

Gauss quadrature

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Quadrature rules

Given a measure α on the interval $[a, b]$ and a function f , a quadrature rule is a relation

$$\int_a^b f(\lambda) d\alpha = \sum_{j=1}^N w_j f(t_j) + R[f]$$

$R[f]$ is the remainder which is usually not known exactly
The real numbers t_j are the nodes and w_j the weights

The rule is said to be of exact degree d if $R[p] = 0$ for all polynomials p of degree d and there are some polynomials q of degree $d + 1$ for which $R[q] \neq 0$

- ▶ Quadrature rules of degree $N - 1$ can be obtained by interpolation
- ▶ Such quadrature rules are called interpolatory
- ▶ **Newton–Cotes** formulas are defined by taking the nodes to be equally spaced
- ▶ A popular choice for the nodes is the zeros of the **Chebyshev** polynomial of degree N . This is called the **Fejér** quadrature rule
- ▶ Another interesting choice is the set of extrema of the **Chebyshev** polynomial of degree $N - 1$. This gives the **Clenshaw–Curtis** quadrature rule

Theorem

Let k be an integer, $0 \leq k \leq N$. The quadrature rule has degree $d = N - 1 + k$ if and only if it is interpolatory and

$$\int_a^b \prod_{j=1}^N (\lambda - t_j) p(x) d\alpha = 0, \quad \forall p \text{ polynomial of degree } \leq k - 1.$$

see Gautschi

If the measure is positive, $k = N$ is maximal for interpolatory quadrature since if $k = N + 1$ the condition in the last theorem would give that the polynomial

$$\prod_{j=1}^N (\lambda - t_j)$$

is orthogonal to itself which is impossible

Gauss quadrature rules

The optimal quadrature rule of degree $2N - 1$ is called a Gauss quadrature

It was introduced by **C.F. Gauss** at the beginning of the nineteenth century

The general formula for a Riemann–Stieltjes integral is

$$I[f] = \int_a^b f(\lambda) d\alpha(\lambda) = \sum_{j=1}^N w_j f(t_j) + \sum_{k=1}^M v_k f(z_k) + R[f], \quad (1)$$

where the weights $[w_j]_{j=1}^N$, $[v_k]_{k=1}^M$ and the nodes $[t_j]_{j=1}^N$ are unknowns and the nodes $[z_k]_{k=1}^M$ are prescribed

see **Davis and Rabinowitz**; **Gautschi**; **Golub and Welsch**

- ▶ If $M = 0$, this is the **Gauss** rule with no prescribed nodes
- ▶ If $M = 1$ and $z_1 = a$ or $z_1 = b$ we have the **Gauss–Radau** rule
- ▶ If $M = 2$ and $z_1 = a, z_2 = b$, this is the **Gauss–Lobatto** rule

The term $R[f]$ is the remainder which generally cannot be explicitly computed

If the measure α is a positive non-decreasing function

$$R[f] = \frac{f^{(2N+M)}(\eta)}{(2N+M)!} \int_a^b \prod_{k=1}^M (\lambda - z_k) \left[\prod_{j=1}^N (\lambda - t_j) \right]^2 d\alpha(\lambda), \quad a < \eta < b \quad (2)$$

Note that for the Gauss rule, the remainder $R[f]$ has the sign of $f^{(2N)}(\eta)$

see **Stoer and Bulirsch**

The Gauss rule

How do we compute the nodes t_j and the weights w_j ?

- ▶ One way to compute the nodes and weights is to use $f(\lambda) = \lambda^i$, $i = 1, \dots, 2N - 1$ and to solve the non linear equations expressing the fact that the quadrature rule is exact
- ▶ Use of the orthogonal polynomials associated with the measure α

$$\int_a^b p_i(\lambda)p_j(\lambda) d\alpha(\lambda) = \delta_{i,j}$$

$$P(\lambda) = [p_0(\lambda) \ p_1(\lambda) \ \cdots \ p_{N-1}(\lambda)]^T, \quad e^N = (0 \ 0 \ \cdots \ 0 \ 1)^T$$

$$\lambda P(\lambda) = J_N P(\lambda) + \gamma_N p_N(\lambda) e^N$$

$$J_N = \begin{pmatrix} \omega_1 & \gamma_1 & & & \\ \gamma_1 & \omega_2 & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & & \gamma_{N-2} & \omega_{N-1} & \gamma_{N-1} \\ & & & & \gamma_{N-1} & \omega_N \end{pmatrix}$$

J_N is a **Jacobi** matrix, its eigenvalues are real and simple

Theorem

The eigenvalues of J_N (the so-called *Ritz* values $\theta_j^{(N)}$ which are also the zeros of p_N) are the nodes t_j of the Gauss quadrature rule. The weights w_j are the squares of the first elements of the normalized eigenvectors of J_N

Proof.

The monic polynomial $\prod_{j=1}^N (\lambda - t_j)$ is orthogonal to all polynomials of degree less than or equal to $N - 1$. Therefore, (up to a multiplicative constant) it is the orthogonal polynomial associated to α and the nodes of the quadrature rule are the zeros of the orthogonal polynomial, that is the eigenvalues of J_N

The vector $P(t_j)$ is an unnormalized eigenvector of J_N corresponding to the eigenvalue t_j

If q is an eigenvector with norm 1, we have $P(t_j) = \omega q$ with a scalar ω . From the Christoffel–Darboux relation

$$w_j P(t_j)^T P(t_j) = 1, j = 1, \dots, N$$

Then

$$w_j P(t_j)^T P(t_j) = w_j \omega^2 \|q\|^2 = w_j \omega^2 = 1$$

Hence, $w_j = 1/\omega^2$. To find ω we can pick any component of the eigenvector q , for instance, the first one which is different from zero $\omega = p_0(t_j)/q_1 = 1/q_1$. Then, the weight is given by

$$w_j = q_1^2$$

If the integral of the measure is not 1

$$w_j = q_1^2 \mu_0 = q_1^2 \int_a^b d\alpha(\lambda)$$

The knowledge of the **Jacobi** matrix and of the first moment allows to compute the nodes and weights of the Gauss quadrature rule

Golub and Welsch showed how the squares of the first components of the eigenvectors can be computed without having to compute the other components with a QR-like method

$$I[f] = \int_a^b f(\lambda) d\alpha(\lambda) = \sum_{j=1}^N w_j^G f(t_j^G) + R_G[f]$$

with

$$R_G[f] = \frac{f^{(2N)}(\eta)}{(2N)!} \int_a^b \left[\prod_{j=1}^N (\lambda - t_j^G) \right]^2 d\alpha(\lambda)$$

The monic polynomial $\prod_{j=1}^N (t_j^G - \lambda)$ which is the determinant χ_N of $J_N - \lambda I$ can be written as $\gamma_1 \cdots \gamma_{N-1} p_N(\lambda)$

Theorem

Suppose f is such that $f^{(2n)}(\xi) > 0$, $\forall n$, $\forall \xi$, $a < \xi < b$, and let

$$L_G[f] = \sum_{j=1}^N w_j^G f(t_j^G)$$

The Gauss rule is exact for polynomials of degree less than or equal to $2N - 1$ and

$$L_G[f] \leq I[f]$$

Moreover $\forall N$, $\exists \eta \in [a, b]$ such that

$$I[f] - L_G[f] = (\gamma_1 \cdots \gamma_{N-1})^2 \frac{f^{(2N)}(\eta)}{(2N)!}$$

The Gauss–Radau rule

To obtain the Gauss–Radau rule, we have to extend the matrix J_N in such a way that it has one prescribed eigenvalue $z_1 = a$ or b

Assume $z_1 = a$. We wish to construct p_{N+1} such that $p_{N+1}(a) = 0$

$$0 = \gamma_{N+1} p_{N+1}(a) = (a - \omega_{N+1}) p_N(a) - \gamma_N p_{N-1}(a)$$

This gives

$$\omega_{N+1} = a - \gamma_N \frac{p_{N-1}(a)}{p_N(a)}$$

Note that

$$(J_N - aI)P(a) = -\gamma_N p_N(a) e^N$$

Let $\delta(a) = [\delta_1(a), \dots, \delta_N(a)]^T$ with

$$\delta_l(a) = -\gamma_N \frac{p_{l-1}(a)}{p_N(a)} \quad l = 1, \dots, N$$

This gives $\omega_{N+1} = a + \delta_N(a)$ and $\delta(a)$ satisfies

$$(J_N - aI)\delta(a) = \gamma_N^2 e^N$$

- ▶ we generate γ_N
- ▶ we solve the tridiagonal system for $\delta(a)$, this gives $\delta_N(a)$
- ▶ we compute $\omega_{N+1} = a + \delta_N(a)$

$$\hat{J}_{N+1} = \begin{pmatrix} J_N & \gamma_N e^N \\ \gamma_N (e^N)^T & \omega_{N+1} \end{pmatrix}$$

gives the nodes and the weights of the Gauss–Radau quadrature rule

Theorem

Suppose f is such that $f^{(2n+1)}(\xi) < 0, \forall n, \forall \xi, a < \xi < b$. Let

$$U_{GR}[f] = \sum_{j=1}^N w_j^a f(t_j^a) + v_1^a f(a)$$

w_j^a, v_1^a, t_j^a being the weights and nodes computed with $z_1 = a$ and let L_{GR}

$$L_{GR}[f] = \sum_{j=1}^N w_j^b f(t_j^b) + v_1^b f(b)$$

w_j^b, v_1^b, t_j^b being the weights and nodes computed with $z_1 = b$.
The Gauss–Radau rule is exact for polynomials of degree less than or equal to $2N$ and we have

$$L_{GR}[f] \leq I[f] \leq U_{GR}[f]$$

Theorem (end)

Moreover $\forall N \exists \eta_U, \eta_L \in [a, b]$ such that

$$I[f] - U_{GR}[f] = \frac{f^{(2N+1)}(\eta_U)}{(2N+1)!} \int_a^b (\lambda - a) \left[\prod_{j=1}^N (\lambda - t_j^a) \right]^2 d\alpha(\lambda)$$

$$I[f] - L_{GR}[f] = \frac{f^{(2N+1)}(\eta_L)}{(2N+1)!} \int_a^b (\lambda - b) \left[\prod_{j=1}^N (\lambda - t_j^b) \right]^2 d\alpha(\lambda)$$

The Gauss–Lobatto rule

We would like to have

$$p_{N+1}(a) = p_{N+1}(b) = 0$$

Using the recurrence relation

$$\begin{pmatrix} p_N(a) & p_{N-1}(a) \\ p_N(b) & p_{N-1}(b) \end{pmatrix} \begin{pmatrix} \omega_{N+1} \\ \gamma_N \end{pmatrix} = \begin{pmatrix} a p_N(a) \\ b p_N(b) \end{pmatrix}$$

Let

$$\delta_l = -\frac{p_{l-1}(a)}{\gamma_N p_N(a)}, \quad \mu_l = -\frac{p_{l-1}(b)}{\gamma_N p_N(b)}, \quad l = 1, \dots, N$$

then

$$(J_N - aI)\delta = e^N, \quad (J_N - bI)\mu = e^N$$

$$\begin{pmatrix} 1 & -\delta_N \\ 1 & -\mu_N \end{pmatrix} \begin{pmatrix} \omega_{N+1} \\ \gamma_N^2 \end{pmatrix} = \begin{pmatrix} a \\ b \end{pmatrix}$$

- ▶ we solve the tridiagonal systems for δ and μ , this gives δ_N and μ_N
- ▶ we compute ω_{N+1} and γ_N

$$\hat{J}_{N+1} = \begin{pmatrix} J_N & \gamma_N e^N \\ \gamma_N (e^N)^T & \omega_{N+1} \end{pmatrix}$$

Theorem

Suppose f is such that $f^{(2n)}(\xi) > 0, \forall n, \forall \xi, a < \xi < b$ and let

$$U_{GL}[f] = \sum_{j=1}^N w_j^{GL} f(t_j^{GL}) + v_1^{GL} f(a) + v_2^{GL} f(b)$$

$t_j^{GL}, w_j^{GL}, v_1^{GL}$ and v_2^{GL} being the nodes and weights computed with a and b as prescribed nodes. The Gauss-Lobatto rule is exact for polynomials of degree less than or equal to $2N + 1$ and

$$I[f] \leq U_{GL}[f]$$

Moreover $\forall N \exists \eta \in [a, b]$ such that

$$I[f] - U_{GL}[f] = \frac{f^{(2N+2)}(\eta)}{(2N+2)!} \int_a^b (\lambda-a)(\lambda-b) \left[\prod_{j=1}^N (\lambda - t_j^{GL}) \right]^2 d\alpha(\lambda)$$

Computation of the Gauss rules

The weights w_i are given by the squares of the first components of the eigenvectors $w_i = (z_1^i)^2 = ((e^1)^T z^i)^2$

Theorem

$$\sum_{l=1}^N w_l f(t_l) = (e^1)^T f(J_N) e^1$$

Proof.

$$\begin{aligned} \sum_{l=1}^N w_l f(t_l) &= \sum_{l=1}^N (e^1)^T z^l f(t_l) (z^l)^T e^1 \\ &= (e^1)^T \left(\sum_{l=1}^N z^l f(t_l) (z^l)^T \right) e^1 \\ &= (e^1)^T Z_N f(\Theta_N) Z_N^T e^1 \\ &= (e^1)^T f(J_N) e^1 \end{aligned}$$

The anti-Gauss rule

A usual way of obtaining an estimate of $I[f] - L_G^N[f]$ is to use another quadrature rule $Q[f]$ of degree greater than $2N - 1$ and to estimate the error as $Q[f] - L_G^N[f]$

Laurie proposed to construct a quadrature rule with $N + 1$ nodes called an anti-Gauss rule

$$H^{N+1}[f] = \sum_{j=1}^{N+1} \varpi_j f(\vartheta_j),$$

such that

$$I[p] - H^{N+1}[p] = -(I[p] - L_G^N[p])$$

for all polynomials of degree $2N + 1$. Then, the error of the Gauss rule can be estimated as

$$\frac{1}{2}(H^{N+1}[f] - L_G^N[f])$$

$$H^{N+1}[p] = 2I[p] - L_G^N[p]$$

for all polynomials p of degree $2N + 1$. Hence, H^{N+1} is a Gauss rule with $N + 1$ nodes for the functional $\mathcal{I}(\cdot) = 2I[\cdot] - L_G^N[\cdot]$

We have

$$I[pq] = \mathcal{I}(pq)$$

for p a polynomial of degree $N - 1$ and q a polynomial of degree N and

$$\mathcal{I}(\tilde{p}_N^2) = 2I(\tilde{p}_N^2)$$

where \tilde{p}_j are the orthogonal polynomials associated to \mathcal{I}
Using the **Stieltjes** formulas for the coefficients we obtain the **Jacobi** matrix

One can construct a quadrature rule $S^{N+1}[f]$ such that

$$I[p] - S^{N+1}[p] = -\gamma(I[p] - L_G^N[p])$$

for all polynomials of degree $2N + 1$. The parameter γ is positive and less than or equal to 1

$$\tilde{J}_{N+1} = \begin{pmatrix} \omega_1 & \gamma_1 & & & & \\ \gamma_1 & \omega_2 & \gamma_2 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \gamma_{N-2} & \omega_{N-1} & \gamma_{N-1} & \\ & & & \gamma_{N-1} & \omega_N & \gamma_N \sqrt{1+\gamma} \\ & & & & \gamma_N \sqrt{1+\gamma} & \omega_{N+1} \end{pmatrix}$$

The error of the Gauss rule can be estimated as

$$\frac{1}{1+\gamma}(S^{N+1}[f] - L_G^N[f])$$

Nonsymmetric Gauss quadrature rules

We consider the case where the measure α can be written as

$$\alpha(\lambda) = \sum_{k=1}^l \alpha_k \delta_k, \quad \lambda_l \leq \lambda < \lambda_{l+1}, \quad l = 1, \dots, N-1$$

where $\alpha_k \neq \delta_k$ and $\alpha_k \delta_k \geq 0$

We assume that there exists two sequences of mutually orthogonal (sometimes called bi-orthogonal) polynomials p and q such that

$$\begin{aligned} \gamma_j p_j(\lambda) &= (\lambda - \omega_j) p_{j-1}(\lambda) - \beta_{j-1} p_{j-2}(\lambda), & p_{-1}(\lambda) &\equiv 0, & p_0(\lambda) &\equiv 1 \\ \beta_j q_j(\lambda) &= (\lambda - \omega_j) q_{j-1}(\lambda) - \gamma_{j-1} q_{j-2}(\lambda), & q_{-1}(\lambda) &\equiv 0, & q_0(\lambda) &\equiv 1 \end{aligned}$$

with $\langle p_i, q_j \rangle = 0, \quad i \neq j$

Let

$$P(\lambda)^T = [p_0(\lambda) \ p_1(\lambda) \ \cdots \ p_{N-1}(\lambda)]$$

$$Q(\lambda)^T = [q_0(\lambda) \ q_1(\lambda) \ \cdots \ q_{N-1}(\lambda)]$$

and

$$J_N = \begin{pmatrix} \omega_1 & \gamma_1 & & & & \\ \beta_1 & \omega_2 & \gamma_2 & & & \\ & \ddots & \ddots & \ddots & & \\ & & & \beta_{N-2} & \omega_{N-1} & \gamma_{N-1} \\ & & & & \beta_{N-1} & \omega_N \end{pmatrix}$$

In matrix form

$$\lambda P(\lambda) = J_N P(\lambda) + \gamma_N p_N(\lambda) e^N$$

$$\lambda Q(\lambda) = J_N^T Q(\lambda) + \beta_N q_N(\lambda) e^N$$

Proposition

$$p_j(\lambda) = \frac{\beta_j \cdots \beta_1}{\gamma_j \cdots \gamma_1} q_j(\lambda)$$

Hence, q_N is a multiple of p_N and the polynomials have the same roots which are also the common real eigenvalues of J_N and J_N^T . We define the quadrature rule as

$$\int_a^b f(\lambda) d\alpha(\lambda) = \sum_{j=1}^N f(\theta_j) s_j t_j + R[f]$$

where θ_j is an eigenvalue of J_N , s_j is the first component of the eigenvector u_j of J_N corresponding to θ_j and t_j is the first component of the eigenvector v_j of J_N^T corresponding to the same eigenvalue, normalized such that $v_j^T u_j = 1$.

Theorem

Assume that $\gamma_j \beta_j \neq 0$, then the nonsymmetric Gauss quadrature rule is exact for polynomials of degree less than or equal to $2N - 1$

The remainder is characterized as

$$R[f] = \frac{f^{(2N)}(\eta)}{(2N)!} \int_a^b p_N(\lambda)^2 d\alpha(\lambda)$$

The extension of the Gauss–Radau and Gauss–Lobatto rules to the nonsymmetric case is almost identical to the symmetric case

The block Gauss quadrature rules

The integral $\int_a^b f(\lambda) d\alpha(\lambda)$ is now a 2×2 symmetric matrix. The most general quadrature formula is of the form

$$\int_a^b f(\lambda) d\alpha(\lambda) = \sum_{j=1}^N W_j f(T_j) W_j + R[f]$$

where W_j and T_j are symmetric 2×2 matrices. This can be reduced to

$$\sum_{j=1}^{2N} f(t_j) u^j (u^j)^T$$

where t_j is a scalar and u^j is a vector with two components

There exist orthogonal matrix polynomials related to α such that

$$\lambda p_{j-1}(\lambda) = p_j(\lambda)\Gamma_j + p_{j-1}(\lambda)\Omega_j + p_{j-2}(\lambda)\Gamma_{j-1}^T$$

$$p_0(\lambda) \equiv I_2, \quad p_{-1}(\lambda) \equiv 0$$

This can be written as

$$\lambda[p_0(\lambda), \dots, p_{N-1}(\lambda)] = [p_0(\lambda), \dots, p_{N-1}(\lambda)]J_N + [0, \dots, 0, p_N(\lambda)\Gamma_N]$$

where

$$J_N = \begin{pmatrix} \Omega_1 & \Gamma_1^T & & & & \\ \Gamma_1 & \Omega_2 & \Gamma_2^T & & & \\ & \ddots & \ddots & \ddots & & \\ & & & \Gamma_{N-2} & \Omega_{N-1} & \Gamma_{N-1}^T \\ & & & & \Gamma_{N-1} & \Omega_N \end{pmatrix}$$

is a symmetric block tridiagonal matrix of order $2N$

The nodes t_j are the zeros of the determinant of the matrix orthogonal polynomials that is the eigenvalues of J_N and u_i is the vector consisting of the two first components of the corresponding eigenvector

However, the eigenvalues may have a multiplicity larger than 1

Let $\theta_i, i = 1, \dots, l$ be the set of distinct eigenvalues and n_i their multiplicities. The quadrature rule is then

$$\sum_{i=1}^l \left(\sum_{j=1}^{n_i} (w_i^j)(w_i^j)^T \right) f(\theta_i)$$

The block quadrature rule is exact for polynomials of degree less than or equal to $2N - 1$ but the proof is rather involved

The block Gauss–Radau rule

We would like a to be a double eigenvalue of J_{N+1}

$$J_{N+1}P(a) = aP(a) - [0, \dots, 0, p_{N+1}(a)\Gamma_{N+1}]^T$$

$$ap_N(a) - p_N(a)\Omega_{N+1} - p_{N-1}(a)\Gamma_N^T = 0$$

If $p_N(a)$ is non singular

$$\Omega_{N+1} = aI_2 - p_N(a)^{-1}p_{N-1}(a)\Gamma_N^T$$

But

$$(J_N - aI) \begin{pmatrix} -p_0(a)^T p_N(a)^{-T} \\ \vdots \\ -p_{N-1}(a)^T p_N(a)^{-T} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ \Gamma_N^T \end{pmatrix}$$

- ▶ We first solve

$$(J_N - aI) \begin{pmatrix} \delta_0(a) \\ \vdots \\ \delta_{N-1}(a) \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ \Gamma_N^T \end{pmatrix}$$

- ▶ We compute

$$\Omega_{N+1} = aI_2 + \delta_{N-1}(a)^T \Gamma_N^T$$

The block Gauss–Lobatto rule

The generalization of the Gauss–Lobatto construction to the block case is a little more difficult

We would like to have a and b as double eigenvalues of the matrix

J_{N+1}

It gives

$$\begin{pmatrix} I_2 & p_N^{-1}(a)p_{N-1}(a) \\ I_2 & p_N^{-1}(b)p_{N-1}(b) \end{pmatrix} \begin{pmatrix} \Omega_{N+1} \\ \Gamma_N^T \end{pmatrix} = \begin{pmatrix} aI_2 \\ bI_2 \end{pmatrix}$$

Let $\delta(\lambda)$ be the solution of

$$(J_N - \lambda I)\delta(\lambda) = (0 \dots 0 \ I_2)^T$$

Then, as before

$$\delta_{N-1}(\lambda) = -p_{N-1}(\lambda)^T p_N(\lambda)^{-T} \Gamma_N^{-T}$$

Solving the 4×4 linear system we obtain

$$\Gamma_N^T \Gamma_N = (b - a)(\delta_{N-1}(a) - \delta_{N-1}(b))^{-1}$$

Thus, Γ_N is given as a Cholesky factorization of the right hand side matrix which is positive definite because $\delta_{N-1}(a)$ is a diagonal block of the inverse of $(J_N - aI)^{-1}$ which is positive definite and $-\delta_{N-1}(b)$ is the negative of a diagonal block of $(J_N - bI)^{-1}$ which is negative definite

From Γ_N , we compute







$$\Omega_{N+1} = aI_2 + \Gamma_N \delta_{N-1}(a) \Gamma_N^T$$

Computation of the block Gauss rules

Theorem

$$\sum_{i=1}^{2N} f(t_i) u_i u_i^T = e^T f(J_N) e$$

where $e^T = (I_2 \ 0 \ \dots \ 0)$

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