Overview

- Integration of polynomial approximant
- Integration operator: continuous and discrete cases, integration matrix
- Definite integration numerical formulas:
  - trapezoid
  - Simpson
  - Second Simpson
- Composite quadrature

- Consider $f\colon \mathbb{R} \to \mathbb{R}$, difficult to compute, and the problem of computation of

$$I_{\mathrm{ab}}(f) = \int_a^b f(t)\,\mathrm{d}t.$$

The integration operator I_{ab} is linear $I_{\mathrm{ab}}(\alpha f + \beta g) = \alpha I_{\mathrm{ab}}(f) + \beta I_{\mathrm{ab}}(g)$

$$\int_a^b [\alpha f(t) + \beta g(t)]\,\mathrm{d}t = \alpha \int_a^b f(t)\,\mathrm{d}t + \beta \int_a^b g(t)\,\mathrm{d}t$$

- Approach to numerical integration is similar to numerical differentiation
  - Construct approximant of f, $g \cong f$
  - Approximate $I_{\mathrm{ab}}(f)$ by $I_{\mathrm{ab}}(g)$, $I_{\mathrm{ab}}(f) \cong I_{\mathrm{ab}}(g)$
- Easiest approximant to work with: g polynomial, e.g., polynomial interpolant

$$f(t) \cong g(t) = a_0 + a_1 t + \cdots + a_n t^n \Rightarrow I_{\mathrm{ab}}(f) = a_0(b-a) + \cdots + a_n \frac{b^{n+1} - a^{n+1}}{n+1}$$

- $f\colon \mathbb{R} \to \mathbb{R}$, dificult to compute, only (partially) known through sample

$$\mathcal{D} = \{(x_i, f_i), i = 0, \ldots, n\},\ f_i = f(x_i).$$

- Continuous-discrete operator analogy

Continuous	Discrete
$f\colon \mathbb{R} \to \mathbb{R}$	$\mathcal{D} = \{(x_i, y_i = f(x_i)), i = 0, \ldots, n\}$
	$\boldsymbol{x} = [\ x_0\ \ \ldots\ \ x_n\ ]^T,\ \boldsymbol{f} = [\ f_0\ \ \ldots\ \ f_n\ ]^T$
$I_{\text{ab}}\colon \mathcal{C}[a,b] \to \mathbb{R}$	$Q_{\text{ab}}\colon \mathbb{R}^{n+1} \to \mathbb{R}$
$f \overset{I_{\text{ab}}}{\to} \int_a^b f(t)\,\mathrm{d}t$	$\boldsymbol{f} \overset{Q_{\text{ab}}}{\to} \sum_{i=0}^{n} w_i f_i$
$\int_a^b f(t)\mathrm{d}t$	$\sum_{i=0}^{n} w_i f_i \cdot 1$, $e.g., h = \frac{b-a}{n}$
	Left Darboux: $w_i = h, i = 0, \ldots, n-1, w_n = 0$
	Right Darboux: $w_0 = 0, w_i = h, i = 0, \ldots, n$
	Note: multiple possible choices for w_i

- Computation of a definite integral yields a scalar from a function sample

$$Q_{\mathrm{ab}}: \mathbb{R}^{n+1} \to \mathbb{R},\ Q(\boldsymbol{f}) = \boldsymbol{w}^T \boldsymbol{f},\ \boldsymbol{w} \in \mathbb{R}^{n+1}$$

- Consider computation of the primitive

$$F(x) = \int_a^x f(t)\,\mathrm{d}t$$

f difficult to compute implies F difficult to compute, known through sample

$$\mathcal{D}' = \{(x_i', F_i' = F(x_i)), i = 0, 1, \ldots, m\}$$

- Discrete analog, a linear mapping from $\mathbb{R}^{n+1}$ (f sample) to $\mathbb{R}^{m+1}$ (F sample)

$$\boldsymbol{F} = \boldsymbol{K}_{\boldsymbol{x},\boldsymbol{x}'}\,\boldsymbol{f}$$

$$\boldsymbol{F} = [\ F_0\ \ \ldots\ \ F_m\ ],\ \boldsymbol{f} = [\ f_0\ \ \ldots\ \ f_n\ ]^T$$

- Lagrange form of polynomial interpolant of $\mathcal{D} = \{(x_i, f_i), i = 0, \ldots, n\}$

$$f(t) \cong p(t) = \sum_{j=0}^{n} f_j \ell_j(t), \ell_j(t) = \prod_{l=0}^{n}{}' \frac{(t - x_l)}{(x_j - x_l)}$$

- Integral of polynomial interpolant

$$F(x_i') \cong \int_a^{x_i'} p(t)\mathrm{d}t = \int_a^{x_i'} \sum_{j=0}^{n} f_j \ell_j(t)\mathrm{d}t = \sum_{j=0}^{n} \left(\int_a^{x_i'} \ell_j(t)\mathrm{d}t \right) f_j = \sum_{j=0}^{n} k_{ij} f_j$$

- In matrix form the above is

$$\boldsymbol{F} = \boldsymbol{K}_{\boldsymbol{x},\boldsymbol{x}'} \boldsymbol{f}, \boldsymbol{K}_{\boldsymbol{x},\boldsymbol{x}'} \in \mathbb{R}^{(m+1)\times(n+1)}$$

- Components of $\boldsymbol{K}_{\boldsymbol{x},\boldsymbol{x}'}$

$$k_{ij} = \left(\int_a^{x_i'} \ell_j(t)\mathrm{d}t \right)$$

- To approximate $I_{\text{ab}}(f) = \int_a^b f(t)\,\mathrm{d}t$, evaluate $Q_{\text{ab}}(\boldsymbol{f}) \cong I_{\text{ab}}(f)$

$$Q_{\text{ab}}: \mathbb{R}^{n+1} \to \mathbb{R},\ Q_{\text{ab}}(\boldsymbol{f}) = \boldsymbol{w}^T \boldsymbol{f},\ \boldsymbol{w} \in \mathbb{R}^{n+1}$$

- $f: \mathbb{R} \to \mathbb{R}$ known through data set (f sample) $\mathcal{D} = \{(x_i, f_i), i = 0, 1, \ldots, n\}$
- Construct polynomial interpolant $f(t) \cong p(t) = \sum_{i=0}^{n} f_i \ell_i(t)$

$$\int_a^b f(t)\,\mathrm{d}t \cong \sum_{i=0}^{n} \left(\int_a^b \ell_i(t)\,\mathrm{d}t \right) f_i = \sum_{i=0}^{n} w_i f_i$$

- *Trapezoid formula*: $n = 1$, p linear, $b = x_1 = x_0 + h = a + h$,

$$\int_a^b f(t)\,\mathrm{d}t \cong \left(\int_{x_0}^{x_1} \frac{t - x_1}{x_0 - x_1}\,\mathrm{d}t \right) f_0 + \left(\int_{x_0}^{x_1} \frac{t - x_0}{x_1 - x_0}\,\mathrm{d}t \right) f_1 \Rightarrow$$

$$\int_a^b f(t)\,\mathrm{d}t \cong Q_{\text{ab}}(f) = \frac{h}{2} f_0 + \frac{h}{2} f_1 = \frac{b-a}{2}(f_0 + f_1) = \boldsymbol{w}^T \boldsymbol{f},\ \boldsymbol{w} = [\ h/2 \quad h/2\ ].$$

- *Simpson formula*: $n=2$, p quadratic, $x_0=a, x_1=a+h, x_2=a+2h=b$,

$$\int_a^b f(t)\,\mathrm{d}t \cong Q_{\mathrm{ab}}(\boldsymbol{f}) = \sum_{i=0}^{n}\left(\int_a^b \ell_i(t)\,\mathrm{d}t\right) f_i$$

$$w_0 = \int_a^b \ell_0(t)\,\mathrm{d}t = \int_{x_0}^{x_2} \frac{(t-x_1)(t-x_2)}{(x_0-x_1)(x_0-x_2)}\,\mathrm{d}t = \frac{h}{3}$$

$$w_1 = \int_a^b \ell_1(t)\,\mathrm{d}t = \int_{x_0}^{x_2} \frac{(t-x_0)(t-x_2)}{(x_1-x_0)(x_1-x_2)}\,\mathrm{d}t = \frac{4h}{3}$$

$$w_2 = \int_a^b \ell_2(t)\,\mathrm{d}t = \int_{x_0}^{x_2} \frac{(t-x_0)(t-x_1)}{(x_2-x_0)(x_2-x_1)}\,\mathrm{d}t = \frac{h}{3}$$

$$\int_a^b f(t)\,\mathrm{d}t \cong Q_{\mathrm{ab}}(\boldsymbol{f}) = \frac{h}{3}(f_0+4f_1+f_2) = \frac{b-a}{6}(f_0+4f_1+f_2)$$

$$\boldsymbol{w}^T = \frac{h}{3}\begin{bmatrix} 1 & 4 & 1 \end{bmatrix}$$

- *Second Simpson formula*: $n=3$, p cubic, $x_i = a + i\,h, h = (b-a)/3$

$$\int_a^b f(t)\,\mathrm{d}t \cong Q_{\mathrm{ab}}(\boldsymbol{f}) = \sum_{i=0}^{n} \left(\int_a^b \ell_i(t)\,\mathrm{d}t \right) f_i$$

$$w_0 = \int_{x_0}^{x_3} \ell_0(t)\,\mathrm{d}t = \int_{x_0}^{x_3} \frac{(t-x_1)(t-x_2)(t-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}\,\mathrm{d}t = \frac{3h}{8}$$

$$w_1 = \int_a^b \ell_1(t)\,\mathrm{d}t = \int_{x_0}^{x_3} \frac{(t-x_0)(t-x_2)(t-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}\,\mathrm{d}t = \frac{9h}{8}$$

$$w_2 = \int_a^b \ell_2(t)\,\mathrm{d}t = \int_{x_0}^{x_3} \frac{(t-x_0)(t-x_1)(t-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}\,\mathrm{d}t = \frac{9h}{8}$$

$$w_3 = \int_a^b \ell_3(t)\,\mathrm{d}t = \int_{x_0}^{x_3} \frac{(t-x_0)(t-x_1)(t-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}\,\mathrm{d}t = \frac{3h}{8}$$

$$Q_{\mathrm{ab}}(\boldsymbol{f}) = \frac{h}{8}(3f_0 + 9f_1 + 9f_2 + 3f_3) = \frac{b-a}{8}(f_0 + 3f_1 + 3f_2 + f_2)$$

- Previous quadrature formulas based upon k-degree polynomial interpolation

$$I_{\mathrm{ab}}(f)=\int_a^b f(t)\mathrm{d}t \cong Q_{\mathrm{ab}}^{(k)}(f)=(b-a)\sum_{i=0}^{k} w_i^{(k)} f_i,\ f_i=f(a+ih),\ h=\frac{b-a}{k+1}$$

k	1	2	3
Name	Trapezoid	Simpson	2^{nd} Simpson
$\boldsymbol{w}$	$\frac{1}{2}\begin{bmatrix}1\\1\end{bmatrix}$	$\frac{1}{6}\begin{bmatrix}1\\4\\1\end{bmatrix}$	$\frac{1}{8}\begin{bmatrix}1\\3\\3\\1\end{bmatrix}$

- Numerical integration error is evaluated by integral of interpolation error

$$e=I_{\mathrm{ab}}(f)-Q_{\mathrm{ab}}^{(k)}(f)=\int_a^b [f(t)-p_k(t)]\mathrm{d}t=\int_a^b \frac{f^{(k+1)}(\xi_t)}{(k+1)!}w(t)\,\mathrm{d}t$$

$$w(t)=\prod_{i=0}^{k}(t-x_i),\ x_i=a+ih$$

- Trapezoid

$$e = \left|\frac{1}{2}\int_a^b f''(\xi_t)\,(t-a)(t-b)\,\mathrm{d}t\right| \leqslant \|f''\|_\infty \frac{1}{2}\left|\int_{-h/2}^{h/2}\left(y^2-\left(\frac{h}{2}\right)^2\right)\mathrm{d}y\right| \Rightarrow$$

$$e \leqslant \|f''\|_\infty \int_0^{h/2}\left(\left(\frac{h}{2}\right)^2 - y^2\right)\mathrm{d}y = \|f''\|_\infty\left(\frac{h^3}{12}\right)$$

- Simpson
  - Try with $k=2$ to obtain $e \leqslant \|f^{(3)}\|_\infty \frac{1}{6}\int_a^b (t-a)\left(t-\frac{a+b}{2}\right)(t-b)\,\mathrm{d}t$

$$\int_a^b (t-a)\left(t-\frac{a+b}{2}\right)(t-b)\,\mathrm{d}t = \int_{-h}^{h}(y-h)y(y+h)\,\mathrm{d}t = 0$$

  - Terms of order $\mathcal{O}(h^4)$ cancel out!
  - Peano kernel theorem is used to obtain

$$e \leqslant \|f^{(4)}\|_\infty \frac{h^5}{90}$$

- Increased accuracy arises from more sample points $\mathcal{D}=\{(x_i, f_i), i=0,\ldots,m\}$
  - Do not use high degree polynomial interpolant (Runge phenomenon)
  - Apply a lower-order formula repeatedly over subintervals $\Rightarrow$ "composite"
- *Composite trapezoid formula*

$$I_{\mathrm{ab}}(f)=\int_a^b f(t)\mathrm{d}t=\sum_{i=1}^{m}\int_{x_{i-1}}^{x_i} f(t)\mathrm{d}t$$

Assume equidistant sampling $x_{i+1}-x_i=h=(b-a)/m$

$$I_{\mathrm{ab}}(f)\cong Q_{\mathrm{ab}}(f)=\frac{h}{2}\sum_{i=1}^{m}(f_{i-1}+f_i)=\frac{h}{2}(f_0+f_m)+h\sum_{i=1}^{m-1} f_i$$

- Composite trapezoid error, over $[x_{i-1}, x_i]$, error is $e_i\leqslant\|f''\|_\infty h^3/12$

$$e\leqslant\sum_{i=1}^{m} e_i\leqslant\|f''\|_\infty m h^3/12=\|f''\|_\infty\frac{b-a}{12}h^2$$

Composite trapezoid is second-order accurate.

- Assume $\mathcal{D} = \{(x_i, f_i), i = 0, 1, \ldots, m\}$, $m = 2p$
- *Composite Simpson formula*

$$I_{\mathrm{ab}}(f) = \int_a^b f(t)\mathrm{d}t = \sum_{i=1}^{p} \int_{x_{2i-2}}^{x_{2i}} f(t)\mathrm{d}t$$

Assume equidistant sampling $h = (b-a)/m = (b-a)/(2p), x_{2i} - x_{2i-2} = 2h$

$$I_{\mathrm{ab}}(f) \cong Q_{\mathrm{ab}}(f) = \frac{h}{3}\sum_{i=1}^{p} (f_{2i-2} + 4f_{2i-1} + f_{2i})$$

- Composite Simpson error, over $[x_{2i-2}, x_{2i}]$, error is $e_i \leqslant \| f^{(4)}\|_\infty h^5/90$

$$e \leqslant \sum_{i=1}^{m} e_i \leqslant \| f^{(4)}\|_\infty h^5/90 = \| f^{(4)}\|_\infty \frac{b-a}{180} h^4$$

Composite Simpson is fourth-order accurate.