Lecture 7: Singular Integrals, Open Quadrature rules, and Gauss Quadrature

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In this lecture we discuss the evaluation of singular integrals using so-called open quadrature formulae. We also discuss various techniques to obtain more accurate approximations to singular integrals such as subtracting out the singularity and transformations to non singular integrals. We next introduce Gauss Integration, which exploits the orthogonality properties of orthogonal polynomials in order to obtain integration rules that can integrate a polynomial of degree $2N-1$ exactly using only N sample points. We also discuss integration on infinite integrals and adaptive integration.

Key Concepts: Singular Integrals, Open Newton-Cotes Formulae, Gauss Integration.

7 Singular Integrals, Open Quadrature rules, and Gauss Quadrature

7.1 Integrating functions with singularities

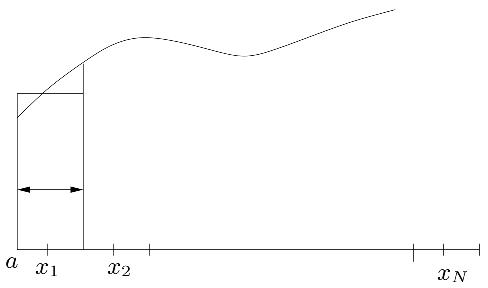
Consider evaluating singular integrals of the form $I = \int_0^1 \frac{e^{-x}}{x^{2/3}} dx$

We cannot just use the trapezoidal rule in this case as $f_0 \to \infty$. Instead we use what are called *open integration formulae* that do not use the endpoints in the numerical approximation of the integrals.

7.1.1 *Open Newton-Cotes formulae*

The Midpoint rule

$$\begin{aligned}
f(x) &= f(x_0) + (x-x_0)f'(x_0) + \frac{(x-x_0)^2}{2}f''(x_0) + \cdots \\
\int_{x_0-h/2}^{x_0+h/2} f(x)dx &= \int_{x_0-h/2}^{x_0+h/2} f_0 + (x-x_0)f_0' + \frac{(x-x_0)^2}{2}f''(\xi)dx \\
&= hf_0 + \int_{-h/2}^{h/2} sf_0' + \frac{s^2}{2}f''(\xi)\,d\xi \\
&= hf_0 + \frac{2s^3}{6}\Big|_0^1 f''(\xi) = hf_0 + \frac{1}{3}\frac{h^3}{8}f''(\xi) = hf_0 + \frac{h^3}{24}f''(\xi)
\end{aligned}$$



The Composite Midpoint rule

$$\begin{aligned} I = \int_a^b f(x)\, dx &= \sum_{k=1}^{N} \int_{x_k-h/2}^{x_k+h/2} f(x)dx \\ &= \sum_{k=1}^{N} \int_{-h/2}^{h/2} f(x_k+s)ds \\ &= \sum_{k=1}^{N} \int_{-h/2}^{h/2} f(x_k) + sf'(x_k) + \frac{s^2}{2} f''(x_k) + \cdots ds \\ &= h\sum_{k=1}^{N} f(x_k) + \sum_{k=1}^{N} f''(x_k) \frac{h^3}{3\cdot 2^3} \\ &= h\sum_{k=1}^{N} f(x_k) + \frac{h^3}{24} \sum_{k=1}^{N} f''(x_k) \\ &= h\sum_{k=1}^{N} f(x_k) + \frac{h^2}{24} \int_a^b f''(x)\, dx \\ &= h\sum_{k=1}^{N} f(x_k) + \frac{h^2}{24} \{f'(b) - f'(a)\} \end{aligned}$$

For 1 cell $\int_{x_k-h/2}^{x_k+h/2} f(x)\, dx = hf(x_k) + \frac{h^3}{24} f''(x_k)$

Open Newton-Cotes Formulae:

$$\int_{x_0}^{x_2} f(x)\, dx = 2hf_1 + \frac{(2h)^3}{24} f''(\xi) \qquad MidpointRule \quad \xi \in (x_0, x_1)$$

$$\int_{x_0}^{x_3} f(x)\, dx = \frac{3h}{2}(f_1+f_2) + \frac{h^3}{4} f^{(2)}(\xi) \qquad \xi \in (x_0, x_3)$$

$$\int_{x_0}^{x_4} f(x)\, dx = \frac{4h}{3}(2f_1 - f_2 + 2f_3) + \frac{28h^5}{90} f^{(4)}(\xi) \qquad \xi \in (x_0, x_4)$$

7.1.2 *Change of variable*

$$\text{(Eg.1)} \qquad I = \int_0^1 x^{-1/n} f(x)\, dx \qquad n \geq 2 \qquad f(t^n)\, t^{-1} n t^{n-1} dt$$

$$\text{let } t = x^{1/n} \qquad x = t^n \qquad dx = n t^{n-1} dt$$

$$\therefore I = n \int_0^1 f(t^n) t^{n-2} dt \qquad \text{which is a proper integral for } n \geq 2$$

$$\text{(Eg. 2)} \qquad I = \int_{-1}^1 \frac{f(x)}{(1-x^2)^{1/2}}\, dx \qquad x = \cos t \qquad dx = -\sin t\, dt$$

$$= \int_0^\pi f(\cos t)\, dt \qquad \text{proper}$$

$$\text{(Eg. 3)} \qquad I = \int_0^1 \frac{f(x)}{[x(1-x)]^{1/2}}\, dx \qquad x = \sin^2 t \qquad dx = 2 \sin t \cos t\, dt$$

$$= \int_0^{\pi/2} \frac{f(\sin^2 t) 2 \sin t \cos t\, dt}{\sin t \cos t} = 2 \int_0^{\pi/2} f(\sin^2 t) dt.$$

7.1.3 *Subtracting the singularity*

Consider evaluating the integral

$$I = \int_0^1 \frac{e^x}{x^{1/2}}\, dx$$

We note that close to the singular point $x = 0$ in the integrand, the numerator can be expanded about the singular point in the Taylor series: $e^x = 1 + x + \frac{x^2}{2!} + \ldots$. We now choose to rearrange the integrand as follows

$$I = \int_0^1 \frac{e^x}{x^{1/2}}\, dx = \int_0^1 \frac{1}{x^{1/2}}\, dx + \int_0^1 \frac{(e^x - 1)}{x^{1/2}}\, dx$$

$$= 2 + \int_0^1 \frac{e^x - 1}{x^{1/2}}\, dx$$

Using this decomposition we can thus evaluate the singular part analytically and the non-singular part numerically. We can expect to obtain a more accurate result than simply using an open integration formula and ignoring the singularity. Since the accuracy of the midpoint rule, for example, depends on the second derivative of the integrand $\frac{(e^x-1)}{x^{1/2}}$, we cannot expect even the midpoint rule to achieve its theoretical rate of convergence for this integral. To retrieve the $O(h^2)$ accuracy of the Midpoint rule we need to subtract at least three terms as follows:

$$\begin{aligned} I &= \int_0^1 \frac{e^x}{x^{1/2}}\, dx \\ &= 2 + \int_0^1 \frac{x}{x^{1/2}}\, dx + \int_0^1 \frac{x^2/2}{x^{1/2}} dx + \int_0^1 \frac{e^x - 1 - x - x^2/2}{x^{1/2}}\, dx \\ &= 2 + \frac{2}{3} x^{3/2}\Big|_0^1 + \frac{2}{5}\frac{x^{3/2}}{2}\Big|_0^1 + \int_0^1 \frac{e^x - 1 - x - x^2/2}{x^{1/2}}\, dx \\ &= \frac{43}{15} + \int_0^1 \frac{e^x - 1 - x - x^2/2}{x^{1/2}}\, dx \end{aligned}$$

In figure 1 we plot the errors obtained when the midpoint rule is used directly as well as the errors when 1 and 3 terms are subtracted from the integrand. The second order accuracy only returns when 3 terms are removed so that g'' is bounded on $[0,1]$, where $g(x) = \frac{e^x - 1 - x - x^2/2}{x^{1/2}}$.

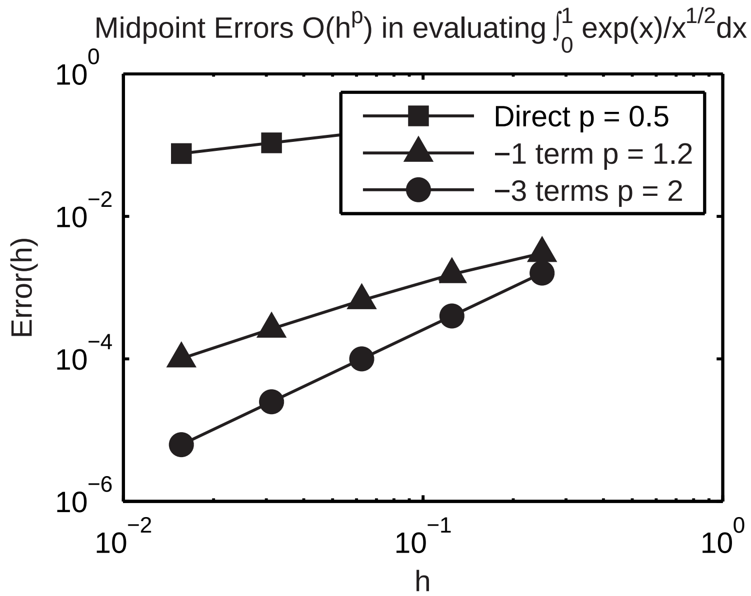


FIGURE 1. Plots of the errors vs h when the midpoint rule is used directly, and when 1 and 3 terms are removed

7.2 Gauss Quadrature

7.2.1 *Orthogonal polynomials*

There exist families of polynomial functions $\{\phi_n(x)\}_{n=0}^{\infty}$ each of which are orthogonal with respect to integration over an interval $[a, b]$ with weight $w(x)$: i.e.:

$$\int_a^b \phi_m(x)\phi_n(x)w(x)dx = \delta_{mn}C_n.$$

Eg. (1) **Legendre Polynomials**: $\{P_n(x)\}$; $[a, b] = [-1, 1]$; $w(x) \equiv 1$.

$$P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \frac{1}{2}(3x^2 - 1), \ldots$$

In general $P_n(x)$ can be constructed by the recursion:

$$P_n(x) = \frac{2n-1}{n}xP_{n-1}(x) - \frac{(n-1)}{n}P_{n-2}(x).$$

$$\text{ODE:} \quad (1 + x^2)y'' - 2xy' + (n + 1)ny = 0; \quad y = P_n(x)$$

Eg. (2) **Laguerre Polynomials**: $\{\mathcal{L}_n(x)\}$; $[a, b) = [0, \infty)$; $w(x) = e^{-x}$

$$\mathcal{L}_0(x) = 1; \quad \mathcal{L}_1(x) = 1 - x, \quad \mathcal{L}_2(x) = 2 - 4x + x^2, \ldots$$

Recursion relation:

$$\mathcal{L}_n(x) = (2n - x - 1)\mathcal{L}_{n-1}(x) - (n - 1)^2\mathcal{L}_{n-2}(x).$$

$$\text{ODE:} \quad xy'' + (1 - x)y' + ny = 0; \qquad y = \mathcal{L}_n(x).$$

Eg. (3) **Chebyshev Polynomials**: $\{T_n(x)\}$, $[a, b] = [-1, 1]$, $w(x) = 1/\sqrt{1 - x^2}$

Definition: $T_n(x) = \cos n\theta$ where $\theta = \cos^{-1} x$.

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_2(x) = \cos 2\theta = 2\cos^2\theta - 1 = 2x^2 - 1, \ldots$$

The recursion relation follows from the identity: $\cos n\theta = 2\cos\theta\cos(n-1)\theta - \cos(n-1)$

$$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

$$\text{ODE:} \ (1 - x^2)y'' - xy' + n^2y = 0 \qquad y = T_n(x)$$

Hermite Polynomials: $\{H_n(x)\}$ $(a,b)=(-\infty,\infty)$ $w(x)=e^{-x^2}$

$$H_0(x)=1, \qquad H_1(x)=2x, \qquad H_2(x)=4x^2-2,\ldots$$

$$\text{Recursion: } H_n(x)=2xH_{n-1}(x)-2(n-1)H_{n-2}(x)$$

$$\textbf{ODE: } y''-2xy'+2ny=0 \qquad y=H_n(x).$$

7.2.2 *Expansion of an arbitrary polynomial in terms of orthogonal polynomials*

Let $q_k(x)=\alpha_0+\alpha_1 x+\cdots+\alpha_k x^k$ be any polynomial of degree k. Then since the orthogonal polynomials $\{\phi_j(x)\}$ are linearly independent, we can also express $q_k(x)$ as a linear combination of $\{\phi_j(x)\},\ j=0,\ldots,k$ as follows:

$$\begin{aligned} q_k(x) &= \alpha_0+\alpha_1 x+\cdots+\alpha_k x^k \\ &= \beta_0\phi_0+\beta_1\phi_1+\cdots+\beta_k\phi_k. \end{aligned} \qquad (*)$$

Example: Expand $q_2(x)=-2x^2+2x-1$ in terms of Legendre Polynomials $P_k(x)$

$$\begin{aligned} q_2(x) &= -2x^2+2x-1 \qquad \text{in terms of Legendre polynomials} \\ &= \beta_0+\beta_1 x+\beta_2\frac{1}{2}(3x^2-1) \\ &= \left(\beta_0-\frac{\beta_2}{2}\right)+\beta_1 x+\frac{3\beta_2}{2}x^2 \\ \frac{3\beta_2}{2} &= -2 \quad \Rightarrow \quad \beta_2=-\frac{4}{3} \\ \beta_1 &= 2 \\ \beta_0+\frac{2}{3} &= -1 \quad \Rightarrow \quad \beta_0=-\frac{5}{3} \\ \therefore q_2(x) &= -\frac{5}{3}P_0(x)+2P_1(x)-\frac{4}{3}P_2(x) \end{aligned}$$

7.2.3 $\phi_n(x)$ *is orthogonal w.r.t the weight* $w(x)$ *to all lower degree polynomials* $q_k(x),\ k=0,\ldots,n-1$

The fact that any polynomial $q_k(x)$ can be expanded as a linear combination of orthogonal polynomials $\{\phi_j(x)\}_{j=0}^k$ up to degree k, as was shown in the expansion $(*)$, implies that an orthogonal polynomial $\phi_n(x)$ is orthogonal with respect to the weight $w(x)$ to any polynomial of a lower degree than n. In other words, if $\{q_k(x)\}_{k=0}^{n-1}$ are any polynomials of degrees $k=0,\ldots,n-1$, then

$$\int_a^b w(x)\phi_n(x)q_k(x)dx=0 \qquad \text{for } k=0,\ldots,n-1$$

To see this, consider any kth degree polynomial $q_k(x)$ and use use the expansion $(*)$ to write

$$\begin{aligned}\int_a^b w(x)\phi_n(x)q_k(x)dx &= \int_a^b w(x)\phi_n(x)\sum_{m=0}^{k}\beta_k\phi_m(x)dx \\ &= \sum_{m=0}^{k}\beta_k\int_a^b w(x)\phi_n(x)\phi_m(x)dx \\ &= 0\end{aligned}$$

The latter integrals vanish because of the orthogonality of polynomials of distinct degree with respect to the weight $w(x)$.

7.3 Gauss-Legendre quadrature

Idea behind Gauss Quadrature:

We assume that the approximation of $\int_a^b f(x)dx$ is given by:

$$\int_a^b f(x)dx \approx \sum_{i=0}^{N} w_i f(x_i)$$

where the w_i are weights given to the function values $f(x_i)$. If we regard the x_i as free then can we do better by choosing these x_i appropriately?

Shift to the interval $[-1,1]$: There is no loss of generality in assuming that $[a,b]=[-1,1]$ since the change of variables $x\in[a,b]$ to $t\in[-1,1]$:

$$x=\frac{t(b-a)}{2}+\frac{(a+b)}{2}$$

will reduce the integral to $\int_{-1}^{1} F(t)dt$ where $F(t)=\frac{(b-a)}{2}f(x(t))$

Let us approximate f on $[-1,1]$ by a polynomial of degree $M-1$ and integrate the resulting polynomial. The error involved is of the form:

$$\begin{aligned}\int_{-1}^{1} f(x)dx &= \int_{-1}^{1} p_{M-1}(x)dx+\frac{f^{(M)}(\xi)}{M!}\int_{-1}^{1}(x-x_1)\dots(x-x_M)dx \\ &= \sum_{k=1}^{M} f_k\int_{-1}^{1}\ell_k(x)dx+\int_{-1}^{1} f[x_1,\dots,x_M,x](x-x_1)\dots(x-x_M)dx \\ &= \sum_{k=1}^{M} f_k w_k+\int_{-1}^{1} f[x_1,\dots,x_M,x](x-x_1)\dots(x-x_M)dx \quad \text{where} \quad \ell_k(x)=\prod_{\substack{j=1\\ j\neq k}}^{M}(x-x_j)/x_k-x_j) \\ & \qquad \text{and} \quad w_k=\int_{-1}^{1}\ell_k(x)dx.\end{aligned}$$

This formula will be exact if f is a polynomial of degree $M-1$ since then $P_{M-1}(x)\equiv f(x)$.

Now let $M = 2N$ and choose $x_1, \dots, x_N$ to be the zeros of the Legendre polynomial $P_N(x)$ of degree N. In this case, all the weights $w_k = 0$ $\boxed{\text{for } k \geq N+1}$ as can be seen from the calculation

$$
\begin{aligned}
w_k = \int_{-1}^{1} \ell_k(x)dx &= \int_{-1}^{1} \frac{\overbrace{(x-x_1)\dots(x-x_N)}\ \overbrace{(x-x_{N+1})\dots(x-x_{k-1})(x-x_{k+1})\dots(x-x_M)}}{(x_k-x_1)\quad\dots\quad(x_k-x_{N+1})\quad\dots\quad(x_k-x_M)}\,dx \quad k \geq N+1 \\
&= \widetilde{C}_k \int_{-1}^{1} P_N(x) q_{k,N-1}(x)\,dx \\
&= \widetilde{C}_k \int_{-1}^{1} P_N(x) \left(\sum_{S=0}^{N-1} \beta_S P_S(x) \right) dx \\
&= 0 \text{ no matter where we choose the } x_{N+1}, \dots, x_{2N}.
\end{aligned}
$$

$$
\begin{aligned}
\therefore \int_{-1}^{1} f(x)\,dx &= \sum_{k=1}^{N} f_k w_k + \frac{f^{(2N)}(\xi)}{(2N)!} \int_{-1}^{1} (x-x_1)^2 \dots (x-x_N)^2\,dx \\
&= \sum_{k=1}^{N} f_k w_k + \frac{f^{(2N)}(\xi)}{(2N)!} \int_{-1}^{1} C_N^2 \left[P_N(x)\right]^2\,dx
\end{aligned}
$$

or $$\int_{-1}^{1} f(x)\,dx = \sum_{k=1}^{N} f_k w_k + \frac{2^{2N+1}(N!)^4}{(2N+1)[(2N)!]^3}\, f^{(2N)}(\xi).$$

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 $w_k = \dfrac{2(1-x_k^2)}{(N+1)^2\left[P_{N+1}(x_k)\right]^2}$

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
$\vdots$			

7.3.1 *Generating the coefficients and weights using the method of undetermined coefficients*

N=2: This quadrature rule must integrate a polynomial of degree $2 \times 2 - 1 = 3$ 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=2: This quadrature rule must integrate a polynomial of degree 5 exactly.

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

$$||$$

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

$$2w_1 + w_2 = 2$$

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

Example: Evaluate $I = \int_0^1 \sin \pi x \, dx$

We make use of the transformation of variables $x = \frac{t(1-0)}{2} + \frac{1}{2} = \frac{t+1}{2} \quad t = 2x - 1$

$$
\begin{aligned}
I &= \int_0^1 \sin \pi x \, dx = 0.636619772 \\
&= \frac{1}{2} \int_{-1}^{1} \sin \pi \frac{(1+t)}{2} \, dt \\
&\approx \frac{1}{2} \left[\sin \pi \frac{\left(1 - \frac{1}{\sqrt{3}}\right)}{2} + \sin \pi \frac{\left(1 + \frac{1}{\sqrt{3}}\right)}{2} \right] \\
&= \cos \frac{\pi}{2\sqrt{3}} \\
&= 0.616190509
\end{aligned}
$$

Compare this result with the trapezium rule using two function evaluations, which yields =0.5000000. Now using three point Gauss-Legendre formula:

$$
\begin{aligned}
I &\overset{N=3}{\approx} \frac{1}{2} \left[\frac{5}{9} . \sin \pi \left(\frac{1 - \sqrt{\frac{3}{5}}}{2} \right) + \frac{8}{9} \sin \frac{\pi}{2} + \frac{5}{9} \sin \left(\frac{1 + \sqrt{\frac{3}{5}}}{2} \right) \right] \\
&= \frac{5}{9} \cos \left(\frac{\pi}{2} \sqrt{\frac{3}{5}} \right) + \frac{4}{9} \\
&= 0.637061877
\end{aligned}
$$

7.3.2 *Other Gauss-Quadrature formulae*

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

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

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

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

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

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

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

7.4 Integrating Functions on Infinite Intervals

Consider evaluating integrals of the form

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

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 $p > 1$.

7.4.1 *Truncate the Infinite Interval*

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

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

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

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

OR use an asymptotic approximation for I_2.

- Evaluate I_1 using the standard integration rules.

7.4.2 *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

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

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

7.4.3 *Specialized Gauss integration rules for infinite intervals*

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

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

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

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

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

7.5 Adaptive Integration

7.5.1 Adaptive Simpson Integration

$$I(0) = \underbrace{\frac{h}{3}[f_0 + 4f_3 + f_5]}_{S_2(h)} - \frac{h^5}{90}f^{(4)}(\xi) \qquad \begin{matrix} f_1 & f_2 & f_3 & f_4 & f_5 \\ \bullet & \circ & \bullet & \circ & \bullet \\ \leftarrow & -- & \rightarrow & & \\ & h & & & \end{matrix}$$

$$I(0) = \underbrace{\frac{(h/2)}{3}\{[f_0 + 4f_2 + 2f_3 + 4f_4 + f_5]\}}_{S_4(h)} - \frac{(h/2)^5}{90}\left\{f^{(4)}(\xi_1) + f^{(4)}(\xi_{2?})\right\}$$

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

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

$$\therefore \quad \frac{h^5}{90}f^{(4)}(\xi) \simeq \frac{16}{15}(S_2 - S_4)$$

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

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

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

NO

$$\begin{matrix} \bullet & \circ & \bullet & \circ & \bullet & \circ & \bullet \\ | & & & & | & & \end{matrix}$$

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

7.5.2 *The Best of Both Worlds – Gauss-Patterson Integration*

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

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

- 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.