0.3.2 Integrating functions with singularities

$$I = \int_0^1 \frac{dx}{x^{1/2}} = 2x^{1/2}\Big|_0^1 = 2$$

$$I = \int_0^1 \frac{e^{-x}}{x^{2/3}} dx$$

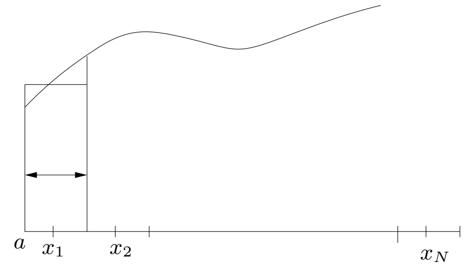
We cannot just use the trapezoidal rule in this case as $f_0 \to \infty$. In this case we use what are called open integration formulae.

1. Open integration 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



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

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:

$$
\begin{aligned}
\int_{x_0}^{x_2} f(x)\,dx &= 2hf_1 + \frac{(2h)^3}{24} f''(\xi) && MidpointRule \quad \xi \in (x_0, x_1) \\
\int_{x_0}^{x_3} f(x)\,dx &= \frac{3h}{2}(f_1+f_2) + \frac{h^3}{4} f^{(2)}(\xi) && \xi \in (x_0, x_3) \\
\int_{x_0}^{x_4} f(x)\,dx &= \frac{4h}{3}(2f_1 - f_2 + 2f_3) + \frac{28h^5}{90} f^{(4)}(\xi) && \xi \in (x_0, x_4)
\end{aligned}
$$

2. Change of variable

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

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

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

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

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

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

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

3. Subtracting the singularity: $\qquad e^x = 1 + x + \frac{x^2}{2!} + \ldots$

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

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

$$= 2 + \frac{2}{3} x^{3/2} \Big|_0^1 + \int_0^1 \frac{e^x - 1 - x}{x^{1/2}}\, dx$$

$$= \frac{8}{3} + \int_0^1 \frac{e^x - 1 - x}{x^{1/2}}\, dx$$

0.3.2 Gauss Quadrature

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: $\cos n\theta = 2\cos\theta\cos(n-1)\theta-\cos(n-1)$

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

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

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

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

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

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

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?

Expansion of an arbitrary polynomial in terms of orthogonal polynomials.

$$\begin{aligned} \text{Let} \quad q_n(x) &= \alpha_0 + \alpha_1 x + \cdots + \alpha_n x^n \\ &= \beta_0\phi_0 + \beta_1\phi_1 + \cdots + \beta_n\phi_n. \end{aligned} \qquad (*)$$

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

Orthogonality of all lower degree polynomials:

An important fact that results from the expansion $(*)$ is

$$\begin{aligned} \int_a^b w(x)P_m(x)q_n(x)dx &= 0 \qquad \text{for } n = 0, \ldots, m-1 \\ \sum_{k=0}^{n} \beta_k \int_a^b w(x)\phi_k(x)\phi_m(x)dx &= 0. \end{aligned}$$

Idea behind Gauss-Legendre quadrature:

Say we wish to integrate $\int_a^b f(x)dx \qquad (*)$

Then 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 $F(t) = \frac{(b-a)}{2} f(x(t))$

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

$$\text{and} \qquad w_k = \int_{-1}^{1} \ell_k(x)dx.$$

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 $\boxed{\underline{\underline{\text{for } k \geq N+1}}}$

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

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