Method to get an n-point Gaussian formula of the form

$$\int_{a}^{b} \omega(x) f(x) dx = \sum_{i=1}^{n} H_{i} f(x_{i}) + C f^{(2n)}(\eta)$$

- 1. Define the inner product.
- 2. Find the monic orthogonal polynomial of degree = n, $\phi_n(x)$.
- 3. Find the *n* zeros, x_i , of ϕ_n .
- 4. Use the method of undetermined coefficients to find H_i .
- 5. Set $f(x) = x^{2n}$ so that

$$C = \frac{1}{(2n)!} \left[\int_a^b \omega(x) x^{2n} \, dx - \sum_{i=1}^n H_i x_i^{2n} \right]$$

EXAMPLE. What is the two point Gauss-Laguerre formula

$$\int_0^\infty e^{-x} f(x) \, \mathrm{d}x \approx H_1 f(x_1) + H_2 f(x_2)?$$

Furthermore, give a formula for the truncation error and then estimate the error in your approximation of

$$\int_0^\infty e^{-x} \cos(\cos(\frac{x}{10})) \, \mathrm{d}x$$

From a previous lecture we know that for the Laguerre inner product

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

the monic orthogonal polynomial of degree = 2 is $\phi_2(x) = x^2 - 4x + 2$ which has zeros at $x_1 = 2 - \sqrt{2}$ and $x_2 = 2 + \sqrt{2}$ which we use as our integration points in our integration formula

$$\int_0^\infty e^{-x} f(x) \, \mathrm{d}x \approx H_1 f(2 - \sqrt{2}) + H_2 f(2 + \sqrt{2}).$$

Now using the method of undetermined coefficients find H_1 and H_2 satisfying

$$f(x) = 1: H_1 + H_2 = \int_0^\infty e^{-x} dx = 1$$

$$f(x) = x: H_1 x_1 + H_2 x_2 = \int_0^\infty x e^{-x} dx = 1$$

$$H_1 = \frac{x_2 - 1}{x_2 - x_1} = \frac{1}{2} + \frac{1}{2\sqrt{2}}$$

$$H_2 = 1 - H_1 = \frac{1}{2} - \frac{1}{2\sqrt{2}}$$

So we know our formula

$$\int_0^\infty e^{-x} f(x) \, \mathrm{d}x \approx \left[\tfrac{1}{2} + \tfrac{1}{2\sqrt{2}} \right] f(2 - \sqrt{2}) + \left[\tfrac{1}{2} - \tfrac{1}{2\sqrt{2}} \right] f(2 + \sqrt{2})$$
 integrates polynomials of degree \leqslant 3 exactly. So let us check that the formula is exact for x^2 , x^3 but not for x^4

$$2! = \int_0^\infty e^{-x} x^2 \, dx = \left[\frac{1}{2} + \frac{1}{2\sqrt{2}} \right] (2 - \sqrt{2})^2 + \left[\frac{1}{2} - \frac{1}{2\sqrt{2}} \right] (2 + \sqrt{2})^2$$

$$= \frac{1}{2} (2(2^2 + (\sqrt{2})^2)) - \frac{1}{2\sqrt{2}} (2(2 \times 2\sqrt{2})) = 6 - 4 = 2\sqrt{2}$$

$$3! = \int_0^\infty e^{-x} x^3 \, dx = \left[\frac{1}{2} + \frac{1}{2\sqrt{2}} \right] (2 - \sqrt{2})^3 + \left[\frac{1}{2} - \frac{1}{2\sqrt{2}} \right] (2 + \sqrt{2})^3$$

$$= \frac{1}{2} (2(2^3 + 3 \times 2(\sqrt{2})^2)) - \frac{1}{2\sqrt{2}} (2(3 \times 2^2 \sqrt{2} + (\sqrt{2})^3)) = 20 - 14 = 6\sqrt{2}$$

$$4! = \int_0^\infty e^{-x} x^4 \, dx \neq \left[\frac{1}{2} + \frac{1}{2\sqrt{2}} \right] (2 - \sqrt{2})^4 + \left[\frac{1}{2} - \frac{1}{2\sqrt{2}} \right] (2 + \sqrt{2})^4$$

$$= \frac{1}{2} (2(2^4 + 6 \times 2^2(\sqrt{2})^2 + (\sqrt{2})^4)) - \frac{1}{2\sqrt{2}} 2(4 \times 2^3 \sqrt{2} + 4 \times 2(\sqrt{2})^3)$$

$$= 68 - 48 = 20$$

For $f, f', \dots, f^{(4)}$ continuous on $[0, \infty)$ by multiplying the Hermite interpolation formula by e^{-x} , integrating over $(0, \infty)$ (noting $\overline{H}_i = 0$ by construction) and using the second integral mean value theorem it follows that

$$\int_0^\infty e^{-x} f(x) dx - \left\{ \left[\frac{1}{2} + \frac{1}{2\sqrt{2}} \right] f(2 - \sqrt{2}) + \left[\frac{1}{2} - \frac{1}{2\sqrt{2}} \right] f(2 + \sqrt{2}) \right\}$$

$$= \frac{1}{4!} \int_0^\infty e^{-x} (x^2 - 4x + 2)^2 f^{(4)}(\xi) dx = \frac{f^{(4)}(\eta)}{4!} \int_0^\infty e^{-x} (x^2 - 4x + 2)^2 dx$$

$$= C f^{(4)}(\eta) \text{ where } C = \frac{1}{4!} (24 - 20) = \frac{1}{6}.$$

Now applying the formula

$$\int_0^\infty e^{-x} \cos(\cos(\frac{x}{10})) \, dx \approx \left[\frac{1}{2} + \frac{1}{2\sqrt{2}}\right] \cos(\cos(\frac{2-\sqrt{2}}{10})) + \left[\frac{1}{2} - \frac{1}{2\sqrt{2}}\right] \cos(\cos(\frac{2+\sqrt{2}}{10})) = 0.5485108$$

correct to 7 decimal places. Noting that

$$|f^{(4)}(x)| = 10^{-4} |\cos(\cos(\frac{x}{10}))(\sin^4(\frac{x}{10}) + 4\sin^2(\frac{x}{10}) - 3\cos^2(\frac{x}{10})) -\sin(\cos(\frac{x}{10}))(6\sin^2(\frac{x}{10})\cos(\frac{x}{10}) + \cos(\frac{x}{10}))| \le 1.5 \times 10^{-3}$$

Hence

$$\left| \int_0^\infty e^{-x} \cos(\cos(\frac{x}{10})) \, dx - 0.5485108 \right| \le \frac{1}{6} |f^{(4)}(\eta)| \le 2.5 \times 10^{-4}.$$

n-point Gauss-Legendre formula

We will find the general n point formula where $\omega(x)\equiv 1$ and [a,b]=[-1,1]. That is

$$\int_{-1}^{1} f(x) \, dx = \sum_{i=1}^{n} H_i f(x_i) + E$$

where the x_i 's are the zeros of the Legendre polynomial given by Rodrigues formula

$$P_n(x) := \frac{1}{2^n n!} \frac{\mathrm{d}^n}{\mathrm{d}x^n} (x^2 - 1)^n = \frac{1}{2^n n!} (2n)(2n - 1) \cdots (n+1)x^n + \cdots$$
$$= \frac{(2n)!}{2^n (n!)^2} x^n + \cdots = \frac{(2n)!}{2^n (n!)^2} w_n(x). \tag{\dagger}$$

We show that $(P_n, P_m) = 0$ for $n \neq m$. Let $n \geqslant m$ then using integration by parts

$$2^{n+m}n!m!(P_n, P_m) = \int_{-1}^{1} \frac{\mathrm{d}^n}{\mathrm{d}x^n} (x^2 - 1)^n \frac{\mathrm{d}^m}{\mathrm{d}x^m} (x^2 - 1)^m \, \mathrm{d}x$$

$$= \left[\frac{\mathrm{d}^{n-1}}{\mathrm{d}x^{n-1}} (x^2 - 1)^n \frac{\mathrm{d}^m}{\mathrm{d}x^m} (x^2 - 1)^m \right]_{-1}^{1}$$

$$- \int_{-1}^{1} \frac{\mathrm{d}^{n-1}}{\mathrm{d}x^{n-1}} (x^2 - 1)^n \frac{\mathrm{d}^{m+1}}{\mathrm{d}x^m} (x^2 - 1)^m \, \mathrm{d}x$$

$$= \dots = (-1)^m \int_{-1}^{1} \frac{\mathrm{d}^{n-m}}{\mathrm{d}x^{n-m}} (x^2 - 1)^n \frac{\mathrm{d}^{2m}}{\mathrm{d}x^{2m}} (x^2 - 1)^m \, \mathrm{d}x$$

$$= (2m)!(-1)^m \int_{-1}^{1} \frac{\mathrm{d}^{n-m}}{\mathrm{d}x^{n-m}} (x^2 - 1)^n \, \mathrm{d}x = \begin{cases} 0 & n > m \\ \frac{2[2^n n!]^2}{(2n+1)} & n = m \end{cases}$$

where we obtain the last relation by noting that $I_n:=\int_{-1}^1 (1-x^2)^n\,\mathrm{d}x$ satisfies the recurrence relation

$$I_n = \frac{2n}{2n+1}I_{n-1}, \ I_0 = 2 \Longrightarrow I_n = \frac{2[2^n n!]^2}{(2n+1)!} \text{ i.e. } (P_n, P_n) = \frac{2}{2n+1}.$$
 (‡)

Now the integration coefficients are given by

$$H_i = \int_{-1}^{1} l_i(x) dx = \int_{-1}^{1} \frac{P_n(x)}{P'_n(x_i)(x - x_i)} dx.$$

Expanding the polynomial $P_{n+1}(x)$ as a Taylor series about x_i we find that

$$P_{n+1}(x) = P_{n+1}(x_i) + \sum_{j=1}^{n} \frac{P_{n+1}^{(j)}(x_i)(x-x_i)^j}{j!} + \frac{P_{n+1}^{(n+1)}(x_i)(x-x_i)^{n+1}}{(n+1)!}$$

it follows on multiplying this formula by $P_n(x)/(x-x_i)$ and integrating over [-1, 1], noting the orthogonality of $\{P_n\}$, (\dagger) and (\ddagger) , that

$$\underbrace{\sum_{i=0}^{1} P_{n+1}(x) \underbrace{\frac{P_{n}(x)}{x_{i}}}_{x=x_{i}} dx}_{=0} \underbrace{\frac{P_{n}-1}{P_{n+1}(x_{i}) \frac{P_{n}(x)}{x_{i}}}_{x=x_{i}} dx}_{=0} + \sum_{j=1}^{n} \underbrace{\int_{-1}^{1} \frac{P_{n+1}^{(j)}(x_{i}) \underbrace{(x_{i} - x_{i})^{j-1}}_{j!}}_{=0} P_{n}(x) dx}_{=0} + \underbrace{\int_{-1}^{1} \frac{P_{n+1}^{(n+1)!}(x_{i})}{P_{n+1}^{(n+1)}(x_{i})}}_{(x_{i} - x_{i})} \underbrace{\frac{P_{n}(x)}{(x_{i} - x_{i})^{n}}}_{(n+1)!} P_{n}(x) dx}_{(n+1)!} = P_{n+1}(x_{i}) \underbrace{\int_{-1}^{1} \frac{P_{n}(x)}{x_{i}}_{x=x_{i}}}_{=2n+1,n+1} dx + \underbrace{\frac{2n(n!)^{2}}{(2n)!}}_{=2n+1,n+1} \times \underbrace{\frac{1}{(2n+1)!}}_{=2n+1,n+1} \underbrace{\frac{P_{n}(x)}{(n+1)!}}_{=2n+1,n+1} \underbrace{\frac{P_{n}(x)}{(2n+1)!}}_{=2n+1,n+1} \underbrace{\frac{P_{n}(x)}{(2n+1)!}}_{=2n+1,n+1}$$

which implies on rearrangement that

$$H_i = \frac{1}{P_n'(x_i)} \int_{-1}^1 \frac{P_n(x)}{(x-x_i)} dx = \frac{1}{P_n'(x_i)} \times \frac{1}{P_{n+1}(x_i)} \times \frac{-2}{n+1}$$

The truncation error, on noting (†), the second integral mean value theorem and (‡), is given by integrating the Hermite interpolation formula and noting that $\overline{H}_i = 0$ by construction

$$E = \int_{-1}^{1} f(x) dx - \sum_{i=1}^{n} H_{i} f(x_{i}) = \int_{-1}^{1} \frac{1}{(2n)!} f^{(2n)}(\xi) (w_{n}(x))^{2} dx$$
$$= \frac{1}{(2n)!} f^{(2n)}(\eta) \left(\frac{2^{n} (n!)^{2}}{(2n)!} \right)^{2} (P_{n}, P_{n}) = \frac{2^{2n+1} (n!)^{4}}{[(2n)!]^{3} (2n+1)} f^{(2n)}(\eta).$$

In an analogous way one can derive the n-point Gauss-Chebyshev formula

$$\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}} dx - \frac{\pi}{n} \sum_{i=1}^{n} f\left(\cos\left[\frac{(2i-1)\pi}{2n}\right]\right) = \frac{\pi}{2^{2n-1}(2n)!} f^{(2n)}(\eta).$$