11-08-17, Wed

Gaussian quadrature:

Theorem:

$$\int_a^b f(x)\,w(x)\,dx \approx \sum_{i=0}^{n} A_i f(x_i) \qquad (*)$$

where

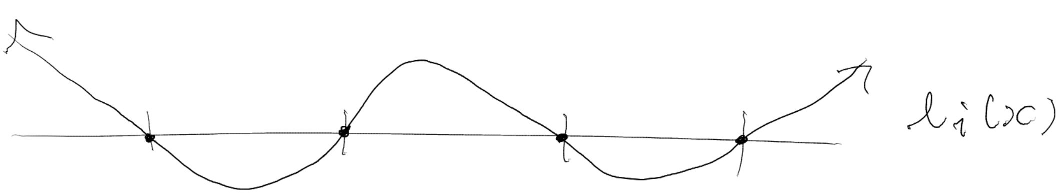
$$A_i = \int_a^b w(x)\, l_i(x)\,dx$$

with

$$l_i(x) = \prod_{\substack{j=0 \\ j\neq i}}^{n} \frac{x - x_j}{x_i - x_j} \qquad \text{(Lagrange polynomial)}$$

and $x_0, x_1, \dots, x_n$ are the roots of q which is w-orthogonal to Π_{n+1}, i.e.

$$\int_a^b q(x)\,p(x)\,w(x)\,dx = 0, \qquad p \in \Pi_{n+1}.$$



The formula $(*)$ is exact for $f \in \Pi_{2n+1}$.

How do we calculate the q's? $q = q_{n+1}$

We need 2 properties.

① q_{n+1} is monic of degree is $n+1$

② $\int q_{n+1}(x) p(x) w(x) dx = 0, \quad p \in \Pi_n$

Let's look at the case where $w(x) \equiv 1$ on $[-1, 1]$.

Need:

$q_0(x) = 1$

$q_1(x) = x$

Check:

$$\int_{-1}^{1} x \cdot 1 dx = 0 \text{ by symmetry.}$$

Then earlier we had a recursion formula:

If $n \geq 2$

$$q_n(x) = (x - a_n) q_{n-1}(x) - b_n q_{n-2}(x)$$

with

$$a_n = \frac{\langle x q_{n-1}, q_{n-1} \rangle}{\langle q_{n-1}, q_{n-1} \rangle}, \text{ and } b_n = \frac{\langle x q_{n-1}, q_{n-2} \rangle}{\langle q_{n-2}, q_{n-2} \rangle}.$$

Idea: You can check if q_{n-1}, q_{n-2} satisfy ① and ② then so does q_n.

$q_2(x) = (x - a_2)x - b_2 1$ where

$$a_2 = \frac{\langle x q_1, q_1 \rangle}{\langle q_1, q_1 \rangle} = \frac{\int_{-1}^{1} x^3 \, dx}{\int_{-1}^{1} x^2 \, dx} = 0.$$

$$b_2 = \frac{\langle x q_1, q_0 \rangle}{\langle q_0, q_0 \rangle} = \frac{\int_{-1}^{1} x^2 \, dx}{\int_{-1}^{1} 1 \, dx} = \frac{1}{3}.$$

So,

$$q_2(x) = x^2 - \frac{1}{3}.$$

Similarly,

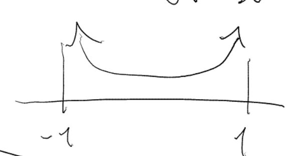
$$q_3(x) = x^3 - \frac{3}{5}x.$$

We have

q_n = Legendre polynomials of degree n.

<u>Chebyshev</u>:

$$w(x) = \frac{1}{\sqrt{1 - x^2}}$$



Penalize boundaries

Lemma:

① $A_i > 0, \quad \forall i$

② $\sum_{i=0}^{n} A_i = \int_a^b w(x)\,dx$

Proof: We have some q with

$$\int_a^b q(x)\,p(x)\,w(x)\,dx = 0, \quad p \in \Pi_n .$$

Choose p in the formula above to be

$$p(x) = \frac{q(x)}{x - x_j}, \qquad (\text{recall } q(x_j) = 0).$$

So p is of degree n. So p^2 is of degree $2n$.
So the GQ formula is exact for p^2. Thus

$$\underset{\underset{(w>0)}{\uparrow}}{0 <} \int_a^b p^2(x)\,w(x)\,dx = \sum_{i=0}^{n} A_i\,p^2(x_i)$$

Then

$$p(x_i) = \frac{q(x_i)}{x - x_j} = 0 \text{ if } i \neq j$$

$$p(x_j) = \text{whatever} \underset{\underset{\text{roots of } q \text{ are distinct}}{\uparrow}}{\neq} 0$$

(Divide by $(x - x_j)^{\ell}$ if x_j higher multiplicity).

So $A_j > 0$. For ②, in general

$$\sum_{i=0}^{n} A_i f(x_i) \approx \int_a^b f(x)\omega(x)\,dx .$$

Pick $f(x) \equiv 1 \in \Pi_0 \subset \Pi_{2n+1}$. So the formula is exact and gives ②. $\square$

Theorem: (on convergence of GC)

If f is continuos on $[a,b]$ then

$$\lim_{n\to\infty} \sum_{i=0}^{n} A_i^{(n)} f(x_i^{(n)}) = \int_a^b f(x)\, w(x)\, dx.$$

Proof: Let $\varepsilon > 0$. By the Weierstrass approximation theorem, there exists a polynomial p (of some indeterminate degree), such that

$$|f(x) - p(x)| < \varepsilon, \qquad x \in [a,b].$$

Let degree of $p = N(\varepsilon) = N$. Then

$$\left| \int_a^b f(x)\, w(x)\, dx - \sum_{i=0}^{N} A_i^{(N)} f(x_i^{(N)}) \right| \leq$$

$$\leq \left| \int_a^b f(x)\, w(x)\, dx - \int_a^b p(x)\, w(x)\, dx \right| +$$

$$\left| \int_a^b p(x)\, w(x)\, dx - \sum_{i=0}^{N} A_i^{(N)} p(x_i^{(N)}) \right| +$$

$$+ \left| \sum_{i=0}^{N} A_i^{(N)} \left[p(x_i^{(N)}) - f(x_i^{(N)}) \right] \right| \leq$$

$$\leq \int_a^b |f(x)-p(x)|\,w(x)\,dx + \overset{\text{GC exact for } p}{\overset{\downarrow}{0}} + \sum_{i=0}^{N} |A_i^{(N)}|\,|p(x_i^{(N)}) - f(x_i^{(N)})|$$

$$\leq \varepsilon \int_a^b w(x)\,dx + \varepsilon \sum_{i=0}^{N} A_i^{(N)}$$

$|A_i^{(N)}| = A_i^{(N)}$ by part 1 in lemma.

$$= 2\varepsilon \int_a^b w(x)\,dx.$$

by lemma part 2

So take $\hat{\varepsilon} = 2\varepsilon \int_a^b w(x)\,dx$ so. $\square$

Adaptive quadrature:

An automatic numerical integration program (e.g. quad integral function in MATLAB) calculates an approximation to

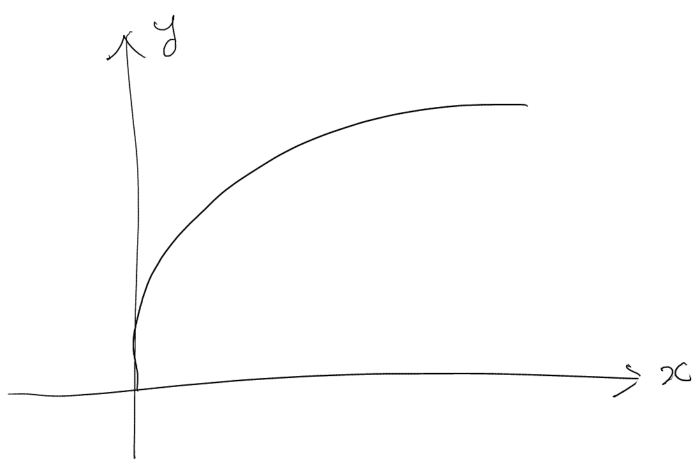
$$\int_a^b f(x)\,dx$$

to within a user-specified accuracy.

In an adaptive integration method, the nodes are chosen "on the fly" to reflect the varying local behavior of the function f.

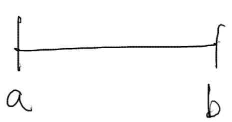
Example:

$$I = \int_0^1 \sqrt{x}\,dx.$$



So the slope of $y = \sqrt{x} \to \infty$ as $x \to 0$.
So we would need small Δx near 0.
But for x near 1, f does not vary as much.
So there is no point in having lots of nodes near $x=1$. With Simpson's rule, for example, we have equally spaced nodes.
So we would need lots of nodes across $[0,1]$ to get required accuracy near $x=0$.
Instead, put nodes where most need them.

<u>Example</u>: Consider applying Simpson's rule as follows.



$$S(a,b) = \frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]$$

with error

$$S(a,b) - \int_a^b f(x)\,dx = +\frac{1}{90}\left[\frac{b-a}{2}\right]^5 f^{(4)}(\xi)$$

with $\xi \in [a,b]$.

Idea: If the interval $[a,b]$ is such that $f^{(4)}$ is big on $[a,b]$ then to get small error need short interval ($(b-a)^5 << 1$).

In more generality,

$$I(f) = \sum_{j=1}^{\frac{n}{2}} \int_{x_{2j-2}}^{x_{2j}} f(x)\,dx \simeq$$

$$\simeq I_n(f) = \sum_{j=1}^{\frac{n}{2}} \left[\frac{x_{2j}-x_{2j-2}}{6}\right]\left[f_{2j-2} + 4f_{2j-1} + f_{2j}\right]$$

and the total error is

$$I(f) - I_n(f) = -\frac{1}{90}\frac{1}{32}\sum_{j=1}^{\frac{n}{2}} (x_{2j} - x_{2j-2})^5 f^{(4)}(\xi)$$

with $x_{2j-2} \leq \xi_j \leq x_{2j}$.

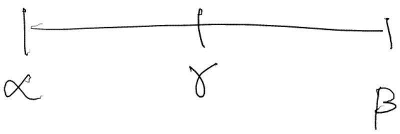
If $f^{(4)}$ varies a lot, you would want to vary

$|x_{2j} - x_{2j-2}|$

a lot to compensate and keep error per subinterval approximately constant.

Notation:

$$I_{\alpha,\beta} = \int_{\alpha}^{\beta} f(x)\,dx ,$$



Pick $\gamma = \frac{\alpha+\beta}{2}$.

First approximation to $I_{\alpha,\beta}$ is

$$I^1_{\alpha,\beta} = \frac{h}{3}\left[f(\alpha) + 4f(\gamma) + f(\beta)\right]$$

with

$$\gamma = \frac{\alpha+\beta}{2} \quad \text{(midpoint), and}$$

$$h = \frac{\beta-\alpha}{2}.$$

Then set

$$I^2_{\alpha,\beta} = I^1_{\alpha,\gamma} + I^1_{\gamma,\beta}.$$

Suppose we are given a tolerance $\varepsilon > 0$ and want

$$\left|I^{\text{true}} - I^{\text{approx}}\right| < \varepsilon .$$

Here is an algorithm to almost ensure this.

(Recall we want $\int_a^b f(x)\,dx$).

Choose $\alpha = a$, $\beta = b$.

① Compute $I^1_{\alpha,\beta}$, $I^2_{\alpha,\beta}$.

② If $|I^2_{\alpha,\beta} - I^1_{\alpha,\beta}| < \varepsilon$ then accept $I^2_{\alpha,\beta}$ as your approximation I^{approx} and stop.

③ Otherwise set $\varepsilon = \frac{\varepsilon}{2}$. Let

$$I_{\alpha,\beta} = I_{\alpha,\gamma} + I_{\gamma,\beta}.$$

Repeat the 2 steps on RHS with new tolerance.