ERROR ESTIMATE FOR THE GAUSS QUADRATURE FORMULA: THE GAUSS-KRONROD vs THE ANTI-GAUSSIAN APPROACH

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Gauss quadrature formula (Gauss 1814)

Let $d\sigma$ be a (nonnegative) measure on the interval $[a,b]$, and

$$\int_a^b f(t)d\sigma(t) = \sum_{\nu=1}^{n} \lambda_\nu f(\tau_\nu) + R_n^G(f), \qquad (1)$$

where:

- The $\tau_\nu = \tau_\nu^{(n)}$ are the zeros of the nth degree (monic) orthogonal polynomial $\pi_n(\cdot) = \pi_n(\cdot; d\sigma)$, hence, they are all in (a,b).
- The $\lambda_\nu = \lambda_\nu^{(n)}$ are all positive.
- Formula (1) has precise degree of exactness $d_n^G = 2n-1$, i.e., $R_n^G(f) = 0$ for all $f \in \mathbb{P}_{2n-1}$.

Methods for studying the error term R_n^G

- Peano kernel methods

  Given that $R_n^G(f) = 0$ for all $f \in \mathbb{P}_{s-1}$, if f has a piecewise continuous derivative of order s on $[a, b]$ (or, less restrictively, $f^{(s-1)}$ is absolutely continuous on $[a, b]$), then, by the Peano representation theorem,

$$|R_n^G(f)| \le c_s \max_{a \le t \le b} |f^{(s)}(t)|, \quad c_s = \int_a^b |K_s(t)| dt, \quad s = 1, 2, \ldots, d_n^G + 1,$$

  where K_s is the s-th Peano kernel of R_n^G.
  For $s = d_n^G + 1 = 2n$, we have $c_{2n} = [(2n)!]^{-1} \int_a^b \pi_n^2(t) d\sigma(t)$.
  Task: Compute or estimate $\int_a^b |K_s(t)| dt$, even asymptotically.

- Contour integration methods

  If f is single-valued holomorphic in a domain D, Γ is a contour in D surrounding $[a, b]$ and $\ell(\Gamma)$ is the length of Γ, then

$$|R_n^G(f)| \le \frac{\ell(\Gamma)}{2\pi} \max_{z \in \Gamma} |\tilde{K}_n(z)| \max_{z \in \Gamma} |f(z)|,$$

  where $\tilde{K}$ is the kernel of R_n^G.
  Task: Compute or estimate $\max_{z \in \Gamma} |\tilde{K}_n(z)|$.

- Hilbert space techniques

  If f is single-valued holomorphic in a domain D and $H = H(D)$ is a Hilbert space, then R_n^G is a bounded linear functional in H and

$$|R_n^G(f)| \le \|R_n^G\| \|f\|,$$

  where $\|R_n^G\|$ is the norm of the error functional R_n^G and $\|f\|$ is the norm of f in the Hilbert space H.
  Task: Compute or estimate $\|R_n^G\|$.

W. Gautschi, A survey of Gauss-Christoffel quadrature formulae, in *E.B. Christoffel: The influence of his work on mathematics and the physical sciences*, P.L. Butzer and F. Fehér, eds., Birkhäuser, Basel, 1981, pp. 72-147.

What can we do if the smoothness of f is quite low of if we have no information on the smoothness of f?

Practical error estimator

Let $I(f) = \int_a^b f(t) d\sigma(t)$, $\quad Q_n^G(f) = \sum_{\nu=1}^n \lambda_\nu f(\tau_\nu)$ and consider a quadrature formula with $m > n$ points, quadrature sum $Q_m(f)$ and degree of exactness greater than $2n-1$. Then, we write

$$|R_n^G(f)| \simeq |Q_n^G(f) - Q_m(f)|, \tag{2}$$

i.e., $Q_m(f)$ plays the role of the "true" value of $I(f)$.

As the Gauss formula has optimal degree of exactness for an n-point quadrature formula, the smallest value for $m = n+1$.

So, what is an appropriate m-point formula?
In particular, using the already known $f(\tau_\nu)$, $\nu = 1, 2, \ldots, n$, can we find a quadrature formula of the highest possible degree of exactness by allowing $n+1$ additional evaluations of the function, i.e., a quadrature formula which uses the τ_ν, $\nu = 1, 2, \ldots, n$, and, in addition, $n+1$ new points τ_μ^*, $\mu = 1, 2, \ldots, n+1$?

Gauss-Kronrod quadrature formula (Kronrod 1964)

Let $d\sigma$ be a (nonnegative) measure on the interval $[a,b]$, and

$$\int_a^b f(t)d\sigma(t) = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*) + R_n^K(f), \tag{3}$$

where:

- The τ_ν are the Gauss nodes.
- The $\tau_\mu^* = \tau_\mu^{*(n)}$, $\sigma_\nu = \sigma_\nu^{(n)}$, $\sigma_\mu^* = \sigma_\mu^{*(n)}$ are chosen such that formula (3) has maximum degree of exactness.
- Formula (3) has degree of exactness (at least) $d_n^K = 3n+1$.

Desirable properties:

- The nodes τ_μ^*, $\mu = 1, 2, \ldots, n+1$, are all real and interlace with the nodes τ_ν, $\nu = 1, 2, \ldots, n$, of the Gauss formula, that is,

$$\tau_{n+1}^* < \tau_n < \tau_n^* < \cdots < \tau_2^* < \tau_1 < \tau_1^*.$$

- The nodes τ_μ^*, $\mu = 1, 2, \ldots, n+1$, are all contained in $[a,b]$.
- The weights σ_ν, $\nu = 1, 2, \ldots, n$, σ_μ^*, $\mu = 1, 2, \ldots, n+1$, are all positive.

The $Q_n^K(f) = \sum_{\nu=1}^{n} \sigma_\nu f(\tau_\nu) + \sum_{\mu=1}^{n+1} \sigma_\mu^* f(\tau_\mu^*)$ can be used in place of $Q_m(f)$ in (2). Advantage: With $n+1$ new evaluations of the function (at the τ_μ^*) the degree of exactness is raised from $2n-1$ to (at least) $3n+1$.

Stieltjes polynomial (Stieltjes 1894)

The Kronrod nodes τ_μ^* are zeros of a polynomial $\pi_{n+1}^*(\cdot) = \pi_{n+1}^*(\cdot; d\sigma)$, discovered by Stieltjes, through his work on continued fractions and the moment problem, which is characterized and can be uniquely defined by the orthogonality condition

$$\int_a^b \pi_{n+1}^*(t)t^k\pi_n(t)d\sigma(t) = 0, \quad k = 0, 1, \ldots, n,$$

i.e., π_{n+1}^* is orthogonal to all polynomials of lower degree relative to the variable-sign measure $d\sigma^*(t) = \pi_n(t)d\sigma(t)$ on $[a, b]$.

In view of the above, the Stieltjes polynomial π_{n+1}^* might have complex zeros, in which case the corresponding Gauss-Kronrod formula fails to exist, with real and distinct nodes in the interval of integration and positive weights. Unfortunately, this happens for several of the classical measures:

- For the Gegenbauer measure $d\sigma_\lambda(t) = (1 - t^2)^{\lambda-1/2}dt$ on $[-1, 1]$, $\lambda > -1/2$, when $\lambda > 3$ and n sufficiently large.
- For the Jacobi measure $d\sigma_{\alpha,\beta}(t) = (1-t)^\alpha(1+t)^\beta dt$ on $[-1, 1]$, $\alpha, \beta > -1$, when $\min(\alpha, \beta) \geq 0$ and $\max(\alpha, \beta) > 5/2$ and n sufficiently large.
- For the Hermite measure $d\sigma^H(t) = e^{-t^2}dt$ on $(-\infty, \infty)$.
- For the Laguerre measure $d\sigma^{(\alpha)}(t) = t^\alpha e^{-t}dt$ on $(0, \infty)$, $\alpha > -1$, when $-1 < \alpha \leq 1$, and n sufficiently large.

We have positive results, i.e., the Gauss-Kronrod formula exists with real and distinct nodes in the interval of integration and positive weights, for several nonclassical measures, in particular, the Bernstein-Szegö mesures, which are defined by

$$d\sigma^{(\pm 1/2)}(t) = \frac{(1-t^2)^{\pm 1/2}}{\rho(t)} dt, \quad -1 < t < 1,$$

$$d\sigma^{(\pm 1/2, \mp 1/2)}(t) = \frac{(1-t)^{\pm 1/2}(1+t)^{\mp 1/2}}{\rho(t)} dt, \quad -1 < t < 1,$$

where ρ is an arbitrary polynomial that remains positive on $[-1, 1]$.

S.N., Gauss-Kronrod quadrature formulae - A survey of fifty years of research, *Electron. Trans. Numer. Anal.*, v. 45, 2016, pp. 371–404.

So, what can we do in those cases that the Gauss-Kronrod formula fails to exist?

Anti-Gaussian quadrature formula (Laurie 1996)

Let $d\sigma$ be a (nonnegative) measure on the interval $[a,b]$, and

$$\int_a^b f(t)d\sigma(t) = \sum_{\mu=1}^{n+1} w_\mu f(t_\mu) + R_{n+1}^{AG}(f), \tag{4}$$

which is designed to have an error precisely opposite to the error of the Gauss formula, that is, if

$$Q_{n+1}^{AG}(f) = \sum_{\mu=1}^{n+1} w_\mu f(t_\mu),$$

then

$$R_{n+1}^{AG}(p) = -R_n^G(p) \quad \text{for all} \quad p \in \mathbb{P}_{2n+1},$$

i.e.,

$$I(p) - Q_{n+1}^{AG}(p) = -[I(p) - Q_n^G(p)] \quad \text{for all} \quad p \in \mathbb{P}_{2n+1}.$$

The anti-Gaussian formula has the following properties:

- The nodes $t_\mu,\ \mu = 1,2,\ldots,n+1$, are zeros of the polynomial

  $$\pi_{n+1}^{AG}(t) = \pi_{n+1}(t) - \beta_n \pi_{n-1}(t),$$

  where β_n are the coefficients in the three-term recurrence relation for the orthogonal polynomials π_n.

- The nodes $t_\mu,\ \mu = 1,2,\ldots,n+1$, are all real and interlace with the nodes $\tau_\nu,\ \nu = 1,2,\ldots,n$, of the Gauss formula.

- The nodes $t_\mu,\ \mu = 2,3,\ldots,n$, are all contained in $[a,b]$.

- The node $t_{n+1} \in [a,b]$ if and only if $\frac{\pi_{n+1}(a)}{\pi_{n-1}(a)} \geq \beta_n$, and the node $t_1 \in [a,b]$ if and only if $\frac{\pi_{n+1}(b)}{\pi_{n-1}(b)} \geq \beta_n$.

- The weights $w_\mu,\ \mu = 1,2,\ldots,n+1$, are all positive.

- The anti-Gaussian formula can easily be constructed.

Averaged Gaussian quadrature formula (Laurie 1996)

This is the $(2n+1)$-point quadrature formula obtained by the quadrature sum

$$Q_{2n+1}^{AvG}(f) = \frac{1}{2}(Q_n^G(f) + Q_{n+1}^{AG}(f)). \tag{5}$$

This formula has degree of exactness (at least) $2n+1$.

The $Q_{2n+1}^{AvG}(f)$ can be used in place of $Q_m(f)$ in (2).
Advantage: With $n+1$ new evaluations of the function (at the t_μ) the degree of exactness is raised from $2n-1$ to (at least) $2n+1$.

Comparison between Gauss-Kronrod formula and averaged Gaussian formula

- The Gauss-Kronrod formula does not always exist with the desirable properties, but whenever it does exist its degree of exactness is (at least) $3n+1$.
- The averaged Gaussian formula does always exist with the desirable properties, but the degree of exactness is (at least) $2n+1$.
- Can we have a formula that combines the advantages of both the Gauss-Kronrod formula and the averaged Gaussian formula, i.e., a formula having the desirable properties as well as degree of exactness (at least) $3n+1$?
- Is it possible for a measure $d\sigma$ on $[a,b]$ to get the same error estimate for the Gauss formula by using either the Gauss-Kronrod formula or the averaged Gaussian formula, i.e., a measure $d\sigma$ on $[a,b]$ for which the Gauss-Kronrod formula coincides with the averaged Gaussian formula?

Measures with constant recurrence coefficients (Gautschi and N. 1996)

Let the (monic) orthogonal polynomials relative to a (nonnegative) measure $d\sigma$ satisfy a three-term recurrence relation of the form,

$$\pi_{n+1}(t) = (t - \alpha_n)\pi_n(t) - \beta_n \pi_{n-1}(t), \quad n = 0, 1, 2, \ldots,$$

$$\alpha_n = \alpha, \quad \beta_n = \beta \ \text{ for all } \ n \geq \ell,$$

where $\alpha_n \in \mathbb{R},\ \beta_n > 0,\ \ell \in \mathbb{N}$, and $\pi_0(t) = 1,\ \pi_{-1}(t) = 0$. Any such measure $d\sigma$ is known to be supported on a finite interval, say $[a, b]$ **(Chihara 1978; Mate, Nevai and VanAssche 1991)**. We write $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a, b]$.

Among the many orthogonal polynomials satisfying a recurrence relation of this kind are the four Chebyshev-type polynomials, as well as those associated with the Bernstein-Szegö measures.

If $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a, b]$, then trivially $\alpha_n \to \alpha,\ \beta_n \to \beta$ as $n \to \infty$, and it follows **(Chihara 1978)** that

$$[\alpha - 2\sqrt{\beta}, \alpha + 2\sqrt{\beta}\,] \tag{6}$$

is the "limiting spectral interval" of $d\sigma$. Although $d\sigma$ might has support points outside the interval (6), for inclusion results we will assume the following property.

Property A The measure $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a, b]$ is such that

$$a = \alpha - 2\sqrt{\beta}, \quad b = \alpha + 2\sqrt{\beta}.$$

Gauss-Kronrod formulae for measures with constant recurrence coefficients (Gautschi and N. 1996)

Theorem 1 Consider a measure $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$. Then the corresponding Stieltjes polynomials are given by

$$\pi_{n+1}^*(t) = \pi_{n+1}(t) - \beta\pi_{n-1}(t) \quad \text{for all} \quad n \geq 2\ell - 1.$$

Proposition 2 Consider a measure $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$ and let τ_ν be the zeros of the corresponding orthogonal polynomial π_n. Then

$$\pi_{n+1}(\tau_\nu) = \frac{1}{2}\pi_{n+1}^*(\tau_\nu), \quad \nu = 1, 2, \ldots, n,$$

for all $n \geq 2\ell - 1$.

Theorem 3 Consider a measure $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$. Then the following holds:

(a) The Gauss-Kronrod formula (3) has the interlacing property for all $n \geq 2\ell - 1$, that is,

$$\tau_{n+1}^* < \tau_n < \tau_n^* < \cdots < \tau_2^* < \tau_1 < \tau_1^*. \tag{7}$$

(b) If $d\sigma$ has Property A, then all τ_μ^* are in $[a,b]$ for all $n \geq 2\ell - 1$.

(c) All weights σ_ν, σ_μ^* in formula (3) are positive for each $n \geq 2\ell - 1$. In particular,

$$\sigma_\nu = \frac{1}{2}\lambda_\nu, \quad \nu = 1, 2, \ldots, n,$$

where λ_ν, $\nu = 1, 2, \ldots, n$, are the weights in the Gauss formula (1).

(d) Formula (3) has degree of exactness (at least) $4n - 2\ell + 2$ if $n \geq 2\ell - 1$.

Anti-Gaussian and averaged Gaussian formulae for measures with constant recurrence coefficients (Spalević 2017, N. 2018)

Theorem 4 Consider a measure $d\sigma \in \mathcal{M}_\ell^{(\alpha,\beta)}[a,b]$. Then the following holds:

(a) The anti-Gaussian formula (4) for all $n \geq 2\ell - 1$ is given by

$$t_\mu = \tau_\mu^*, \quad w_\mu = 2\sigma_\mu^*, \quad \mu = 1, 2, \ldots, n+1,$$

where τ_μ^* are the Stieltjes nodes and σ_μ^* the corresponding weights in the respective Gauss-Kronrod formula (3).

(b) The averaged Gaussian formula obtained by the quadrature sum (5) for all $n \geq 2\ell - 1$ gives the same error estimate for $R_n^G(f)$ as the Gauss-Kronrod formula (3), that is,

$$|R_n^G(f)| \simeq |Q_n^G(f) - Q_n^K(f)| = |Q_n^G(f) - Q_{2n+1}^{AvG}(f)| = \frac{|Q_n^G(f) - Q_{n+1}^{AG}(f)|}{2}.$$

(c) The averaged Gaussian formula obtained by the quadrature sum (5) for all $n \geq 2\ell - 1$ has degree of exactness (at least) $4n - 2\ell + 2$.

Modified anti-Gaussian quadrature formula **(Calvetti and Reichel 2003)**

Let $d\sigma$ be a (nonnegative) measure on the interval $[a, b]$, and

$$\int_a^b f(t)d\sigma(t) = \sum_{\mu=1}^{n+1} w_\mu f(t_\mu) + R_{n+1}^{MAG}(f), \tag{8}$$

which, if

$$Q_{n+1}^{MAG}(f) = \sum_{\mu=1}^{n+1} w_\mu f(t_\mu),$$

is designed such that

$$R_{n+1}^{AG}(p) = -\gamma R_n^G(p) \quad \text{for all} \quad p \in \mathbb{P}_{2n+1}, \quad \gamma > 0,$$

i.e.,

$$I(p) - Q_{n+1}^{AG}(p) = -\gamma[I(p) - Q_n^G(p)] \quad \text{for all} \quad p \in \mathbb{P}_{2n+1}, \quad \gamma > 0.$$

Generalized averaged Gaussian quadrature formula **(Spalević 2007)**

This is the $(2n+1)$-point quadrature formula obtained by the quadrature sum

$$Q_{2n+1}^{GAvG}(f) = \frac{1}{1+\gamma}(\gamma Q_n^G(f) + Q_{n+1}^{MAG}(f)), \quad \gamma > 0. \tag{9}$$

Theorem 5 (N. 2018) Let the (nonnegative) measure $d\sigma$ on the interval $[a,b]$, and assume that the respective orthogonal polynomial $\pi_{n+1}(\cdot) = \pi_{n+1}(\cdot; d\sigma)$ and Stieltjes polynomial $\pi^*_{n+1}(\cdot) = \pi^*_{n+1}(\cdot; d\sigma)$ satisfy

$$\pi_{n+1}(\tau_\nu) = \frac{1}{1+\gamma}\pi^*_{n+1}(\tau_\nu), \quad \nu = 1, 2, \ldots, n, \quad \gamma > 0,$$

where τ_ν, $\nu = 1, 2, \ldots, n$, are the zeros of the orthogonal polynomial $\pi_n(\cdot) = \pi_n(\cdot; d\sigma)$. Then the following hold:

(a) The Gauss-Kronrod formula (3) has the interlacing property (7) and all weights $\sigma_\nu,\ \nu = 1, 2, \ldots, n,\ \sigma^*_\mu,\ \mu = 1, 2, \ldots, n+1$, are positive.

(b) The modified anti-Gaussian formula (8) is given by

$$t_\mu = \tau^*_\mu, \quad w_\mu = (1+\gamma)\sigma^*_\mu, \quad \mu = 1, 2, \ldots, n+1, \quad \gamma > 0.$$

(c) The generalized averaged Gaussian formula (9) gives the same error estimate for $R^G_n(f)$ as the Gauss-Kronrod formula (3), that is,

$$|R^G_n(f)| \simeq |Q^G_n(f) - Q^K_n(f)| = |Q^G_n(f) - Q^{GAvG}_{2n+1}(f)| = \frac{1}{1+\gamma}|Q^G_n(f) - Q^{MAG}_{n+1}(f)|, \ \gamma > 0.$$

(d) The generalized averaged Gaussian formula obtained by the quadrature sum (9) has degree of exactness (at least) $3n+1$.

Measures with constant recurrence coefficients extended (N. submitted)

Let the (monic) orthogonal polynomials relative to a (nonnegative) measure $d\sigma$ satisfy a three-term recurrence relation of the form,

$$\pi_{n+1}(t) = (t - \alpha_n)\pi_n(t) - \beta_n \pi_{n-1}(t), \quad n = 0, 1, 2, \ldots,$$
$$\alpha_n = \begin{cases} \alpha_e, & n \text{ even}, \\ \alpha_o, & n \text{ odd}, \end{cases} \quad \beta_n = \beta \ \text{ for } \ n \geq \ell,$$

where $\alpha_n \in \mathbb{R}$, $\beta_n > 0$, $\ell \in \mathbb{N}$, and $\pi_0(t) = 1$, $\pi_{-1}(t) = 0$. Any such measure $d\sigma$ is known to be supported on a finite interval, say $[a, b]$ **(Chihara 1978)**. We write $d\sigma \in \mathcal{M}_\ell^{(\alpha_e, \alpha_o, \beta)}[a, b]$.

If $d\sigma \in \mathcal{M}_\ell^{(\alpha_e, \alpha_o, \beta)}[a, b]$, then trivially $\alpha_{2n} \to \alpha_e$, $\alpha_{2n-1} \to \alpha_o$ and $\beta_n \to \beta$ as $n \to \infty$, and it follows **(Chihara 1978)** that

$$\left[\frac{\alpha_e + \alpha_o - \sqrt{(\alpha_e - \alpha_o)^2 + 16\beta}}{2}, a^*\right] \cup \left[b^*, \frac{\alpha_e + \alpha_o + \sqrt{(\alpha_e - \alpha_o)^2 + 16\beta}}{2}\right], \tag{10}$$
$$a^* = \min(\alpha_e, \alpha_o), \quad b^* = \max(\alpha_e, \alpha_o),$$

is the "limiting spectral interval" of $d\sigma$. Although $d\sigma$ might has support points outside the interval (10), for inclusion results we will assume the following property.

Property $\mathrm{A_e}$ The measure $d\sigma \in \mathcal{M}_\ell^{(\alpha_e, \alpha_o, \beta)}[a, b]$ is such that

$$a = \frac{\alpha_e + \alpha_o - \sqrt{(\alpha_e - \alpha_o)^2 + 16\beta}}{2}, \quad b = \frac{\alpha_e + \alpha_o + \sqrt{(\alpha_e - \alpha_o)^2 + 16\beta}}{2}.$$

Gauss-Kronrod formulae for measures with constant recurrence coefficients extended (N. submitted)

Theorem 6 Consider a measure $d\sigma \in \mathcal{M}_\ell^{(\alpha_e,\alpha_o,\beta)}[a,b]$. Then the corresponding Stieltjes polynomials are given by

$$\pi^*_{n+1}(t) = \pi_{n+1}(t) - \beta\pi_{n-1}(t) \quad \text{for all} \quad n \geq 2\ell - 1. \tag{11}$$

Are there any other measures, besides those in the class $\mathcal{M}_\ell^{(\alpha_e,\alpha_o,\beta)}[a,b]$, for which the corresponding Stieltjes polynomials are given by (11)?

Theorem 7 Consider a (nonnegative) measure $d\sigma$ on the interval $[a,b]$, and let the respective monic orthogonal polynomials $\pi_n(\,\cdot\,) = \pi_n(\,\cdot\,; d\sigma)$ satisfy a three-term recurrence relation of the form

$$\pi_{n+1}(t) = (t-\alpha_n)\pi_n(t) - \beta_n\pi_{n-1}(t), \quad n = 0,1,2,\ldots,$$
$$\pi_0(t) = 1, \quad \pi_{-1}(t) = 0,$$

where $\alpha_n = \alpha_n(d\sigma) \in \mathbb{R}$ and $\beta_n = \beta_n(d\sigma) > 0$. If the corresponding monic Stieltjes polynomial $\pi^*_{n+1}(\,\cdot\,) = \pi^*_{n+1}(\,\cdot\,; d\sigma)$ is given by

$$\pi^*_{n+1}(t) = \pi_{n+1}(t) - \hat{\beta}\pi_{n-1}(t) \quad \text{for} \quad n \geq 2\ell - 1,$$

where $\hat{\beta} > 0$, then

$$\alpha_n = \alpha_{n+2} \quad \text{for} \quad n \geq 2\ell - 2,$$
$$\beta_n = \hat{\beta} \quad \text{for} \quad n \geq 2\ell.$$

The first of these relations immediately leads to

$$\alpha_n = \begin{cases} \hat{\alpha}_e, & n \text{ even}, \\ \hat{\alpha}_o, & n \text{ odd}, \end{cases} \qquad n \geq 2\ell - 2.$$

Proposition 8 Consider a measure $d\sigma \in \mathcal{M}_\ell^{(\alpha_e,\alpha_o,\beta)}[a,b]$ and let τ_ν be the zeros of the corresponding orthogonal polynomial π_n. Then

$$\pi_{n+1}(\tau_\nu) = \frac{1}{2}\pi^*_{n+1}(\tau_\nu), \quad \nu = 1, 2, \ldots, n, \tag{12}$$

for all $n \geq 2\ell - 1$.

Are there any other measures, besides those in the class $\mathcal{M}_\ell^{(\alpha_e,\alpha_o,\beta)}[a,b]$, for which the corresponding Stieltjes polynomials satisfy a functional relation of the form (12) (which is of even broader scope than (11))?

Theorem 9 Consider a (nonnegative) measure $d\sigma$ on the interval $[a,b]$, and assume that the respective monic orthogonal polynomial $\pi_{n+1}(\,\cdot\,) = \pi_{n+1}(\,\cdot\,; d\sigma)$ and monic Stieltjes polynomial $\pi^*_{n+1}(\,\cdot\,) = \pi^*_{n+1}(\,\cdot\,; d\sigma)$, both of degree $n+1$, satisfy, at the zeros τ_ν of the nth degree monic orthogonal polynomial $\pi_n(\,\cdot\,) = \pi_n(\,\cdot\,; d\sigma)$, the functional relation (12) for all $n \geq 2\ell - 1$. Then, for the coefficients $\alpha_n = \alpha_n(d\sigma) \in \mathbb{R}$ and $\beta_n = \beta_n(d\sigma) > 0$ of the three-term recurrence relation for the π_n's, there hold

$$\alpha_n = \alpha_{n+2} \quad \text{for} \quad n \geq 2\ell - 2,$$
$$\beta_n = \beta_{n+1} \quad \text{for} \quad n \geq 2\ell - 1.$$

From this, there immediately follows that

$$\alpha_n = \begin{cases} \hat{\alpha}_e, & n \text{ even}, \\ \hat{\alpha}_o, & n \text{ odd}, \end{cases} \qquad n \geq 2\ell - 2,$$

$$\beta_n = \hat{\beta}, \quad n \geq 2\ell - 1.$$

Theorem 10 Consider a measure $d\sigma \in \mathcal{M}_\ell^{(\alpha_e,\alpha_o,\beta)}[a,b]$. Then the following holds:

(a) The Gauss-Kronrod formula (3) has the interlacing property for all $n \geq 2\ell-1$, that is,

$$\tau_{n+1}^* < \tau_n < \tau_n^* < \cdots < \tau_2^* < \tau_1 < \tau_1^*.$$

(b) If $d\sigma$ has Property $\mathrm{A_e}$, then all τ_μ^* are in $[a,b]$ for all $n \geq 2\ell - 1$.

(c) All weights $\sigma_\nu,\ \sigma_\mu^*$ in formula (3) are positive for each $n \geq 2\ell-1$. In particular,

$$\sigma_\nu = \frac{1}{2}\lambda_\nu, \quad \nu = 1, 2, \ldots, n,$$

where $\lambda_\nu,\ \nu = 1, 2, \ldots, n$, are the weights in the Gauss formula (1).

(d) Formula (3) has degree of exactness (at least) $4n - 2\ell + 2$ if $n \geq 2\ell - 1$.

Anti-Gaussian and averaged Gaussian formulae for measures with constant recurrence coefficients extended (N. submitted)

Theorem 11 Consider a measure $d\sigma \in \mathcal{M}_\ell^{(\alpha_e,\alpha_o,\beta)}[a,b]$. Then the following holds:

(a) The anti-Gaussian formula (4) for all $n \geq 2\ell - 1$ is given by

$$t_\mu = \tau_\mu^*, \quad w_\mu = 2\sigma_\mu^*, \quad \mu = 1, 2, \ldots, n+1,$$

where τ_μ^* are the Stieltjes nodes and σ_μ^* the corresponding weights in the respective Gauss-Kronrod formula (3).

(b) The averaged Gaussian formula obtained by the quadrature sum (5) for all $n \geq 2\ell - 1$ gives the same error estimate for $R_n^G(f)$ as the Gauss-Kronrod formula (3), that is,

$$|R_n^G(f)| \simeq |Q_n^G(f) - Q_n^K(f)| = |Q_n^G(f) - Q_{2n+1}^{AvG}(f)| = \frac{|Q_n^G(f) - Q_{n+1}^{AG}(f)|}{2}.$$

(c) The averaged Gaussian formula obtained by the quadrature sum (5) for all $n \geq 2\ell - 1$ has degree of exactness (at least) $4n - 2\ell + 2$.

Numerical examples

1. We approximate the integral

$$\int_{-1}^{1} \frac{e^{\omega t^2}\sqrt{1-t^2}}{1+8t^2}dt,$$

using the Gauss formula (1) for the Bernstein-Szegö measure $d\sigma(t) = \frac{(1-t^2)^{1/2}}{1+8t^2}dt,\ -1 \leq t \leq 1$, which is symmetric and belongs to the class $\mathcal{M}_2^{(0,1/4)}[-1,1]$. We want to estimate the error by means of either the Gauss-Kronrod formula (3) or the anti-Gaussian formula (4) or the averaged Gaussian formula obtained by the quadrature sum (5), all for the measure $d\sigma$.

We have the following estimates

$$|R_n^G(f)| \simeq |Q_n^G(f) - Q_n^K(f)| = |Q_n^G(f) - Q_{2n+1}^{AvG}(f)| = \frac{|Q_n^G(f) - Q_{n+1}^{AG}(f)|}{2}, \qquad (13)$$

and

$$|R_n^G(f)| \simeq |Q_n^G(f) - Q_{n+1}^{AG}(f)|. \qquad (14)$$

ω	n	Estimate (13)	Error
0.25	5	0.34293879340445752667(-8)	0.34293879340998812119(-8)
0.5	5	0.12071257186969120661(-6)	0.12071257193337309965(-6)
1.0	5	0.46884850418394618087(-5)	0.46884851244292840060(-5)
	10	0.15976103307723944006(-12)	0.15976103307723944018(-12)
2.0	5	0.22385466978816500828(-3)	0.22385480636040099772(-3)
	10	0.25588826185324556767(-9)	0.25588826185324577168(-9)
4.0	5	0.16801749617265879605(-1)	0.16802124385775649115(-1)
	10	0.66155361907837291451(-6)	0.66155361907895200196(-6)

ω	n	Estimate (14)	Error
0.25	5	0.68587758680891505335(-8)	0.34293879340998812119(-8)
0.5	5	0.24142514373938241321(-6)	0.12071257193337309965(-6)
1.0	5	0.93769700836789236173(-5)	0.46884851244292840060(-5)
	10	0.31952206615447888013(-12)	0.15976103307723944018(-12)
2.0	5	0.44770933957633001655(-3)	0.22385480636040099772(-3)
	10	0.51177652370649113534(-9)	0.25588826185324577168(-9)
4.0	5	0.33603499234531759210(-1)	0.16802124385775649115(-1)
	10	0.13231072381567458290(-5)	0.66155361907895200196(-6)

2. We approximate the integral

$$\int_{-2}^{2} \frac{\cos 2t}{a^2 + t^2} d\sigma(t),$$

using the Gauss formula (1) for the measure $d\sigma$ on the interval $[-2, 2]$, which is such that the corresponding orthogonal polynomials satisfy the three-term recurrence relation

$$\pi_{n+1}(t) = t\pi_n(t) - \beta_n \pi_{n-1}(t), \quad n = 0, 1, 2, \ldots,$$
$$\pi_0(t) = 1, \ \pi_{-1}(t) = 0,$$

with

$$\beta_0 = 2\pi, \quad \beta_1 = 2, \quad \beta_n = 1, \ n \geq 2.$$

Obviously, $d\sigma$ is symmetric and belongs to the class $\mathcal{M}_2^{(0,1)}[-2, 2]$. We want to estimate the error of the Gauss formula (1) by means of either the Gauss-Kronrod formula (3) or the anti-Gaussian formula (4) or the averaged Gaussian formula obtained by the quadrature sum (5), all for the measure $d\sigma$.

a	n	Estimate (13)	Error
0.5	5	0.15950252604625732883(1)	0.17293193666037607515(1)
	10	0.13334890750170194607(0)	0.13240370886221642898(0)
	15	0.11226247409308208931(-1)	0.11232946796027654841(-1)
	20	0.94515115316491529235(-3)	0.94510366684431348902(-3)
1.0	5	0.17183249892423693967(0)	0.17323028963303109824(0)
	10	0.13976983112059154117(-2)	0.13976059136176722502(-2)
	15	0.11364152054685362994(-4)	0.11364158162809131302(-4)
	20	0.92397587839372000735(-7)	0.92397587435582498851(-7)
2.0	5	0.89285471186899925240(-2)	0.89298880754113225641(-2)
	10	0.13409566916884800128(-5)	0.13409566620469198678(-5)
	15	0.19936912912780380925(-9)	0.19936912912845902956(-9)
	20	0.29641560144932457723(-13)	0.29641560144932443240(-13)
4.0	5	0.43856789247808432022(-3)	0.43856819491682257127(-3)
	10	0.30243873825096542187(-9)	0.30243873825087803545(-9)

a	n	Estimate (14)	Error
0.5	5	0.31900505209251465766(1)	0.17293193666037607515(1)
	10	0.26669781500340389215(0)	0.13240370886221642898(0)
	15	0.22452494818616417862(-1)	0.11232946796027654841(-1)
	20	0.18903023063298305847(-2)	0.94510366684431348902(-3)
1.0	5	0.34366499784847387933(0)	0.17323028963303109824(0)
	10	0.27953966224118308235(-2)	0.13976059136176722502(-2)
	15	0.22728304109370725988(-4)	0.11364158162809131302(-4)
	20	0.18479517567874400147(-6)	0.92397587435582498851(-7)
2.0	5	0.17857094237379985048(-1)	0.89298880754113225641(-2)
	10	0.26819133833769600255(-5)	0.13409566620469198678(-5)
	15	0.39873825825560761849(-9)	0.19936912912845902956(-9)
	20	0.59283120289864915446(-13)	0.29641560144932443240(-13)
4.0	5	0.87713578495616864044(-3)	0.43856819491682257127(-3)
	10	0.60487747650193084374(-9)	0.30243873825087803545(-9)

Open questions

- Identify the measures $d\sigma \in \mathcal{M}_\ell^{(\alpha_e,\alpha_o,\beta)}[a,b]$.
- Are other measures $d\sigma$ on the interval $[a,b]$ such that the Stieltjes polynomial $\pi_{n+1}^*(\cdot) = \pi_{n+1}^*(\cdot; d\sigma)$ has a special form (like $\pi_{n+1}^*(t) = \pi_{n+1}(t) - \beta\pi_{n-1}(t)$)?
- Are other measures $d\sigma$ on the interval $[a,b]$ such that the corresponding Gauss-Kronrod and averaged Gaussian formulae coincide?
- Are measures $d\sigma$ on the interval $[a,b]$ such that the corresponding averaged Gaussian formula has maximum degree of exactness and anyway better than $2n+1$?

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