Gauss quadrature

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Consider $[a, b] \subset \mathbf{R}$ and

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and $w(x)$ is a weight function. Given $x_0 < x_1 \cdots < x_n, \quad x_i \in [a, b]$, Consider $[a,b] \subset \mathbf{R}$ and

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$$p_{2n+1}(x) = \sum_{i=0}^{n} H_i(x) f(x_i) + \sum_{i=0}^{n} K_i(x) f'(x_i),$$

$$\begin{aligned} H_i(x) &= (L_i(x))^2(1-2L_i'(x_i)(x-x_i)), \\ K_i(x) &= (L_i(x))^2(x-x_i), \end{aligned} \qquad \begin{aligned} L_i(x) &:= \prod_{j=0, j\neq i}^{n} \frac{x-x_j}{x_i-x_j} \\ L_0(x) &\equiv 1, \end{aligned}$$

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putting p_{2n+1} in place of f in the integral gives an approximation of the integral:

$$\int_a^b w(x)\, f(x)\, dx \approx \sum_{i=0}^{n} W_i f(x_i) + \sum_{i=0}^{n} V_i f'(x_i), \qquad \begin{aligned} W_i &:= \textstyle\int_a^b w(x) H_i(x)\, dx, \\ V_i &:= \textstyle\int_a^b w(x) K_i(x)\, dx. \end{aligned}$$

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Finally we choose $x_0, \ldots, x_n$ such that $V_i = 0$.
We found that this is possible iff

$$0 = V_i = \int_a^b w(x)\, (L_i(x))^2 (x - x_i)\, dx = c_j \int_a^b w(x)\, \omega(x)\, L_i(x)\, dx$$

so

$$0 = V_i \Leftrightarrow \langle \omega, q \rangle_w = 0, \quad \forall q \in \Pi_n$$

which means we should choose $x_0, \ldots, x_n$ to be the zeros of a polynomial $\omega(x) \in \Pi_{n+1}$ belonging to a system of orthogonal polynomials w.r.t. $\langle \cdot, \cdot \rangle_w$.

Summarizing

$$\int_a^b w(x)\, f(x)\, dx \approx \mathcal{G}_n(f) := \sum_{i=0}^{n} W_i f(x_i)$$

where

$$W_i := \int_a^b w(x)\, [L_i(x)]^2\, dx$$

$x_0, \ldots, x_n$ to be the zeros of a polynomial of degree $n+1$ belonging to a system of orthogonal polynomials w.r.t. $\langle \cdot, \cdot \rangle_w$

Theorem 10.1. Let w (weight function) be defined, integrable, continuous and positive on (a, b) and $f \in C^{(2n+2)}[a, b]$ (continuous differentiable with $2n+2$ continuous derivatives) and $n \geq 0$. Then for the Gauss quadrature $\exists\, \eta \in (a, b)$ s.t.

$$\int_a^b w(x) f(x)\, dx - \sum_{k=0}^{n} W_k f(x_k) = K_n\, f^{(2n+2)}(\eta), \tag{1}$$

and

$$K_n = \frac{1}{(2n+2)!} \int_a^b w(x)[\omega(x)]^2\, dx.$$

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So the the Gauss quadrature is exact for polynomials of degree $2n + 1$.
Rough estimate:

$$\max_{k=0,..,n} |x - x_k| = b - a, \quad |\omega(x)|^2 \leq \big((n+1)(b-a)\big)^2$$

$$K_n \leq \frac{1}{(2n+2)!}(n+1)^2(b-a)^2 \int_a^b w(x)\, dx.$$

Convergence of Gauss quadrature to the integral

Let us denote the Gauss quadrature formula with

$$\mathcal{G}_n(f) := \sum_{k=0}^{n} W_k f(x_k)$$

Theorem 10.2. Let w (weight function) be defined, integrable, continuous and positive on (a, b) and $f \in C^0[a, b]$ (continuous in the closed interval $[a, b]$). Then

$$\lim_{n\to\infty} \mathcal{G}_n(f) = \int_a^b w(x)f(x)\,dx.$$

Proof. Weierstrass theorem: $\forall \epsilon_0 > 0$, $\exists$ p_N (polynomial) such that

$$|f(x) - p_N(x)| \leq \epsilon_0, \quad \forall x \in [a, b], \quad p_N \in \Pi_N$$

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$$\begin{aligned}\int_a^b w(x)f(x)\,dx - G_n(f) \quad &= \quad \int_a^b w(x)(f(x) - p_N(x))\,dx \\ &\quad + \int_a^b w(x)p_N\,dx - \mathcal{G}_n(p_N) \\ &\quad + \mathcal{G}_n(p_N) - \mathcal{G}_n(f).\end{aligned}$$

$$\int_a^b f(x)\,dx = \sum_{j=1}^{m} \int_{x_{j-1}}^{x_j} f(x)\,dx,$$

$x_j - x_{j-1} = h = \frac{b-a}{m}$, $x_j = a + j\,h$.

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Change of variables: $[x_{j-1}, x_j] \to [-1, 1]$:

$$x = \frac{1}{2}(x_{j-1} + x_j) + \frac{1}{2}ht, \quad t \in [-1, 1],$$

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$$\int_a^b f(x)\,dx = \frac{h}{2}\sum_{j=1}^{m} \int_{-1}^{1} f(\frac{1}{2}(x_{j-1} + x_j) + \frac{1}{2}ht)\,dt = \frac{h}{2}\sum_{j=1}^{m} I_j$$

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approximate each I_j with a Gauss quadrature formula:

$$\int_a^b f(x)\,dx \approx \frac{h}{2}\sum_{j=1}^{m}\sum_{k=0}^{n} W_k f(\frac{1}{2}(x_{j-1}+x_j) + \frac{1}{2}h\xi_k)$$

W_k and ξ_k weights and nodes of Gauss quadrature on $[-1, 1]$.

a) Show that $\forall p_{2n-1} \in \Pi_{2n-1}$ on the interval, we have

$$p_{2n-1}(x) = (x-a)(b-x)q_{2n-3}(x) + r(x-a) + s(b-x),$$

$q_{2n-3} \in \Pi_{2n-3}, \quad a, b, r, s \in \mathbf{R}$, with a and b not simultaneously zero.
Note: $(x-a), (x-b), (x-a)(b-x)x^k$ and $k = 0, \dots, 2n-3$ with a and b not simultaneously zero is a basis for Π_{2n-1}.

Exercise on Lobatto quadrature: exercise 10.7

a) Show that $\forall p_{2n-1} \in \Pi_{2n-1}$ on the interval, we have

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Solution: using the given basis we can write

$$p_{2n-1}(x) = (x-a)(b-x)\sum_{k=0}^{2n-3} \lambda_k x^k + \lambda_{2n-2}(x-a) + \lambda_{2n-1}(b-x),$$

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and so taking $q_{2n-3}(x) := \sum_{k=0}^{2n-3} \lambda_k x^k$ and $r := \lambda_{2n-2}$, $s := \lambda_{2n-1}$, we see that there exist $q_{2n-3} \in \Pi_{2n-3}, \quad a, b, r, s \in \mathbf{R}$, such that any $p_{2n-1} \in \Pi_{2n-1}$ can be written in the given form.

Exercise on Lobatto quadrature: exercise 10.7

b) Construct the Lobatto quadrature formula

$$\int_a^b w(x)f(x)\,dx \approx W_0 f(a) + \sum_{k=1}^{n-1} W_k f(x_k) + W_n f(b)$$

which is exact when $f \in \Pi_{2n-1}$. Here $w(x)$ is a weight function.

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which is exact when $f \in \Pi_{2n-1}$. Here $w(x)$ is a weight function.
Solution: using the formula obtained in a), $\tilde{w}(x) := w(x)(x-a)(b-x)$

$$\int_a^b w(x)p_{2n-1}(x)dx = \int_a^b \tilde{w}(x)q_{2n-3}(x)dx + r\int_a^b w(x)(x-a)dx + s\int_a^b w(x)(b-x)dx,$$

and using the Gauss quadrature with $n-1$ weights and nodes (W_k^*, x_k^*) wrt $\tilde{w}(x)$ one gets,

$$\int_a^b w(x)p_{2n-1}(x)dx = \sum_{k=1}^{n-1} W_k^* q_{2n-3}(x_k^*) + r\int_a^b w(x)(x-a)dx + s\int_a^b w(x)(b-x)dx,$$

for an arbitrary polynomial $p_{2n-1} \in \Pi_{2n-1}$. Since

$$q_{2n-3}(x_k^*) = \frac{p_{2n-1}(x_k^*) - r(x_k^* - a) - s(b - x_k^*)}{(x_k^* - a)(b - x_k^*)}$$

$$r = p_{2n-1}(b)/(b-a), \quad s = p_{2n-1}(a)/(b-a).$$

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which is exact when $f \in \Pi_{2n-1}$. Here $w(x)$ is a weight function.
Solution: using the formula obtained in a) and the Gauss quadrature with $n-1$ weights and nodes (W_k^*, x_k^*) wrt $\tilde{w}(x) = w(x)(x-a)(b-x)$ one gets,

$$\int_a^b w(x)p_{2n-1}(x)dx = W_0 p_{2n-1}(a) + \sum_{k=1}^{n-1} W_k p_{2n-1}(x_k) + W_n p_{2n-1}(b)$$

$$x_0 := a, x_n := b, x_k := x_k^*, \quad W_k := \frac{W_k^*}{(x_k^*-a)(b-x_k^*)}, \quad k = 1, \dots, n-1,$$

$$W_0 := \frac{1}{b-a}\left(\int_a^b w(x)(b-x)dx - \sum_{k=1}^{n-1} \frac{W_k^*}{x_k^*-a}\right),$$

$$W_n := \frac{1}{b-a}\left(\int_a^b w(x)(x-a)dx - \sum_{k=1}^{n-1} \frac{W_k^*}{b-x_k^*}\right).$$

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$$W_0 := \frac{1}{b-a}\left(\int_a^b w(x)(b-x)\frac{(x-a)}{(x-a)}dx - \sum_{k=1}^{n-1}\frac{W_k^*}{x_k^*-a}\right),$$

with $\tilde{w}(x) = w(x)(x-a)(b-x)$

$$W_0 = \frac{1}{b-a}\left(\int_a^b \tilde{w}(x)\frac{1}{(x-a)}dx - \sum_{k=1}^{n-1}\frac{W_k^*}{x_k^*-a}\right),$$

this is the error for the Gauss quadrature on $m+1 = n-1$ nodes for $\frac{1}{x-a}$ wrt $\tilde{w}$.

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this is the error for the Gauss quadrature on $m+1 = n-1$ nodes for $\frac{1}{x-a}$ wrt $\tilde{w}$. Using theorem 10.1 (with n in the theorem replaced by m and $m = n-2$) we get

$$W_0 = \frac{1}{b-a} K_m \frac{d^{2m+2}}{dx^{2m+2}}\left(\frac{1}{x-a}\right).$$

$K_m = \frac{1}{(2m+2)!}\int_a^b w(x)(\omega(x))^2\,dx$ (see theorem 10.1) is always positive, and the even derivatives of $\frac{1}{x-a}$ are always positive.

Exercise relevant for the project

Show that

$$|f(x) - s(x)| \leq \frac{7}{8} h^2 \|f''\|_\infty, \quad \forall x \in [a, b],$$

where $f \in C^2[a, b]$ and s is the natural cubic spline on the equidistant knots $a = x_0 < x_1 < \cdots < x_n = b$, $x_i - x_{i-1} = h$, $i = 1, \ldots, n$.

Plan:

a) Show first: $|f(x) - s(x)| \leq \frac{h^2}{8}(\|f''\|_\infty + \max_i |s_i''|)$;

b) show then that $|s_i''| \leq 6 \|f''\|_\infty$ to obtain the result. (For the solution see problem set 5 exercise 3.)

Solution of point a)

Recall $f(x_j) = s(x_j)$ and $f(x_{j-1}) = s(x_{j-1})$. Fix a $\bar{x} \in [x_{j-1}, x_j]$ and consider

$$g(x) := f(x) - s(x) - \frac{(x - x_{j-1})(x - x_j)}{(\bar{x} - x_{j-1})(\bar{x} - x_j)}(f(\bar{x}) - s(\bar{x})), \quad \forall x \in [x_{j-1}, x_j],$$

and $0 = g(\bar{x}) = g(x_{j-1}) = g(x_j)$. So there exists $\xi_j(\bar{x}) \in (x_{j-1}, x_j)$ such that

$$0 = g''(\xi_j) = f''(\xi_j) - s''(\xi_j) - \frac{2}{(\bar{x} - x_{j-1})(\bar{x} - x_j)}(f(\bar{x}) - s(\bar{x})),$$

this imples

$$f(\bar{x}) - s(\bar{x}) = (\bar{x} - x_{j-1})(\bar{x} - x_j)\frac{f''(\xi_j) - s''(\xi_j)}{2},$$

and $|(\bar{x} - x_{j-1})(\bar{x} - x_j)| \leq h^2/4$,

$$|f(\bar{x}) - s(\bar{x})| \leq \frac{h^2}{8}(|f''(\xi_j)| + |s''(\xi_j)|),$$

leading to the proof of point a).

Adaptive quadrature: given a tolerance TOL find $\tilde{I} \approx I$ s.t.

$$|I - \tilde{I}| \leq TOL.$$

Consider

$$I = \int_a^b f(x)\,dx,$$

Simpson:

$$S(a,b) := \frac{b-a}{6}\left[f(a) + f\left(\frac{a+b}{2}\right) + f(b)\right]$$

error

$$E(a,b) = -\frac{1}{90}\left(\frac{b-a}{2}\right)^5 f^{(4)}(\xi), \quad \xi \in (a,b),$$

$$I = S + E$$

Plan:

1. Subdivide $[a,b]$ recursively in disjoint subintervals;
2. apply S on each subinterval;
3. stop when $|I - \tilde{I}| \leq TOL$ is satisfied.

Error estimate

Case of two subintervals $[a, b] = [a, c] \cup [c, b]$ $c := \frac{a+b}{2}$, $h = b - a$. Let

$$I_0 = S(a, b), \quad E_0 = E(a, b), \quad I = I_0 + E_0$$

$$\tilde{I} = S(a, c) + S(c, b), \quad \tilde{E} = E(a, c) + E(c, b), \quad I = \tilde{I} + \tilde{E}$$

$$\tilde{E} = -\frac{1}{90}\left(\frac{1}{2}\frac{h}{2}\right)^5 \left(f^{(4)}(\xi_1) + f^{(4)}(\xi_2)\right), \quad \xi_1 \in (a, c), \quad \xi_2 \in (c, b)$$

by the intermediate value theorem, since f^4 is assumed continuous, we have

$$\tilde{E} = -\frac{1}{90}\frac{1}{16}\left(\frac{h}{2}\right)^5 \left(f^{(4)}(\tilde{\xi})\right), \quad \tilde{\xi} \in (a, b),$$

we will assume that for h small $f^{(4)}(\tilde{\xi}) \approx f^{(4)}(\xi)$ this gives

$$E_0 \approx 16\,\tilde{E}, \quad |\tilde{I} - I_0| = |E_0 - \tilde{E}| \approx 15|\tilde{E}| \Rightarrow |\tilde{E}| \approx \frac{|\tilde{I} - I_0|}{15}$$

adaptiveS$(f,\ a,\ b,\mathrm{TOL})$

$I_0 = S(a, b)$

$c := \frac{b+a}{2}$

$\tilde{I} = S(a, c) + S(c, b)$

IF $\quad \frac{1}{15}\,|\tilde{I} - I_0| \leq TOL \quad$ then $\quad \hat{I} = \tilde{I} + \frac{1}{15}(\tilde{I} - I_0)$

ELSE

$\tilde{I} =$**adaptiveS**$(f,\ a,\ c,\ \frac{TOL}{2})$+**adaptiveS**$(f,\ c,\ b,\ \frac{TOL}{2})$

END

RETURN $\hat{I}$