Thus for only N points we can integrate a polynomial of degree $2N-1$ exactly. For arbitrarily chosen sample points $\{x_k\}$, we would have required $2N$ points to achieve the same accuracy.

Expressions for the abscissae and the weights

The $\{x_k\}_{k=1}^{N}$ are the zeros of the Legendre polynomial of degree N.

The weights $w_k = \dfrac{2(1-x_k^2)}{(N+1)^2\,[P_{N+1}(x_k)]^2}$

m	x_k	w_k	
1	0	2	
2	$\pm 0.5773502692 = 1/\sqrt{3}$	1	
3	0	$0.8\dot{8}$	8/9
	$\pm 0.7745966692 = \sqrt{\frac{3}{5}}$	$0.5\dot{5}$	5/9
$\vdots$			

Neat way to generate the coefficients and weights with your bare hands.

$\mathbf{N=2}$: Must integrate a poly of deg $2\times 2-1=3$ exactly:

$$\int_{-1}^{1} a_0 + a_1 x + a_2 x^2 + a_3 x^3 dx = 2a_0 + \frac{2}{3}a_2$$

$$||$$

$$w_1 f(x_1) + w_2 f(x_2) \qquad w_1 = w_2 \quad x_1 = -x_2$$

$$= 2w_1(a_0 + a_2 x_1^2)$$

$$w_1 = 1$$

$$x_1^2 = \frac{1}{3} \qquad x_1 = \frac{1}{\sqrt{3}}$$

N=3: *FIGURE* must integrate a ploy of degree 5 exactly.

$$\int_{-1}^{1} a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5 dx = 2a_0 + \frac{2}{3}a_2 + \frac{2}{5}a_4$$

$$||$$

$$2w_1\left(a_0 + a_2 x_1^2 + a_4 x_1^4\right) + w_2 a_0$$

$$2w_1 + w_2 = 2$$

$$\left.\begin{array}{l} 2w_1x_1^2 = \frac{2}{3} \\ \\ 2w_1x_1^4 = \frac{2}{5} \end{array}\right\} \Rightarrow \begin{array}{l} x_1^2 = \frac{\frac{2}{5}}{2/3} = \frac{3}{5} \Rightarrow \boxed{x_1 = -\sqrt{\frac{3}{5}}} \\ 2w_1\frac{3}{5} = \frac{2}{3} \Rightarrow \boxed{w_1 = \frac{5}{9}} \\ \frac{2.5}{9} + w_2 = 2 \Rightarrow \boxed{w_2 = \frac{8}{9}} \end{array}$$

Other Gauss-Quadrature formulae:

1) **Hermite-Gauss**: $w(x) = e^{-x^2}$ $(a, b) = (-\infty, \infty)$

$$\int_{-\infty}^{\infty} e^{-x^2} f(x)\, dx = \sum_{k=1}^{N} w_k f(x_k) + \frac{N!\sqrt{\pi}}{2^N (2N)!}\, f^{(2N)}(\xi)$$

$$w_k = \frac{2^{N+1} N! \sqrt{\pi}}{[H_{N+1}(x_k)]^2}$$

m	x_k	w_k
2	±0.707107	0.886227
3	0.0	1.181636
	±1.224745	0.295409

2) **Chebyshev-Gauss Quadrature**: $w(x) = (1-x^2)^{-\frac{1}{2}}$ $[a,b] = [-1,1]$.

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\,dx = \sum_{k=1}^{N} w_k f(x_k) + \frac{2\pi}{2^{2N}(2N)!} f^{(2N)}(\xi)$$

$$w_k = \frac{-\pi}{T'_N(x_k)T_{N+1}(x_k)} = \frac{\pi}{N} \qquad \text{(weights are all equal).}$$

$$x = \frac{t(1-0)}{2} + \frac{1}{2} = \frac{t+1}{2} \quad t = 2x-1$$

Eg: $I = \int_0^1 \sin \pi x \, dx = \frac{1}{2}\int_{-1}^{1} \sin \pi \frac{(1+t)}{2}\,dt = 0.636619772$ EXACT

$$\stackrel{N=2}{\approx} \frac{1}{2}\left[\sin \pi \frac{\left(1-\frac{1}{\sqrt{3}}\right)}{2} + \sin \pi \frac{\left(1+\frac{1}{\sqrt{3}}\right)}{2}\right]$$

FIGURE

$$= \cos \frac{\pi}{2\sqrt{3}}$$

$$= 0.616190509$$

Compare with TRAPEZIUM RULE with N=2 yields =0.5000000.

$$I \stackrel{N=3}{\approx} \frac{1}{2}\left[\frac{5}{9}.\sin \pi \left(\frac{1-\sqrt{\frac{3}{5}}}{2}\right) + \frac{8}{9}\sin\frac{\pi}{2} + \frac{5}{9}\sin\left(\frac{1+\sqrt{\frac{3}{5}}}{2}\right)\right]$$

$$= \frac{5}{9}\cos\left(\frac{\pi}{2}\sqrt{\frac{3}{5}}\right) + \frac{4}{9}$$

$$= 0.637061877$$

Integrating Functions on Infinite Intervals:
Eg.

$$I = \int_0^\infty f(x)\,dx$$

If $f(x) \sim x^{-p}$ as $x \to \infty$ then

$$\int_a^\infty x^{-p}\,dx = \frac{x^{1-p}}{1-p}\Big|_a^\infty$$

exists only if $p > 1$.

Truncate the Infinite Interval:

$$\begin{aligned} I &= \int_a^c f(x)\,dx + \int_c^\infty f(x)\,dx \\ &= I_1 + I_2 \end{aligned}$$

- Use the asymptotic behaviour of f to determine how large c should be for $I_2 < \epsilon/2$

$$\text{Eg.} \qquad \int_0^\infty \cos x e^{-x}\,dx$$

$$\begin{aligned} |I_2| &= \left| \int_c^\infty \cos x e^{-x}\,dx \right| \le \int_c^\infty e^{-x}\,dx = e^{-c} \\ \therefore c &= -\ln(\epsilon/2) = 18.4 \qquad \epsilon = 10^{-8} \end{aligned}$$

  OR use an asymptotic approximation for I_2.

- Evaluate I_1 using the standard integration rules.

Map to a Finite Interval

$$I = \int_a^\infty f(x)\,dx \qquad \text{where } f(x) \overset{x\to\infty}{\sim} x^{-p}$$

- Choose the map such that $x^{-p}\,dx \to dt$

$$\text{Eg. } p = 2: \quad -x^{1-p} = -x^{-1} = t \quad dx = t^{-2}\,dt$$
$$x = -\frac{1}{t}$$

$$\therefore I = \int_a^\infty f(x)\,dx = \int_{-\frac{1}{a}}^0 f\left(-\frac{1}{t}\right)\frac{dt}{t^2}$$

  Now as $t \to 0$ $f\left(-\frac{1}{t}\right) \sim \left(-\frac{1}{t}\right)^{-2} = t^2$ so integrand is finite

- OR

$$\begin{aligned} t &= e^{-x} \\ x &= -\ln t \end{aligned} \qquad \Rightarrow \int_0^\infty f(x)\,dx = \int_0^1 \frac{f(-\ln t)}{t}\,dt$$

- OR $[0,\infty) = [0,S] \cup [S,\infty)$ and on $[0,S]$ set $t = x/S$ on $[S,\infty)$ set $t = S/x$

Specialized Gauss integration rules for infinite intervals

(a) Gauss-Laguerre Integration: $(0,\infty)$ $w = e^{-x}$

$$\int_0^\infty e^{-x} f(x)\,dx = \sum_{k=1}^{N} w_k f(\xi_k)$$

$$\int_0^\infty g(x)\,dx = \int_0^\infty e^{-x} \underbrace{(e^x g(x))}_{f(x)}\,dx$$

(b) Gauss-Hermite integration: $(-\infty,\infty)$ $w = e^{-x^2}$

$$\int_{-\infty}^\infty e^{-x^2} f(x)\,dx = \sum_{k=1}^{N} w_k f(\xi_k)$$

Adaptive Simpson Integration:

$$
\begin{array}{lll}
I(0) & = & \underbrace{\frac{h}{3}[f_0 + 4f_3 + f_5]}_{S_2(h)} - \frac{h^5}{90} f^{(4)}(\xi) \qquad \begin{array}{ccccc} f_1 & f_2 & f_3 & f_4 & f_5 \\ \bullet & \circ & \bullet & \circ & \bullet \\ \leftarrow & -- & \rightarrow & & \\ & h & & & \end{array} \\
I(0) & = & \underbrace{\frac{(h/2)}{3}\{[f_0 + 4f_2 + 2f_3 + 4f_4 + f_5]\}}_{S_4(h)} - \frac{(h/2)^5}{90}\left\{ f^{(4)}(\xi_1) + f^{(4)}(\xi_{2?}) \right\}
\end{array}
$$

Assume $f^{(4)}(\xi) = f^{(4)}(\xi_2) \sim f^{(4)}(\xi)$ approximately constant.
Substract

$$
0 = S_2 - S_4 - \frac{h^5}{90} f^{(4)}(\xi) \left[1 - \frac{1}{2^5} \times 2 \right] = \frac{15}{16} \left(\frac{h^5}{90} f^{(4)}(\xi) \right)
$$

$$
\begin{array}{lll}
\therefore \quad \frac{h^5}{90} f^{(4)}(\xi) & \simeq & \frac{16}{15}(S_2 - S_4) \\
\therefore \quad |I(0) - S_4| & \simeq & \frac{h^5}{90} f^{(4)}(\xi) \left(\frac{1}{2^4} \right) = \frac{1}{15}|S_2 - S_4|
\end{array}
$$

$$
\bullet \quad \circ \quad \bullet \quad \circ \quad \bullet \qquad I_2, I_4
$$

is $\frac{1}{15}|S_2 - S_4| < \text{TOL} \ \star |S_4|$ YES $\rightarrow$ DONE

NO

$$
\begin{array}{ccccccc} \bullet & \circ & \bullet & \circ & \bullet & \circ & \bullet \\ | & & & & | & & \end{array}
$$

$$
\text{is } \frac{1}{15} \left| S_2\left(\frac{h}{2}\right) - S_4\left(\frac{h}{2}\right) \right| < \ \text{TOL}
$$

The Best of Both Worlds – Gauss-Patterson Integration

- Gauss Quadrature Rules obtain the highest accuracy for the least number of function evaluations.

$$| \bullet \quad \bullet \quad \bullet | \qquad | \; x \quad x \quad \bullet \quad x \quad x \; |$$

- Newton-Cotes Formulae allow for automatic and adaptive integration rules because the regular grid allows one to use all previous function evaluations toward subsequent refinements - the adaptive Trapezium rule is an example of this.

$$\bullet \quad \circ \quad \bullet \quad \circ \quad \bullet$$

- The Gauss-Patterson integration rules allow one to build higher order integration schemes which make use of previous function evaluations in subsequent calculations. These rules have the attractive high order accuracy typical of Gauss quadrature rules. This is ideal for adaptive integration.

- Patterson, T.N.L. 1968, "The Optimum Addition of Points T Quadrature Formulas", Math. Comp., **122**, p. 847–856.