now, using the change of variables $s = 4t$, $\mathrm{d}s = 4\mathrm{d}t$, we obtain

$$I = \frac{1}{4}\int_{-4}^{4} \frac{1}{1+s^2}\mathrm{d}s = \frac{1}{4}(\mathrm{atan}(4) - \mathrm{atan}(-4)),$$

and since atan is an odd function, the true value of the integral is

$$I = \frac{\mathrm{atan}(4)}{2}.$$

In Tables 4.7 and 4.8, we give the numerical results for estimates (4.1) and (4.2), respectively, together with the modulus of the actual error.

Table 4.7: Estimate (4.1) and actual error for $I = \int_{-1}^{1} \frac{1}{1+16t^2}\mathrm{d}t$.

n	Estimate (4.1)	Actual error
5	0.205122811304407	0.109245922960595
10	0.017286883438072	0.008596090847809
20	1.228738477782558e-04	6.143472340767940e-05
40	6.182453875566150e-09	3.091228257710790e-09
80	1.561774927512982e-17	7.808875064548930e-18

Table 4.8: Estimate (4.2) and actual error for $I = \int_{-1}^{1} \frac{1}{1+16t^2}\mathrm{d}t$.

n	Estimate (4.2)	Actual error
5	0.102561405652204	0.109245922960595
10	0.008643441719036	0.008596090847809
20	6.143692388912789e-05	6.143472340767940e-05
40	3.091226937783075e-09	3.091228257710790e-09
80	7.808874637564909e-18	7.808875064548930e-18

Using precision up to 1000 decimal digits and the Legendre weight function, we see that the anti-Gauss formula is a reliable estimation method for the Gauss formula, since in almost all cases estimate (4.1) provides the correct order of magnitude for the actual error. Estimate (4.2), on the other hand, which results from halving the value of estimate (4.1), provides a substantial improvement.

4.2 Jacobi

In this section, we will study the behaviour of the anti-Gauss formula for the Jacobi weight function $w(t) = (1-t)^{\alpha}(1+t)^{\beta}$. We will approximate the integral

$$I = \int_{-1}^{1} \frac{e^{\omega t^2}(1-t)^{\alpha}(1+t)^{\beta}}{1+8t^2}\mathrm{d}t, \ \omega > 0. \tag{4.8}$$

All computations were performed in double precision. The true value of the integral was computed by the *integral* function of MATLAB.

Example 4.2.1. Initially, we consider $\alpha = \beta = \frac{1}{2}$, that is, the Chebyshev weight function of the second kind $w(t) = (1 - t^2)^{\frac{1}{2}}$. As in the previous section, Tables 4.9 and 4.10, contain the error estimates (4.1) and (4.2), respectively, together with the modulus of the actual error.

Table 4.9: Estimate (4.1) and actual error for $I = \int_{-1}^{1} \frac{e^{\omega t^2}(1-t^2)^{\frac{1}{2}}}{1+8t^2} \mathrm{d}t$.

ω	n	Estimate (4.1)	Actual error
0.25	5	0.071383115088757	0.036249238132116
	10	0.002230178272716	0.001114544659241
	20	2.177907950207114e-06	1.088953455075092e-06
0.5	5	0.069186877779459	0.035133961449588
	10	0.002161562900724	0.001080253725044
	20	2.110900767293700e-06	1.055449879383552e-06
1	5	0.064994311764058	0.033004929835505
	10	0.002030600425047	0.001014804460467
	20	1.983007755224087e-06	9.915034041574344e-07
2	5	0.057288369395571	0.029092293638008
	10	0.001791998629716	8.955618152033384e-04
	20	1.749998201905356e-06	8.749986832867762e-07
4	5	0.034907027011926	0.017802491820914
	10	0.001395827683353	6.975731166041221e-04
	20	1.362899972212617e-06	6.814496613660737e-07

Table 4.10: Estimate (4.2) and actual error for $I = \int_{-1}^{1} \frac{e^{\omega t^2}(1-t^2)^{\frac{1}{2}}}{1+8t^2} \mathrm{d}t$.

ω	n	Estimate (4.2)	Actual error
0.25	5	0.035691557544379	0.036249238132116
	10	0.001115089136358	0.001114544659241
	20	1.088953975103557e-06	1.088953455075092e-06
0.5	5	0.034593438889730	0.035133961449588
	10	0.001080781450362	0.001080253725044
	20	1.055450383646850e-06	1.055449879383552e-06
1	5	0.032497155882029	0.033004929835505
	10	0.001015300212523	0.001014804460467
	20	9.915038776120433e-07	9.915034041574344e-07
2	5	0.028644184697786	0.029092293638008
	10	8.959993148578427e-04	8.955618152033384e-04
	20	8.749991009526781e-07	8.749986832867762e-07
4	5	0.017453513505963	0.017802491820914
	10	6.979138416766117e-04	6.975731166041221e-04
	20	6.814499861063084e-07	6.814496613660737e-07

Example 4.2.2. We will approximate the integral (4.8), with $\alpha = \beta = \frac{3}{2}$, that is, the Gegenbauer weight function $w(t) = (1-t^2)^{\lambda - \frac{1}{2}}$ with $\lambda = 2$. In Tables 4.11 and 4.12, we give the numerical results for estimates (4.1) and (4.2), respectively, together with the modulus of the actual error.

Table 4.11: Estimate (4.1) and actual error for $I = \int_{-1}^{1} \frac{e^{\omega t^2}(1-t^2)^{\frac{3}{2}}}{1+8t^2} \mathrm{d}t$.

ω	n	Estimate (4.1)	Actual error
0.25	5	0.044199092686496	0.022270143659878
	10	0.001326388493740	6.629085408508262e-04
	20	1.262802994728141e-06	6.313837364047004e-07
0.5	5	0.042839226400849	0.021584961789048
	10	0.001285579809960	6.425129892110304e-04
	20	1.223950630846460e-06	6.119581009711439e-07
1	5	0.040243493377848	0.020277077254218
	10	0.001207690466769	6.035850950940613e-04
	20	1.149795210819704e-06	5.748814339012753e-07
2	5	0.035494167217541	0.017884150331034
	10	0.001065783108368	5.326619829488788e-04
	20	1.014690712120014e-06	5.073310849201818e-07
4	5	0.025075336234975	0.012640272704681
	10	8.300882254255182e-04	4.148653301361271e-04
	20	7.902419214556033e-07	3.951098468402137e-07

Table 4.12: Estimate (4.2) and actual error for $I = \int_{-1}^{1} \frac{e^{\omega t^2}(1-t^2)^{\frac{3}{2}}}{1+8t^2} \mathrm{d}t$.

ω	n	Estimate (4.2)	Actual error
0.25	5	0.022099546343248	0.022270143659878
	10	6.631942468698360e-04	6.629085408508262e-04
	20	6.314014973640703e-07	6.313837364047004e-07
0.5	5	0.021419613200424	0.021584961789048
	10	6.427899049798458e-04	6.425129892110304e-04
	20	6.119753154232299e-07	6.119581009711439e-07
1	5	0.020121746688924	0.020277077254218
	10	6.038452333846922e-04	6.035850950940613e-04
	20	5.748976054098520e-07	5.748814339012753e-07
2	5	0.017747083608771	0.017884150331034
	10	5.328915541839563e-04	5.326619829488788e-04
	20	5.073453560600072e-07	5.073310849201818e-07
4	5	0.012537668117487	0.012640272704681
	10	4.150441127127591e-04	4.148653301361271e-04
	20	3.951209607278017e-07	3.951098468402137e-07

Example 4.2.3. Finally, we approximate the integral I with $\alpha = \frac{1}{3}$ and $\beta = -\frac{1}{4}$.

Table 4.13: Estimate (4.1) and actual error for $I = \int_{-1}^{1} \frac{e^{\omega t^2}(1-t)^{\frac{1}{3}}(1+t)^{-\frac{1}{4}}}{1+8t^2}\mathrm{d}t$.

ω	n	Estimate (4.1)	Actual error
0.25	5	0.069496127215217	0.034696534494634
	10	0.002179184883428	0.001089661935765
	20	2.131488573975382e-06	1.064313069787381e-06
0.5	5	0.067357937796257	0.033629019306656
	10	0.002112138413087	0.001056142425478
	20	2.065909564752388e-06	1.037430589434507e-06
1	5	0.063275481561782	0.031590799285776
	10	0.001984170415751	9.921722478754003e-04
	20	1.940742432315901e-06	9.928330242381378e-07
2	5	0.055698534594749	0.027807866746119
	10	0.001751024333993	8.755778952291848e-04
	20	1.712699185807409e-06	8.650877718618943e-07
4	5	0.020662164821396	0.010305147019150
	10	0.001364163421496	6.821495847706416e-04
	20	1.333851475937564e-06	6.904236546922959e-07

Table 4.14: Estimate (4.2) and actual error for $I = \int_{-1}^{1} \frac{e^{\omega t^2}(1-t)^{\frac{1}{3}}(1+t)^{-\frac{1}{4}}}{1+8t^2} \mathrm{d}t$.

ω	n	Estimate (4.2)	Actual error
0.25	5	0.034748063607609	0.034696534494634
	10	0.001089592441714	0.001089661935765
	20	1.065744286987691e-06	1.064313069787381e-06
0.5	5	0.033678968898128	0.033629019306656
	10	0.001056069206543	0.001056142425478
	20	1.032954782376194e-06	1.037430589434507e-06
1	5	0.031637740780891	0.031590799285776
	10	9.920852078753040e-04	9.921722478754003e-04
	20	9.703712161579503e-07	9.928330242381378e-07
2	5	0.027849267297374	0.027807866746119
	10	8.755121669966615e-04	8.755778952291848e-04
	20	8.563495929037046e-07	8.650877718618943e-07
4	5	0.010331082410698	0.010305147019150
	10	6.820817107482391e-04	6.821495847706416e-04
	20	6.669257379687821e-07	6.904236546922959e-07

Again, estimate (4.1) is close to the actual error, while an improvement is made by estimate (4.2), which is even closer to the actual error.

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