Gaussian Quadrature: N-point Gauss Rule; $G_N(f) = \sum_{i=1}^{N} A_i f(\xi_i)$

of precision $2N-1$

approximates integrals of the form $I(f) = \int_a^b w(x)\cdot f(x)\,dx$

for finite or infinite (a,b)

and various cont's weight functions $w(x) \geq 0$

e.g. $\int_{-1}^{1} f(x)\,dx$, $\int_0^\infty e^{-x} f(x)\,dx$, $\int_{-\infty}^{\infty} e^{-x^2} f(x)\,dx$, ...

Given an interval (a,b) and a continuous weight function $w(x)\geq 0$,
we choose nodes ξ_i and coefficients (weights) A_i so that the
<u>N-point Gauss Rule</u> $G_N(f) = \sum_{i=1}^{N} A_i \cdot f(\xi_i)$ is exact for polynomials of deg $\leq 2N-1$
(of precision $2N-1$)

That this can be done, and how, is <u>not</u> obvious at all!
but it is possible thanks to <u>orthogonal polynomials</u> (and Gauss's ingenuity)

Facts: Given (a,b) and $w(x)\geq 0$, there exists a sequence of polynomials $\{p_n(x)\}_{n=0,1,\ldots}$
$p_n(x)$ has degree n and has n distinct zeros in (a,b), and they are
<u>orthogonal</u> in $L^2_w(a,b)$: $\int_a^b w(x)\,p_k(x)\,p_\ell(x)\,dx = \begin{cases} 0 & \text{if } k\neq \ell \\ \neq 0 & \text{if } k=\ell \end{cases}$

Therefore $\{p_0, p_1, \ldots, p_N\}$ forms a basis for the vector space of polynomials of deg $\leq N$ in $L^2_w(a,b)$.

Turns out that for an N-point Gauss Rule, the nodes ξ_i must be the zeros of $p_N(x)$
and the weights A_i can be found in terms of these ξ_i's:

$$A_i = \int_a^b w(x)\left[\prod_{j=1}^{N} \frac{x-\xi_i}{\xi_i-\xi_j}\right]^2 dx$$

Thus, for each (a,b), $w(x)$ the ξ_i and A_i need to found once and be tabulated!

Standard families: Legendre for $\int_{-1}^{1} f(x)\,dx$, Chebychev for $\int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x)\,dx$,
Laguerre for $\int_0^\infty e^{-x} f(x)\,dx$, Hermite for $\int_{-\infty}^{\infty} e^{-x^2} f(x)\,dx$.

With composite Gauss rules we can choose low N on many subintervals.

Advantages:
1. Few function evaluations needed (but at weird points ξ_i) for high accuracy. Most efficient of all quadrature rules!
2. Can approximate improper integrals that other methods cannot touch

<u>Standard intervals</u>: only need $\int_{-1}^{1}$, $\int_{0}^{\infty}$, $\int_{-\infty}^{\infty}$, any $\int_a^b$ can be transformed to one of these

Any $\int_a^b$ with finite a, b can be transformed to $\int_{-1}^{1}$: $x = \frac{a+b}{2} + \frac{b-a}{2}\cdot t$, $-1 \le t \le 1$

Any $\int_a^\infty \underset{x-a=t}{\longrightarrow} \int_0^\infty$, any $\int_{-\infty}^{b} \underset{b-x=t}{\longrightarrow} \int_0^\infty$

e.g. $\int_{-2}^{3}(x^2+1)\cdot\cos 4x\,dx$ $\left(\begin{array}{l}\text{set } x = \frac{1}{2}+\frac{5}{2}t \\ dx = \frac{5}{2}\,dt\end{array}\right)$ $= \frac{5}{2}\int_{-1}^{1}\left[\left(\frac{1+5t}{2}\right)^2+1\right]\cdot\cos\left(4\left(\frac{1+5t}{2}\right)\right)dt$

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e.g. <u>1-point Gauss-Legendre</u>: $\int_{-1}^{1} f(x)\,dx \approx GL_1(f) = A\cdot f(\xi)$, of precision $2\cdot1-1=1$

so exact for $f(x)=1$ and $f(x)=x$:

For $f(x)=1$: want $A\cdot 1 = \int_{-1}^{1} 1\cdot dx = 2$. For $f(x)=x$ want $A\cdot\xi = \int_{-1}^{1} x\,dx = \frac{x^2}{2}\Big|_{-1}^{1} = 0$

$\Rightarrow A=2$, $\xi=0$, so the 1-pt rule is $GL_1(f) = 2f(0)$, of precision 1, like Trapezoidal

$$\int_{-1}^{1} f(x)\,dx \approx GL_1(f) = 2\cdot f(0) \qquad \text{open rule}$$

e.g. <u>2-point Gauss-Legendre</u>: $\int_{-1}^{1} f(x)\,dx \approx GL_2(f) = A_1\cdot f(\xi_1) + A_2\cdot f(\xi_2)$, of precision $2\cdot2-1=3$

should be exact for $1, x, x^2, x^3$:

nonlinear system for A_1, A_2, ξ_1, ξ_2

unclear if solvable, how many sols

$$\begin{cases} A_1 + A_2 = 2 & = \int_{-1}^{1} dx \\ A_1\cdot\xi_1 + A_2\cdot\xi_2 = 0 & = \int_{-1}^{1} x\,dx = \frac{x^2}{2}\Big|_{-1}^{1} = 0 \\ A_1\cdot\xi_1^2 + A_2\cdot\xi_2^2 = \frac{2}{3} & = \int_{-1}^{1} x^2\,dx = \frac{x^3}{3}\Big|_{-1}^{1} \\ A_1\cdot\xi_1^3 + A_2\cdot\xi_2^3 = 0 & = \int_{-1}^{1} x^3\,dx = \frac{x^4}{4}\Big|_{-1}^{1} \end{cases}$$

Instead of $\{x^n\}$, use the <u>Legendre polys</u>: $L_0(x)=1$, $L_1(x)=x$, $L_2=\frac{3}{2}\left(x^2-\frac{1}{3}\right)$, $L_3=\frac{5}{2}\left(x^3-\frac{3}{5}x\right)$

which are <u>orthogonal</u> in $L^2(-1,1)$:

$$\begin{array}{ll} \text{for } f(x)=L_0(x): & A_1 + A_2 = 2 \\ L_1(x): & A_1\cdot\xi_1 + A_2\cdot\xi_2 = 0 \\ L_2(x): & A_1\cdot\frac{3}{2}\left(\xi_1^2-\frac{1}{3}\right) + A_2\cdot\frac{3}{2}\left(\xi_2^2-\frac{1}{3}\right) = \int_{-1}^{1}\frac{3}{2}\left(x^2-\frac{1}{3}\right)dx = \ldots = \frac{3}{2}\left(\frac{2}{3}-\frac{2}{3}\right) = 0 \\ L_3(x): & A_1\cdot\frac{5}{2}\left(\xi_1^3-\frac{3}{5}\xi_1\right) + A_2\cdot\frac{5}{2}\left(\xi_2^3-\frac{3}{5}\xi_2\right) = \int_{-1}^{1}\frac{5}{2}\left(x^3-\frac{3}{5}x\right)dx = \ldots = 0 \end{array}$$

$\Rightarrow \xi_1 = -\frac{1}{\sqrt{3}}$, $\xi_2 = \frac{1}{\sqrt{3}}$, then $\begin{array}{l} A_1 + A_2 = 2 \\ A_1 - A_2 = 0 \end{array} \Rightarrow A_1 = 1$, $A_2 = 1$

last equ: $1\cdot\frac{5}{2}\left(-3^{-3/2} + \frac{3}{5}\cdot 3^{-\frac{1}{2}}\right) + 1\cdot\frac{3}{2}\left(+3^{-3/2} - \frac{3}{5}\cdot 3^{-1/2}\right) \equiv 0$!

$\therefore$ $\boxed{GL_2(f) = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(+\frac{1}{\sqrt{3}}\right)}$ the 2-pt Gauss-Legendre rule has precision 3,

exact up to cubics! like Simpson

using only 2 evaluations!

Standard Gauss Quadrature Rules: N-point rule for $I(f)=\int_a^b w(x)f(x)\,dx$

$$G_N(f) = \sum_{i=1}^{N} A_i \cdot f(\xi_i)$$, of precision $2N-1$. Nodes ξ_i and weights A_i are tabulated for several N

1. Gauss-Legendre for $I(f)=\int_{-1}^{1} f(x)\,dx$. Here $(a,b)=(-1,1)$, $w(x)\equiv 1$
   nodes $\{\xi_i\}_1^N$ are the zeros of the Legendre poly. $L_N(x)$.
   $L_0(x)=1$, $L_1(x)=x$, $L_2(x)=\frac{3}{2}(x^2-\frac{1}{3})$, $L_3(x)=\frac{1}{2}(5x^3-3x)$, etc.
   For $N=2$: $\xi_1=-\frac{1}{\sqrt{3}}$, $\xi_2=\frac{1}{\sqrt{3}}$, $A_1=A_2=1$.

2. Gauss-Chebyshev for $I(f)=\int_{-1}^{1}\frac{1}{\sqrt{1-x^2}}f(x)\,dx$. Here $(a,b)=(-1,1)$, $w(x)=\frac{1}{\sqrt{1-x^2}}$
   nodes $\{\xi_i\}$ are the zeros of Chebyshev polynomials $T_N(x)=\cos(N\arccos x)$:
   $T_0(x)=1$, $T_1(x)=x$, $T_2(x)=2x^2-1$, $T_3(x)=4x^3-3x$, ...
   For $N=2$: $\xi_1=-\frac{1}{\sqrt{2}}$, $\xi_2=\frac{1}{\sqrt{2}}$, $A_1=A_2=\frac{\pi}{2}$

3. Gauss-Laguerre for $I(f)=\int_0^{\infty} e^{-x}\cdot f(x)\,dx$. Here $(a,b)=(0,\infty)$, $w(x)=e^{-x}$.
   nodes $\{\xi_i\}$ are the zeros of Laguerre polynomials $Q_N(x)$:
   $Q_0(x)=1$, $Q_1(x)=1-x$, $Q_2(x)=x^2-4x+2$, $Q_3(x)=-x^3+9x^2-18x+6$, ...
   For $N=2$: $\xi_1=2-\sqrt{2}$, $\xi_2=2+\sqrt{2}$, $A_1=0.85355...$, $A_2=0.14644...$

4. Gauss-Hermite for $I(f)=\int_{-\infty}^{\infty} e^{-x^2} f(x)\,dx$. Here $(a,b)=(-\infty,\infty)$, $w(x)=e^{-x^2}$.
   nodes $\{\xi_i\}$ are the zeros of Hermite polynomials $H_N(x)$:
   $H_0(x)=1$, $H_1(x)=4x$, $H_2(x)=4x^2-2$, $H_3(x)=8x^3-12x$, ...
   For $N=2$: $\xi_1=-\frac{1}{\sqrt{2}}$, $\xi_2=\frac{1}{\sqrt{2}}$, $A_1=A_2=\frac{\sqrt{\pi}}{2}\approx 0.88622...$

5. Gauss-Kronrod adaptive, very high precision $3N+1$!!!
   uses G_N and K_{2N+1} $\left(= G_N + \sum_{i=1}^{N+1} b_i f(\xi_i)\right.$, reuses nodes of $\left.G_N\right)$
   estimates the error by $\left(200\cdot|G_N-K_{2N+1}|\right)^{3/2}$
   Efficient, high accuracy, provides error estimate

netlib/quadpack/qk61.f for $\int_a^b f(x)\,dx$, uses G_{30} and K_{61}

Matlab, octave: quadgk(@FCN, a, b, TOL).

Examples of Gaussian Quadrature

Ex. 1: $I = \int_{-1}^{1} (3x^2 - 2x + 5)\,dx \quad (= 12)$

1-pt $GL_1 = 2f(0) = 2 \cdot 5 = 10$ it's off, has precision 1

2-pt $GL_2 = f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}}) = (\cancel{3} \cdot \frac{1}{\cancel{3}} + \cancel{\frac{2}{\sqrt{3}}} + 5) + (\cancel{3} \cdot \frac{1}{\cancel{3}} - \cancel{\frac{2}{\sqrt{3}}} + 5) = 2 + 10 = 12$ exact!

GL_2 has precision 3

Ex. 2: $I = \int_1^3 x^x\,dx$. Transform to $\int_{-1}^{1}$: set $x = \frac{1+3}{2} + \frac{3-1}{2} \cdot t = 2 + t$, $dx = dt$

$= \int_{-1}^{1} (2+t)^{2+t}\,dt$. $GL_2 = f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}}) \approx \ldots = 13.125831$

$GL_6 = \ldots \approx 13.725105$

To get same accuracy, Trap. needs 8193 evaluations, Simpson needs 129.

Ex. 3: $I = \int_0^{\infty} e^{-x} \sin x\,dx \quad (= \frac{1}{2})$. Use Gauss-Laguerre

$GLag_6(f) = \sum_{i=1}^{6} A_i f(\xi_i)$ with tabulated A_i, ξ_i produces 0.500049475

remarkably good accuracy with only 6 evaluations!

Ex. 4: $I = \int_{-\infty}^{\infty} x^2 e^{-x^2}\,dx \quad (= \frac{\sqrt{\pi}}{2})$. Use Gauss-Hermite with 2 pts

$GH_2(f) = \frac{\sqrt{\pi}}{2} \cdot \left[f(-\frac{1}{\sqrt{2}}) + f(\frac{1}{\sqrt{2}})\right] = \frac{\sqrt{\pi}}{2} \cdot \left[(-\frac{1}{\sqrt{2}})^2 + (\frac{1}{\sqrt{2}})^2\right] = \frac{\sqrt{\pi}}{2}$, exact!

exact value because 2-pt rule has precision 3, exact up to cubic $f(x)$!

Impoper integrals

I. ∞ limits: transform to $\int_0^\infty e^{-x} f(x)dx$ and use Gauss-Laguerre

or to $\int_{-\infty}^\infty e^{-x^2} f(x)dx$ and use Gauss-Hermite

Weight function can be inserted (if not present already):

e.g. $$\int_0^\infty g(x)dx = \int_0^\infty e^{-x} \cdot [\underbrace{e^x g(x)}_{f(x)}]dx$$

II. singularity in (a,b): split off the singularity: $\int_{x_0-\varepsilon}^{x_0+\varepsilon}$, approximate via Taylor

the rest $\left(\int_a^{x_0-\varepsilon}, \int_{x_0+\varepsilon}^b\right)$ by some standard rule.

Multiple integrals (high dimensional) not easy!

1. Double or triple integrals or low dimensions:
   apply Fubini Thm to transform to iterated integrals, then Trapez. or Simpson

2. (Very) high dimensional; Monte Carlo Integration

$$\int_\Omega f(x)dV \approx \mathrm{vol}(\Omega) \cdot (\text{average of } f \text{ over } N \text{ random points in } \Omega)$$
$$= \mathrm{vol}(\Omega) \cdot \frac{1}{N} \sum_{i=1}^N f(x_i)$$