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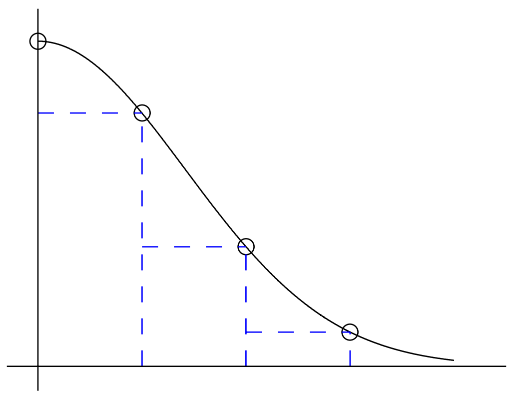
<u>chapter 6</u> : numerical integration

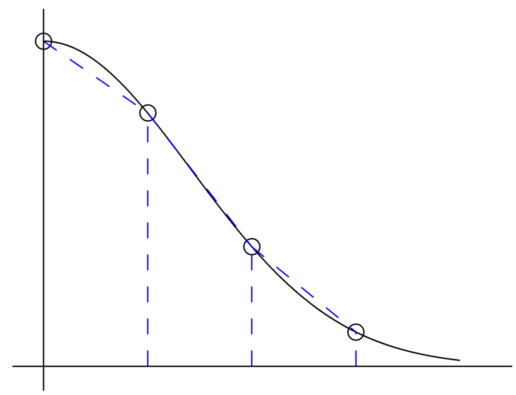
$$\int_0^1 f(x)dx \approx \sum_{i=0}^{n} c_i f_i \ , \ c_i : \text{coefficients} \ , \ f_i = f(x_i) \ , \ x_i : \text{points}$$

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

<u>right-hand Riemann sum</u>



<u>trapezoid rule</u>



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

h	$R(h)$	error	error$/h$	error$/h^2$
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

$$T(h) = \tfrac{1}{2}(f_0 + f_1)h + \tfrac{1}{2}(f_1 + f_2)h + \cdots + \tfrac{1}{2}(f_{n-1} + f_n)h$$
$$= (\tfrac{1}{2}f_0 + f_1 + \cdots + f_{n-1} + \tfrac{1}{2}f_n)h$$

h	$T(h)$	error	error/h	error$/h^2$
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

<u>question</u> : 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)

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

$$R_0(h) = T(h) = \int_0^1 f(x)dx \;+\; c_2h^2 \;+\; c_4h^4 \;+\; c_6h^6 \;+\; \cdots \;:\; \text{2nd order accurate}$$

note : finding $c_2, c_4, c_6, \ldots$ is a good exercise, but the values are not needed here

$$R_0(2h) = T(2h) = \int_0^1 f(x)dx \;+\; c_2(2h)^2 \;+\; c_4(2h)^4 \;+\; c_6(2h)^6 \;+\; \cdots$$

$$= \int_0^1 f(x)dx \;+\; 4c_2h^2 \;+\; 16c_4h^4 \;+\; 64c_6h^6 \;+\; \cdots$$

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

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

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

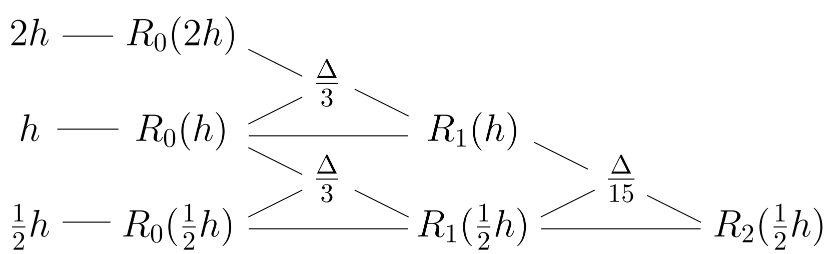
$$R_1(2h) \;=\; \int_0^1 f(x)dx \;+\; \tilde{c}_4(2h)^4 \;+\; \tilde{c}_6(2h)^6 \;+\; \cdots$$

$$= \int_0^1 f(x)dx \;+\; 16\tilde{c}_4h^4 \;+\; 64\tilde{c}_6h^6 \;+\; \cdots$$

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

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

<u>extrapolation table</u> 21 Tue 4/6



<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	0.7471800		
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.

<u>orthogonal polynomials</u>

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 : <u>inner product</u> of two functions on the interval $[-1,1]$

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

<u>properties</u>

1. $\langle f,f\rangle \ge 0$, $\langle f,f\rangle^{1/2} = ||f||$: <u>norm</u> of f , $||f|| = 0 \Leftrightarrow f = 0$
2. $\langle f,\alpha g + h\rangle = \alpha\langle f,g\rangle + \langle f,h\rangle$

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

<u>examples</u>

$$\langle \sin\pi x, \cos\pi x\rangle = \int_{-1}^{1} \sin\pi x\cos\pi x dx = \frac{1}{2\pi}\sin^2\pi x\Big|_{-1}^{1} = 0 \text{ : orthogonal}$$ 22 Thu 4/8

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

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

<u>note</u>

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

$$P_0(x) = 1$$

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

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

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

check : $\langle P_2,P_0\rangle = \cdots = 0$, $\langle P_2,P_1\rangle = 0$ <u>ok</u>

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

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

check : $\langle P_3,P_0\rangle = 0$, $\langle P_3,P_1\rangle = \cdots = 0$, $\langle P_3,P_2\rangle = 0$ <u>ok</u>

<u>Gaussian quadrature</u>

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 <u>exact</u> when $f(x)$ is any polynomial of degree $\leq 2n-1$.

<u>pf of 1</u> :
Assume $n \geq 1$.
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 $1 \leq j \leq n$.
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, $\langle P_n, q\rangle = \int_{-1}^{1} P_n(x)q(x)dx \neq 0$.
But then degree$(q) \geq n$, because degree$(q) < n \Rightarrow \langle P_n, q\rangle = 0$.
Hence $j \geq n, j \leq n \Rightarrow j = n$. <u>ok</u>

<u>pf of 2</u> : omit (see end of the note if interested)

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

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

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

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

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

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

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

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

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

<u>ex</u>

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

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

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.

<u>pf of 2</u> : omit (requires a little bit of Lagrange interpolations)

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

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

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

$$\int_{-1}^1 f(x)dx = \sum_{i=1}^n f(x_i)\int_{-1}^1 L_i(x)dx = \sum_{i=1}^n c_i f(x_i)\ ,\ \text{where } c_i = \int_{-1}^1 L_i(x)dx \quad \underline{\text{ok}}$$

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

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

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

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

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

$$= \sum_{i=1}^n c_i f(x_i) \quad \underline{\text{ok}}$$