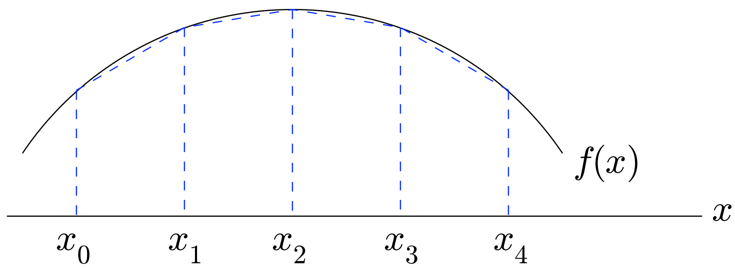
chapter 6 : numerical integration

$$\int_a^b f(x)dx \approx \sum_{i=1}^n c_i f(x_i)$$

For now, assume $x_i = a + ih$, $h = \frac{b-a}{n}$, $i = 0, \ldots, n$: uniform points.

trapezoid rule



$$T(h) = h \cdot \tfrac{1}{2}(f(x_0) + f(x_1)) + h \cdot \tfrac{1}{2}(f(x_1) + f(x_2)) + \cdots + h \cdot \tfrac{1}{2}(f(x_{n-1}) + f(x_n))$$
$$= h\left(\tfrac{1}{2}f(x_0) + f(x_1) + \cdots + f(x_{n-1}) + \tfrac{1}{2}f(x_n)\right)$$

note : The trapezoid rule computes the area under the piecewise linear interpolant to $f(x)$.

ex : $\int_0^1 e^{-x^2} dx = 0.746824\ldots$

h	$T(h)$	error	error/h^2
1	0.683940	0.062884	0.062884
0.5	0.731370	0.015454	0.061816
0.25	0.742984	0.003840	0.061440
0.125	0.745866	0.000958	0.061312

Hence the trapezoid rule is 2nd order accurate. Let's prove it analytically.

local error

$$\int_{x_i}^{x_{i+1}} f(x)dx = h \cdot \tfrac{1}{2}(f(x_i) + f(x_{i+1})) - \tfrac{1}{12}f''(\zeta)h^3$$

pf

$p_1(x) = f[x_i] + f[x_i, x_{i+1}](x - x_i)$: linear interpolating polynomial

$f(x) = p_1(x) + \frac{1}{2}f''(\zeta)(x - x_i)(x - x_{i+1})$: error in polynomial interpolation

$$\int_{x_i}^{x_{i+1}} f(x)dx = \int_{x_i}^{x_{i+1}} p_1(x)dx + \int_{x_i}^{x_{i+1}} \tfrac{1}{2}f''(\zeta)(x - x_i)(x - x_{i+1})dx$$

$$\int_{x_i}^{x_{i+1}} p_1(x)dx \;= hf[x_i] \;+ f[x_i,x_{i+1}]\frac{(x-x_i)^2}{2}\Bigg|_{x_i}^{x_{i+1}} = hf(x_i) + \left(\frac{f(x_{i+1})-f(x_i)}{h}\right)\frac{h^2}{2}$$

$$= h\cdot\tfrac{1}{2}(f(x_i)+f(x_{i+1})) \;\;:\;\; \text{trapezoid rule}$$

$$\int_{x_i}^{x_{i+1}} \tfrac{1}{2}f''(\zeta)(x-x_i)(x-x_{i+1})dx$$

$$= \tfrac{1}{2}f''(\hat{\zeta})\int_{x_1}^{x_{i+1}}(x-x_i)(x-x_{i+1})dx \;\;:\;\; \text{generalized Mean Value Theorem}$$

change variables : $s = \dfrac{x-x_i}{h}\ ,\ \dfrac{x-x_{i+1}}{h} = \dfrac{x-(x_i+h)}{h} = s-1\ ,\ ds = \dfrac{dx}{h}$

$$= \tfrac{1}{2}f''(\hat{\zeta})\int_0^1 hs\cdot h(s-1)\cdot hds \;=\; \tfrac{1}{2}f''(\hat{\zeta})\,h^3\int_0^1(s^2-s)ds$$

$$= \tfrac{1}{2}f''(\hat{\zeta})\,h^3\left(\tfrac{1}{3}s^3-\tfrac{1}{2}s^2\right)\Big|_0^1 \;=\; -\tfrac{1}{12}f''(\hat{\zeta})h^3 \qquad \underline{\text{ok}}$$

<u>global error</u>

$$\int_a^b f(x)dx \;=\; T(h) - \tfrac{1}{12}(b-a)f''(\zeta)h^2 \;\;:\;\; \text{2nd order accurate}$$

<u>pf</u>

$$\int_a^b f(x)dx \;=\; \sum_{i=0}^{n-1}\int_{x_i}^{x_{i+1}} f(x)dx$$

$$= \sum_{i=0}^{n}\Big(h\cdot\tfrac{1}{2}(f(x_i)+f(x_{i+1})) - \tfrac{1}{12}f''(\zeta_i)h^3\Big) \;\;:\;\; \text{local error}$$

$$= T(h) - \tfrac{1}{12}\sum_{i=0}^{n} f''(\zeta_i)h^3 \;=\; T(h) - \tfrac{1}{12}\,n\cdot f''(\zeta)h^3 \qquad \underline{\text{ok}}$$

<u>question</u> : how can we get more accurate results?

1. piecewise quadratic interpolant (Simpson's rule)
2. cubic spline interpolant
3. non-uniform points

<u>asymptotic expansion</u>

$T(h) \;=\; \int_a^b f(x)dx \;+\; c_2h^2 \;+\; c_4h^4 \;+\; c_6h^6 \;+\; \cdots$, where c_i are independent of h

<u>Richardson extrapolation</u> (Romberg's method)

$$T(2h) \;=\; \int_a^b f(x)dx \;+\; c_2(2h)^2 \;+\; c_4(2h)^4 \;+\; c_6(2h)^6 \;+\; \cdots$$

$$= \int_a^b f(x)dx \;+\; 4c_2h^2 \;+\; 16c_4h^4 \;+\; 64c_6h^6 \;+\; \cdots$$

$$\Rightarrow \ \frac{4T(h)-T(2h)}{3} = \int_a^b f(x)dx \ - \ 4c_4h^4 \ - \ 20c_6h^6 \ + \ \cdots$$

define $R_0(h) = T(h)$: 2nd order accurate

define $R_1(h) = R_0(h) + \dfrac{R_0(h)-R_0(2h)}{3}$: 4th order accurate

$$R_1(h) \ = \int_a^b f(x)dx \ + \ \tilde{c}_4h^4 \ + \ \tilde{c}_6h^6 \ + \ \cdots$$

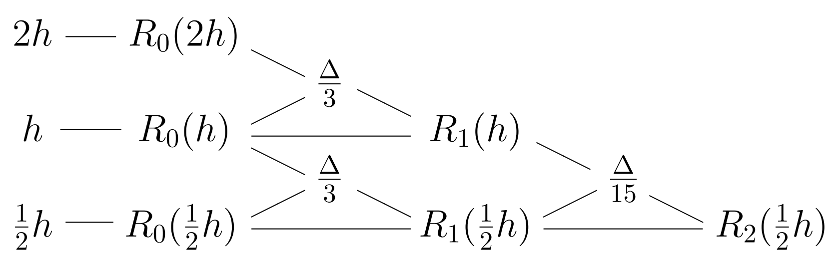
$$R_1(2h) \ = \int_a^b f(x)dx \ + \ \tilde{c}_4(2h)^4 \ + \ \tilde{c}_6(2h)^6 \ + \ \cdots$$

$$= \int_a^b f(x)dx \ + \ 16\tilde{c}_4h^4 \ + \ 64\tilde{c}_6h^6 \ + \ \cdots$$

$$\Rightarrow \ \frac{16R_1(h)-R_1(2h)}{15} = \int_a^b f(x)dx \ - \ \tfrac{16}{5}\tilde{c}_6h^6 \ + \ \cdots$$

define $R_2(h) = R_1(h) + \dfrac{R_1(h)-R_1(2h)}{15}$: 6th order accurate

<u>table</u>



<u>ex</u> : $\displaystyle\int_0^1 e^{-x^2}dx = 0.74682413\ldots$

h	$R_0(h)$	$R_1(h)$	$R_2(h)$	$R_3(h)$
1.0	0.683940			
0.5	0.731370	0.747180		
0.25	0.742984	0.7468553	0.7468336	
0.125	0.745866	0.7468266	0.7468246	0.7468244

<u>note</u>

1. The last column $R_3(h)$ uses $\frac{\Delta}{63}$.
2. down a column : decreasing h , fixed order of accuracy

   across a row : fixed h , increasing order of accuracy orthogonal polynomials

recall : inner product of two vectors in n-dimensional space

$$x^T \cdot y = \sum_{i=1}^{n} x_i y_i$$

define : inner product of two functions on the interval $[-1, 1]$

$$f(x)\,,\ g(x)\ \Rightarrow\ \langle f, g\rangle = \int_{-1}^{1} f(x)g(x)dx$$

properties

1. $\langle f, f\rangle \geq 0\ ,\ \langle f, f\rangle^{1/2} = ||f||$: norm of f , $||f|| = 0 \Leftrightarrow f = 0$

2. $\langle f, \alpha g + h\rangle = \alpha\langle f, g\rangle + \langle f, h\rangle$

def : We say that f and g are orthogonal if $\langle f, g\rangle = 0$.

ex

$$\langle \sin \pi x, \cos \pi x\rangle = \int_{-1}^{1} \sin \pi x \cos \pi x dx\ = \frac{1}{2\pi} \sin^2 \pi x \Big|_{-1}^{1} = 0 \ :\ \text{orthogonal}$$

$$\langle 1, x\rangle = \int_{-1}^{1} 1 \cdot x dx = 0\ :\ \text{orthogonal}$$

$$\langle 1, x^2\rangle = \int_{-1}^{1} 1 \cdot x^2 dx = \tfrac{2}{3}\ :\ \text{not orthogonal}$$

note

Given the functions $\{1, x, x^2, \ldots\}$, the Gram-Schmidt process produces a set of orthogonal polynomials $\{P_0(x), P_1(x), P_2(x), \ldots\}$ called the Legendre polynomials.

$$P_0(x) = 1$$

$$P_1(x) = x - \frac{\langle x, P_0\rangle}{||P_0||^2} P_0 = x$$

$$P_2(x) = x^2 - \frac{\langle x^2, P_0\rangle}{||P_0||^2} P_0 - \frac{\langle x^2, P_1\rangle}{||P_1||^2} P_1 = x^2 - \tfrac{1}{3}$$

$$\langle x^2, P_0\rangle = \int_{-1}^{1} x^2 dx = \tfrac{2}{3}\ ,\ ||P_0||^2 = \int_{-1}^{1} dx = 2\ ,\ \langle x^2, P_1\rangle = \int_{-1}^{1} x^3 dx = 0$$

check : $\langle P_2, P_0\rangle = \int_{-1}^{1}(x^3 - \tfrac{1}{3})dx = 0\ ,\ \langle P_2, P_1\rangle = \int_{-1}^{1}(x^3 - \tfrac{1}{3})x dx = 0$ ok

$$P_3(x) = x^3 - \frac{\langle x^3, P_0\rangle}{||P_0||^2}P_0 - \frac{\langle x^3, P_1\rangle}{||P_1||^2}P_1 - \frac{\langle x^3, P_1\rangle}{||P_1||^2}P_1 = x^3 - \tfrac{3}{5}x$$

$$\langle x^3, P_0\rangle = \int_{-1}^{1} x^3 dx = 0$$

$$\langle x^3, P_1\rangle = \int_{-1}^{1} x^3 \cdot x dx = \tfrac{2}{5}\ ,\ ||p_1||^2 = \int_{-1}^{1} x^2 dx = \tfrac{2}{3}$$

$$\langle x^3, P_2\rangle = \int_{-1}^{1} x^3(x^2 - \tfrac{1}{3})dx = 0$$

note

1. $P_n(x)$ is a polynomial of degree n.
2. Any polynomial $q(x)$ of degree $\le n$ can be written $q(x) = \sum_{i=1}^{n} c_i P_i(x)$,

i.e. $\{P_0, \ldots, P_n\}$ form a basis for the vector space of polynomials of degree $\le n$.

Gaussian quadrature

1. $P_n(x)$ has n distinct roots in $(-1, 1)$, call them $x_1, \ldots, x_n$
2. There exist constants $c_1, \ldots, c_n$ such that the integration rule

$\int_{-1}^{1} f(x)dx \approx \sum_{i=1}^{n} c_i f(x_i)$ is exact for polynomials of degree $\le 2n-1$ (for $n \ge 1$).

ex : $\int_0^1 e^{-x^2}dx = \int_{-1}^{1} e^{-(\frac{1}{2}(t+1))^2}\frac{1}{2}dt = 0.746824$,

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

n	G_n
2	0.746595
3	0.746816
4	0.746824

recall : $T(0.125) = 0.745866$, so Gaussian quadrature is more accurate than the trapezoid rule.

pf of 1 : omit

Assume $n \ge 1$.

Then $0 = \langle P_n, P_0\rangle = \int_{-1}^{1} P_n(x)dx$, so P_n changes sign at least once in $(-1, 1)$.

Let $x_1, \ldots, x_j$ be the points in $(-1, 1)$ at which P_n changes sign, so $1 \le j \le n$.

Let $q(x) = (x - x_1)\cdots(x - x_j)$ and note that q also changes sign at $x_1, \ldots, x_j$ and degree$(q) = j$.

Now consider the intervals $(-1, x_1), (x_1, x_2), \ldots, (x_j, 1)$, and note that P_n and q always have the same sign or always have the opposite sign on each interval.

In either case, $\langle P_n, q\rangle = \int_{-1}^{1} P_n(x)q(x)dx \ne 0$.

But then degree$(q) \ge n$, because degree$(q) < n \Rightarrow \langle P_n, q\rangle = 0$.

Hence $j \ge n, j \le n \Rightarrow j = n$. ok

<u>pf of 2</u> : omit

Let $f(x)$ be a polynomial of degree $\leq 2n-1$.

<u>case 1</u> : degree$(f) \leq n-1$

$f(x) = \sum_{i=1}^{n} f(x_i)L_i(x)$: Lagrange interpolating polynomial at $x_1, \ldots, x_n$

$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{n} f(x_i) \int_{-1}^{1} L_i(x)dx = \sum_{i=1}^{n} c_i f(x_i)$, where $c_i = \int_{-1}^{1} L_i(x)dx$ <u>ok</u>

<u>case 2</u> : degree$(f) \leq 2n-1$

$f = qP_n + r$, where q : quotient , degree$(q) \leq n-1$

r : remainder , degree$(r) \leq n-1$

$\Rightarrow \; f(x_i) = q(x_i)P_n(x_i) + r(x_i) = r(x_i)$

$$\int_{-1}^{1} f(x)dx = \int_{-1}^{1} q(x)P_n(x)dx + \int_{-1}^{1} r(x)dx = \langle q, P_n \rangle + \sum_{i=1}^{n} c_i r(x_i) \; : \text{ by case 1}$$
$$= \sum_{i=1}^{n} c_i f(x_i) \quad \underline{\text{ok}}$$

<u>ex</u> : 3-point Gaussian quadrature

$\int_{-1}^{1} f(x)dx \approx c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)$

$P_3(x) = x^3 - \frac{3}{5}x = x(x^2 - \frac{3}{5})$, $x_1 = -\sqrt{\frac{3}{5}}$, $x_2 = 0$, $x_3 = \sqrt{\frac{3}{5}}$

$c_i = \int_{-1}^{1} L_i(x)dx$: could be computed, but we'll use an alternative method

$f(x) = 1 \Rightarrow \int_{-1}^{1} dx = 2 = c_1 + c_2 + c_3$

$f(x) = x \Rightarrow \int_{-1}^{1} xdx = 0 = c_1 \cdot -\sqrt{\frac{3}{5}} + c_2 \cdot 0 + c_3 \cdot \sqrt{\frac{3}{5}}$

$f(x) = x^2 \Rightarrow \int_{-1}^{1} x^2 dx = \frac{2}{3} = c_1 \cdot \frac{3}{5} + c_2 \cdot 0 + c_3 \cdot \frac{3}{5}$

$c_1 = c_3 = \frac{5}{9}$, $c_2 = \frac{8}{9}$

$\int_{-1}^{1} f(x)dx \approx \frac{5}{9} f(-\sqrt{\frac{3}{5}}) + \frac{8}{9} f(0) + \frac{5}{9} f(\sqrt{\frac{3}{5}})$: exact for polynomials of degree ≤ 5

$f(x) = x^3 \Rightarrow \int_{-1}^{1} x^3 dx = 0$: ok , also x^5

$f(x) = x^4 \Rightarrow \int_{-1}^{1} x^2 dx = \frac{2}{5} = \frac{5}{9} \cdot \frac{9}{25} \cdot 2$: ok

Gauss-Laguerre quadrature

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

method 1 : truncate the domain

method 2 : map $[0,\infty) \to [0,1)$

method 3 : define a new inner product : $\langle f, g\rangle = \int_0^\infty f(x)g(x)e^{-x}dx$

The Laguerre polynomials are orthogonal with respect to this inner product and they are obtained by applying Gram-Schmidt to $\{1, x, x^2, \ldots\}$.

$\mathcal{L}_0(x) = 1$

$\mathcal{L}_1(x) = x - 1$

$\mathcal{L}_2(x) = x^2 - 4x + 2$

Let $x_1, \ldots, x_n$ be the roots of $L_n(x)$ and set $c_i = \int_0^\infty L_i(x)e^{-x}dx$.

Then $\int_0^\infty f(x)e^{-x}dx \approx \sum_{i=1}^{n} c_i f(x_i)$ is exact for polynomials of degree $\leq 2n-1$.

ex : 2-point Gauss-Laguerre rule

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

$$\approx 0.854 \cdot f(0.586) + 0.146 \cdot f(3.414)$$