

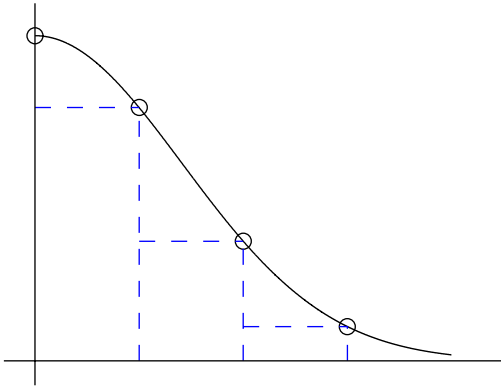
## chapter 6 : numerical integration

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Tues
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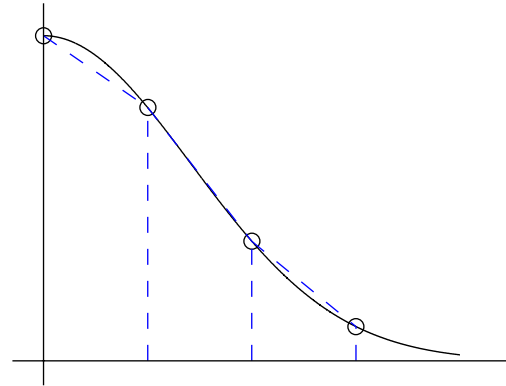
$$\int_0^1 f(x)dx \approx \sum_{i=0}^n c_i f_i \quad , \quad c_i : \text{coefficients} \quad , \quad f_i = f(x_i) \quad , \quad x_i : \text{points}$$

ex :  $\int_0^1 e^{-x^2} dx = 0.7468\dots$  , consider  $x_i = ih$  ,  $h = \frac{1}{n}$  ,  $i = 0, \dots, n$  : uniform

right-hand Riemann sum



trapezoid rule



$$R(h) = f_1 h + f_2 h + \dots + f_n h = (f_1 + f_2 + \dots + f_n)h$$

$h$	$R(h)$	error	error/h	error/h <sup>2</sup>
1	0.3679	0.3789	0.3789	0.3789
0.5	0.5733	0.1735	0.3470	0.6939
0.25	0.6640	0.0829	0.3314	1.3257
0.125	0.7064	0.0405	0.3237	2.5898

$\Rightarrow$  error =  $O(h)$  , 1st order accurate

$$\begin{aligned} T(h) &= \frac{1}{2}(f_0 + f_1)h + \frac{1}{2}(f_1 + f_2)h + \dots + \frac{1}{2}(f_{n-1} + f_n)h \\ &= \left(\frac{1}{2}f_0 + f_1 + \dots + f_{n-1} + \frac{1}{2}f_n\right)h \end{aligned}$$

$h$	$T(h)$	error	error/h	error/h <sup>2</sup>
1	0.6839	0.0629	0.0629	0.0629
0.5	0.7314	0.0155	0.0309	0.0618
0.25	0.7430	0.0038	0.0154	0.0614
0.125	0.7459	0.0010	0.0077	0.0613

$\Rightarrow$  error =  $O(h^2)$  , 2nd order accurate

question : How can we obtain a more accurate integration formula?

1. piecewise quadratic interpolant (Simpson's rule)
2. cubic spline interpolant
3. non-uniform points (e.g. Chebyshev, adapted)
4. extrapolation (explained next)

Richardson extrapolation (Romberg's method)

$R_0(h) = T(h) = \int_0^1 f(x)dx + c_2h^2 + c_4h^4 + c_6h^6 + \dots$  : 2nd order accurate  
note : finding  $c_2, c_4, c_6, \dots$  is a good exercise, but the values are not needed here

$$\begin{aligned} R_0(2h) &= T(2h) = \int_0^1 f(x)dx + c_2(2h)^2 + c_4(2h)^4 + c_6(2h)^6 + \dots \\ &= \int_0^1 f(x)dx + 4c_2h^2 + 16c_4h^4 + 64c_6h^6 + \dots \end{aligned}$$

$\Rightarrow \frac{1}{3}(4R_0(h) - R_0(2h)) = \int_0^1 f(x)dx - 4c_4h^4 - 20c_6h^6 + \dots$  : 4th order accurate

define  $R_1(h) = \frac{1}{3}(4R_0(h) - R_0(2h)) = R_0(h) + \frac{1}{3}(R_0(h) - R_0(2h))$

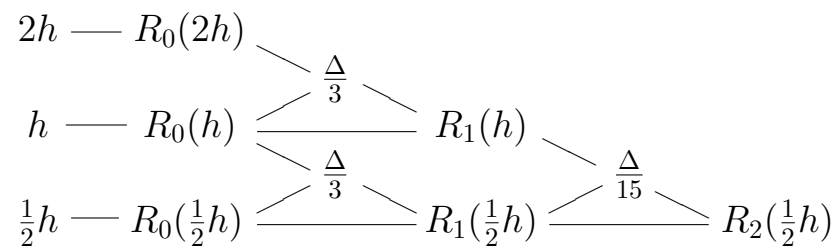
$$R_1(h) = \int_0^1 f(x)dx + \tilde{c}_4h^4 + \tilde{c}_6h^6 + \dots$$

$$\begin{aligned} R_1(2h) &= \int_0^1 f(x)dx + \tilde{c}_4(2h)^4 + \tilde{c}_6(2h)^6 + \dots \\ &= \int_0^1 f(x)dx + 16\tilde{c}_4h^4 + 64\tilde{c}_6h^6 + \dots \end{aligned}$$

$\Rightarrow \frac{1}{15}(16R_1(h) - R_1(2h)) = \int_0^1 f(x)dx - \frac{16}{5}\tilde{c}_6h^6 + \dots$  : 6th order accurate

define  $R_2(h) = \frac{1}{15}(16R_1(h) - R_1(2h)) = R_1(h) + \frac{1}{15}(R_1(h) - R_1(2h))$

extrapolation table



ex :  $\int_0^1 e^{-x^2} dx = 0.74682413\dots$

$h$	$R_0(h)$	$R_1(h)$	$R_2(h)$	$R_3(h)$
1.0	0.683940			
0.5	0.731370	0.7471800		
0.25	0.742984	0.7468553	0.7468336	
0.125	0.745866	0.7468266	0.7468246	0.7468244 : more accurate

1. The last column  $R_3(h)$  uses  $\frac{\Delta}{63}$ .
2. down a column  $\Rightarrow$  decreasing  $h$ , fixed order of accuracy  
across a row  $\Rightarrow$  fixed  $h$ , increasing order of accuracy
3. Extrapolation can be applied to any numerical approximation if the error has an expansion in powers of  $h$ .

orthogonal polynomials

recall : dot product of two vectors in  $n$ -dimensional space

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

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

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

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

def : Two functions  $f$  and  $g$  are orthogonal if  $\langle f, g \rangle = 0$ .

examples

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

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

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

note

1. If  $f(x)$  is even and  $g(x)$  is odd (or vice versa), then  $f$  and  $g$  are orthogonal.
2. Starting from  $\{1, x, x^2, \dots\}$ , the Gram-Schmidt process yields a set of orthogonal polynomials  $\{P_0(x), P_1(x), P_2(x), \dots\}$  called the Legendre polynomials.

$$P_0(x) = 1$$

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

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

$$\langle x^2, P_0 \rangle = \int_{-1}^1 x^2 dx = \frac{2}{3}, \quad \|P_0\|^2 = \int_{-1}^1 dx = 2$$

check :  $\langle P_2, P_0 \rangle = \dots = 0, \langle P_2, P_1 \rangle = 0$  ok

$$P_3(x) = x^3 - \frac{\langle x^3, P_0 \rangle}{\|P_0\|^2} P_0 - \frac{\langle x^3, P_1 \rangle}{\|P_1\|^2} P_1 - \frac{\langle x^3, P_2 \rangle}{\|P_2\|^2} P_2 = x^3 - \frac{3}{5}x$$

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

check :  $\langle P_3, P_0 \rangle = 0, \langle P_3, P_1 \rangle = \dots = 0, \langle P_3, P_2 \rangle = 0$  ok

## Gaussian quadrature

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

$$\int_{-1}^1 f(x) dx \approx \sum_{i=1}^n c_i f(x_i) \text{ is exact when } f(x) \text{ is any polynomial of degree } \leq 2n-1.$$

pf : omit

ex

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

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

$n$	$G_n$
2	0.746595
3	0.746816
4	0.746824

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

ex : 3-point Gaussian quadrature

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

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

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

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

$$f(x) = x^2 \Rightarrow \int_{-1}^1 x^2 dx = c_1 \cdot \frac{3}{5} + c_2 \cdot 0 + c_3 \cdot \frac{3}{5} = \frac{2}{3} \Rightarrow c_1 = \frac{5}{9}, c_2 = \frac{8}{9}$$

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

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

$$f(x) = x^4 \Rightarrow \int_{-1}^1 x^4 dx = \frac{5}{9} \cdot \frac{9}{25} + \frac{8}{9} \cdot 0 + \frac{5}{9} \cdot \frac{9}{25} = \frac{2}{5} : \text{ ok}$$