6. 수치 적분과 미분

(Numerical integration and differentiation)

1. 수치적분 (Numerical integration)

1.1 Basic Quadrature Rules

- Newton interpolatory divided-difference formula

$$f_n(x) = f(x_0) + (x - x_0) f[x_1, x_0] + (x - x_0)(x - x_1) f[x_2, x_1, x_0]$$

$$+ \cdots + (x - x_0)(x - x_1) \cdots (x - x_{n-1}) f[x_n, x_{n-1}, \cdots, x_0]$$

$$f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

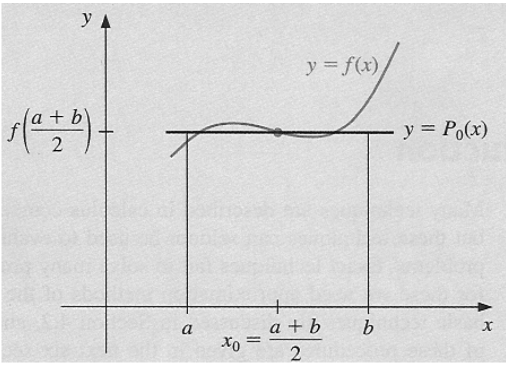
$$f[x_0, x_1, x_2] = \frac{\dfrac{f(x_2) - f(x_1)}{x_2 - x_1} - \dfrac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_o}$$

$$f(x) - f_n(x) = \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x - x_0)(x - x_1) \cdots (x - x_n)$$

몇 개의 항을 사용하느냐에 따라 다른 접근 방법이 된다.
Different methods depending on the number of terms
(Midpoint, Trapezoidal, Simpson Rule)
각각의 경우 error level 은?
Error level in individual cases?

- Midpoint Rule

$$\int_a^b f(x)\ dx \approx \int_a^b f[x_o]\ dx = f[x_o](b-a) = f\left(\frac{a+b}{2}\right)(b-a)$$



Error estimation

$$\int_a^b f[x_0, x_1](x - x_0)\,dx = \frac{f[x_0, x_1]}{2}(x - x_0)^2\Big]_a^b$$

$$= \frac{f[x_0, x_1]}{2}\left(x - \frac{a+b}{2}\right)^2\Big]_a^b$$

$$= \frac{f[x_0, x_1]}{2}\left[\left(b - \frac{a+b}{2}\right)^2 - \left(a - \frac{a+b}{2}\right)^2\right]$$

$$= \frac{f[x_0, x_1]}{2}\left[\left(\frac{b-a}{2}\right)^2 - \left(\frac{a-b}{2}\right)^2\right] = 0.$$

Suppose that the arbitrary x_1 was chosen to be the same value as x_0.

$$\int_a^b \frac{(x - x_0)^2}{2} f''(\xi(x))\,dx = f''(\xi)\int_a^b \frac{(x - x_0)^2}{2}\,dx = \frac{f''(\xi)}{6}(x - x_0)^3\Big]_a^b$$

$$= \frac{f''(\xi)}{6}\left[\left(b - \frac{b+a}{2}\right)^3 - \left(a - \frac{b+a}{2}\right)^3\right]$$

$$= \frac{f''(\xi)}{6}\frac{(b-a)^3}{4} = \frac{f''(\xi)}{24}(b-a)^3.$$

Midpoint Rule

If $f \in C^2[a, b]$, then a number ξ in (a, b) exists with

$$\int_a^b f(x)\,dx = (b-a)f\left(\frac{a+b}{2}\right) + \frac{f''(\xi)}{24}(b-a)^3.$$

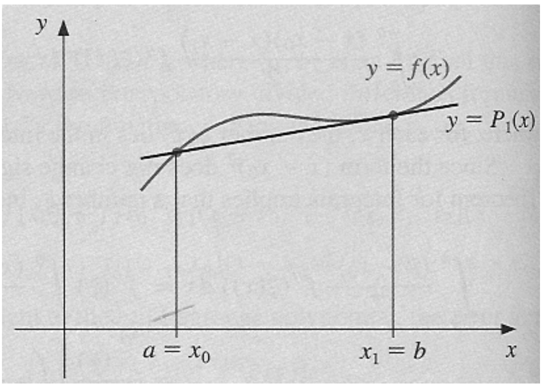
- Trapezoidal Rule

$$\int_a^b \{f[x_0] + f[x_0, x_1](x - x_0)\}\, dx$$

$$= \left[f[a]x + f[a, b]\frac{(x-a)^2}{2} \right]_a^b$$

$$= f(a)(b-a) + \frac{f(b) - f(a)}{b-a}\left[\frac{(b-a)^2}{2} - \frac{(a-a)^2}{2} \right]$$

$$= (b-a)\frac{f(a) + f(b)}{2}.$$



Error estimation

$$\int_a^b \frac{(x-a)(x-b)}{2} f''(\xi(x))\, dx = \frac{f''(\xi)}{2}\int_a^b (x-a)[(x-a)+(a-b)]\, dx$$

$$= \frac{f''(\xi)}{2}\left[\frac{(x-a)^3}{3} + \frac{(x-a)^2}{2}(a-b) \right]_a^b$$

$$= \frac{f''(\xi)}{2}\left[\frac{(b-a)^3}{3} + \frac{(b-a)^2}{2}(a-b) \right].$$

Trapezoidal Rule

If $f \in C^2[a, b]$, then a number ξ in (a, b) exists with

$$\int_a^b f(x)\, dx = (b-a)\frac{f(a) + f(b)}{2} - \frac{f''(\xi)}{12}(b-a)^3.$$

- Simpson Rule

$$\int_a^b \left\{ f(a) + f\left[a, \frac{a+b}{2}\right](x-a) + f\left[a, \frac{a+b}{2}, b\right](x-a)\left(x - \frac{a+b}{2}\right)\right\} dx$$

$$= \left[f(a)x + f\left[a, \frac{a+b}{2}\right]\frac{(x-a)^2}{2}\right]_a^b$$

$$+ f\left[a, \frac{a+b}{2}, b\right]\int_a^b (x-a)\left[(x-a) + \left(a - \frac{a+b}{2}\right)\right] dx$$

$$= f(a)(b-a) + \frac{f(\frac{a+b}{2}) - f(a)}{\frac{a+b}{2} - a}\frac{(b-a)^2}{2}$$

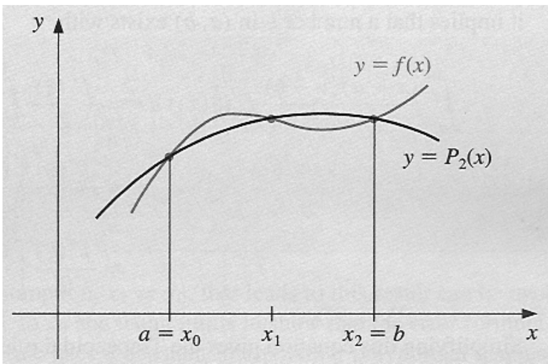
$$+ \frac{f[\frac{a+b}{2}, b] - f[a, \frac{a+b}{2}]}{b-a}\left[\frac{(x-a)^3}{3} + \frac{(x-a)^2}{2}\left(\frac{a-b}{2}\right)\right]_a^b$$

$$= (b-a)\left[f(a) + f\left(\frac{a+b}{2}\right) - f(a)\right]$$

$$+ \left(\frac{1}{b-a}\right)\left[\frac{f(b) - f(\frac{a+b}{2})}{\frac{b-a}{2}} - \frac{f(\frac{a+b}{2}) - f(a)}{\frac{b-a}{2}}\right]\left[\frac{(b-a)^3}{3} - \frac{(b-a)^3}{4}\right]$$

$$= (b-a)f\left(\frac{a+b}{2}\right) + \frac{2}{(b-a)^2}\left[f(b) - 2f\left(\frac{a+b}{2}\right) + f(a)\right]\frac{(b-a)^3}{12}.$$

$$\int_a^b f(x)\, dx \approx \frac{(b-a)}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right].$$



Simpson's Rule

If $f \in C^4[a, b]$, then a number ξ in (a, b) exists with

$$\int_a^b f(x)\, dx = \frac{(b-a)}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] - \frac{f^{(4)}(\xi)}{2880}(b-a)^5.$$

- Comparisons

Table 4.1 Integrals on the Interval [1, 1.2]

$f(x)$	x^2	x^4	$1/(x+1)$	$\sqrt{1+x^2}$	$\sin x$	e^x
Exact value	0.24267	0.29766	0.09531	0.29742	0.17794	0.60184
Midpoint	0.24200	0.29282	0.09524	0.29732	0.17824	0.60083
Trapezoidal	0.24400	0.30736	0.09545	0.29626	0.17735	0.60384
Simpson's	0.24267	0.29767	0.09531	0.29742	0.17794	0.60184

Table 4.2 Integrals on the Interval [0, 2]

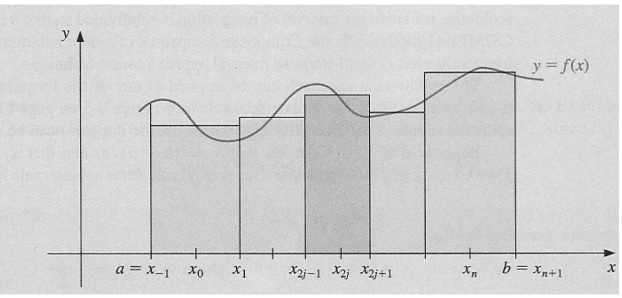
$f(x)$	x^2	x^4	$1/(x+1)$	$\sqrt{1+x^2}$	$\sin x$	e^x
Exact value	2.667	6.400	1.099	2.958	1.416	6.389
Midpoint	2.000	2.000	1.000	2.818	1.682	5.436
Trapezoidal	4.000	16.000	1.333	3.326	0.909	8.389
Simpson's	2.667	6.667	1.111	2.964	1.425	6.421

1.2 Composite Quadrature Rules

Composite Midpoint Rule

Suppose that $f \in C^2[a, b]$. Then for some μ in (a, b) we have

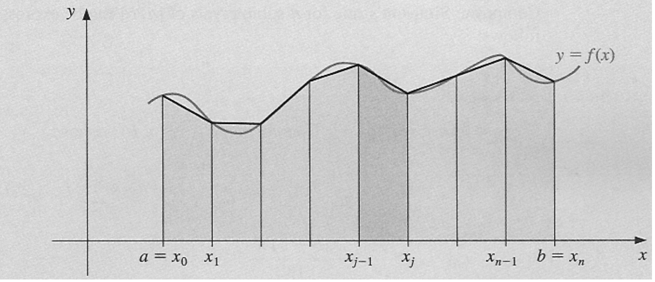
$$\int_a^b f(x)\,dx = 2h \sum_{j=0}^{n/2} f(x_{2j}) + \frac{(b-a)h^2}{6} f''(\mu).$$



Composite Trapezoidal Rule

Suppose that $f \in C^2[a, b]$. Then for some μ in (a, b) we have

$$\int_a^b f(x)\,dx = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{j=1}^{n-1} f(x_j)\right] - \frac{(b-a)h^2}{12} f''(\mu).$$

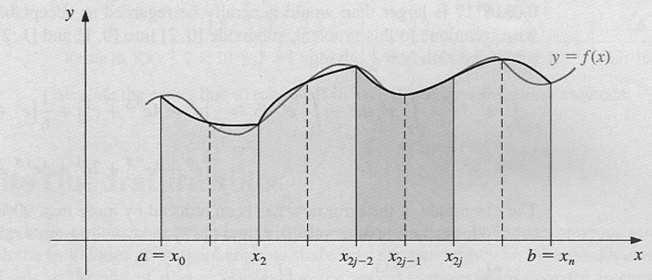


Composite Simpson's Rule

Suppose that $f \in C^4[a, b]$. Then for some μ in (a, b) we have

$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(b)\right]$$

$$- \frac{(b-a)h^4}{180} f^{(4)}(\mu).$$



- Simpson 3/8 공식 (Simpson 3/8 Formula)

3 차까지의 다항식을 이용하여 네 개의 data point 들을 보간하여 적분 값을 구한다.

$$\int_a^b f(x)dx \cong (b-a)\frac{f(x_o)+3f(x_1)+3f(x_2)+f(x_3)}{8}$$

Error, $E = -\frac{f^{(4)}(\xi)}{6480}(b-a)^5$

세 개의 data point 로도 같은 정도의 정확도를 얻을 수 있는 일반 Simpson (1/3) 공식이 더 선호되지만 Simpson 3/8 공식은 구간의 개수가 홀수일 때 Simpson 1/3 공식에 대한 보완으로 활용된다.
Used for the last three intervals with an odd number of intervals

Problem) x = 0 ~ 0.8 의 구간에서 다음의 식을 적분하라.

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

Mid point, Trapezoidal, Simpson 법을 이용하되, 각 방법에서 구간의 크기를 줄여 가면서, 오차가 줄어드는 정도를 비교하시오. (정답: 1.64053334)

```
FUNCTION TrapEq (n, a, b)
        h = (b – a)/n
        x = a
        sum = f(x)
        DO i = 1, n–1
            x = x + h
            sum = sum + 2 * f(x)
        ENDDO
        sum = sum + f(b)
        TrapEq = (b – a) * sum / (2*n)
END TrapEq
```

```
FUNCTION SimpEq (n, a, b)
        h = (b – a)/n
        x = a
        sum = f(x)
        DO i = 1, n–2, 2
            x = x + h
            sum = sum + 4 * f(x)
            x = x + h
            sum = sum + 2 * f(x)
        ENDDO
        x = x + h
        sum = sum + 4 * f(x)
        sum = sum + f(b)
        SimpEq = (b – a) * sum / (3*n)
END SimpEq
```

1.3 방정식의 적분

구간의 크기를 임의로 조절할 수 있을 때. 즉, 요구되는 수준의 정확도를 얻기 위해 필요한 만큼의 f(x) 값을 생성해 낼 수 있을 때.
Used when one can generate any necessary number of data points easily.

- Richardson Extrapolation

$$M = N(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots \qquad \text{Eq.(1)}$$

Replace the parameter *h* by half its value,

$$M = N(\frac{h}{2}) + K_1 \frac{h}{2} + K_2 \frac{h^2}{4} + K_3 \frac{h^3}{8} + \cdots \qquad \text{Eq.(2)}$$

2 Eq.(2) – Eq.(1) = M

$$M = \left[N(\frac{h}{2}) + \left(N(\frac{h}{2}) - N(h) \right) \right] + K_2 \left(\frac{h^2}{2} - h^2 \right) + K_3 \left(\frac{h^3}{4} - h^3 \right) + \cdots$$

define

$$N_1(h) = N(h)$$

$$N_2(h) = N_1(\frac{h}{2}) + \left(N_1(\frac{h}{2}) - N_1(h) \right)$$

By combining two *O(h)* approximations, an *O(h²)* approximation is produced.

$$M = N_2(h) - \frac{K_2}{2} h^2 - \frac{3K_3}{4} h^3 - \cdots \qquad \text{Eq.(3)}$$

Replace *h* by *h*/2 in Eq.(3),

$$M = N_2(\frac{h}{2}) - \frac{K_2}{8}h^2 - \frac{3K_3}{32}h^3 - \cdots \qquad \text{Eq.(4)}$$

Combine Eqs.(3) and (4) to eliminate the h^2 term
4 Eq.(4) – Eq.(3) = 3M

$$3M = 4N_2(\frac{h}{2}) - N_2(h) + \frac{3K_3}{4}\left(-\frac{h^3}{2} + h^3 \right) + \cdots$$

$$M = \left[N_2(\frac{h}{2}) + \frac{N_2(h/2) - N_2(h)}{3} \right] + \frac{K_3}{8}h^3 + \cdots$$

define $$N_3(h) = N_2(\frac{h}{2}) + \frac{N_2(h/2) - N_2(h)}{3}$$

By combining two $O(h^2)$ approximations, an $O(h^3)$ approximation is produced.

$$M = N_3(h) + \frac{K_3}{8}h^3 + \cdots$$

By continuing the process, $O(h^4)$ and $O(h^5)$ approximations are reproduced

$$N_4(h) = N_3(\frac{h}{2}) + \frac{N_3(h/2) - N_3(h)}{7}$$

$$N_5(h) = N_4(\frac{h}{2}) + \frac{N_4(h/2) - N_4(h)}{15}$$

$$N_j(h) = N_{j-1}(\frac{h}{2}) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{2^{j-1} - 1}$$

- Romberg Integration

  Richardson extrapolation is performed to speed the convergence

  Composite Trapezoidal rule in [a,b] using *m* subintervals

$$\int_a^b f(x)\ dx = \frac{h}{2}\left[f(a) + f(b) + 2\sum_{j=1}^{m-1} f(x_j) \right] - \frac{(b-a)}{12} h^2 f''(\xi)$$

where h = (b−a)/m, x_j = a + jh for j = 0, 1, 2, ⋯, m

with m_1 = 1, m_2 = 2, m_3 = 4, ⋯, and $m_n = 2^{n-1}$

h_k corresponding to m_k is $h_k = (b-a)/m_k = (b-a)/2^{k-1}$

$$\int_a^b f(x)\ dx = \frac{h_k}{2}\left[f(a) + f(b) + 2\sum_{i=1}^{2^{k-1}-1} f(a + ih_k) \right] - \frac{(b-a)}{12} h_k^2 f''(\xi_k)$$

Introduction of the notation $R_{k,1}$

$$R_{1,1} = \frac{h_1}{2}[f(a) + f(b)] = \frac{(b-a)}{2}[f(a) + f(b)]$$

$$R_{2,1} = \frac{1}{2}[R_{1,1} + h_1 f(a + h_2)]$$

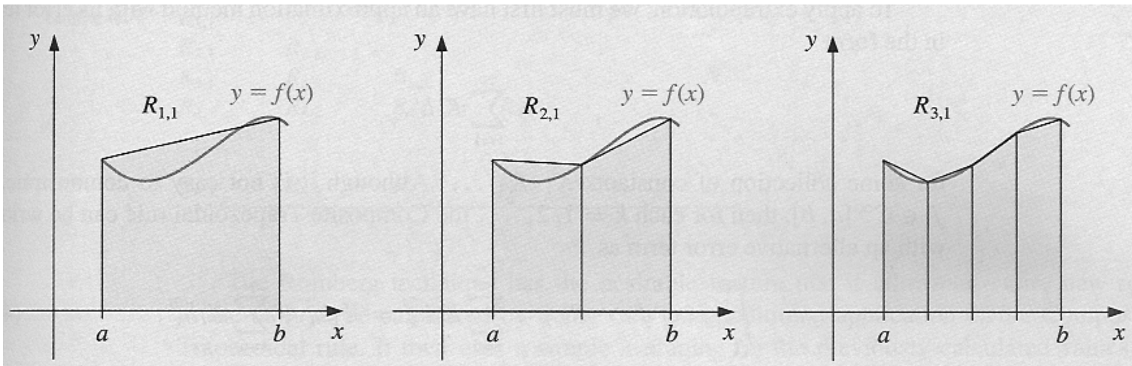
$$R_{3,1} = \frac{1}{2}\left\{R_{2,1} + h_2[f(a + h_3) + f(a + 3h_3)]\right\}$$

in General
$$R_{k,1} = \frac{1}{2}\left\{ R_{k-1,1} + h_{k-1}\sum_{i=1}^{2^{k-2}} f(a + (2i-1)h_k \right\}$$

for *k* = 2, 3, ⋯, n.

Extrapolation
$$R_{k,2} = R_{k,1} + \frac{R_{k,1} - R_{k-1,1}}{3}$$

$$R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}$$



Example 1 Using the Composite Trapezoidal rule to perform the first step of the Romberg Integration scheme for approximating $\int_0^\pi \sin x\, dx$ with $n = 6$ leads to

$$R_{1,1} = \frac{\pi}{2}[\sin 0 + \sin \pi] = 0,$$

$$R_{2,1} = \frac{1}{2}\left[R_{1,1} + \pi \sin \frac{\pi}{2}\right] = 1.57079633,$$

$$R_{3,1} = \frac{1}{2}\left[R_{2,1} + \frac{\pi}{2}\left(\sin \frac{\pi}{4} + \sin \frac{3\pi}{4}\right)\right] = 1.89611890,$$

$$R_{4,1} = \frac{1}{2}\left[R_{3,1} + \frac{\pi}{4}\left(\sin \frac{\pi}{8} + \sin \frac{3\pi}{8} + \sin \frac{5\pi}{8} + \sin \frac{7\pi}{8}\right)\right] = 1.97423160,$$

$$R_{5,1} = 1.99357034, \quad \text{and} \quad R_{6,1} = 1.99839336.$$

■

Example 2 In Example 1, the values for $R_{1,1}$ through $R_{n,1}$ were obtained by approximating $\int_0^\pi \sin x\, dx$ with $n = 6$. The output from ROMBRG42 produces the Romberg table shown in Table 4.5. Although there are 21 entries in the table, only the six entries in the first column require function evaluations since these are the only entries generated by the Composite Trapezoidal rule. The other entries are obtained by a simple averaging process. Notice that all the extrapolated values except for the first (in the first row of the second column) are more accurate than the best Composite Trapezoidal approximation (in the last row of the first column). ■

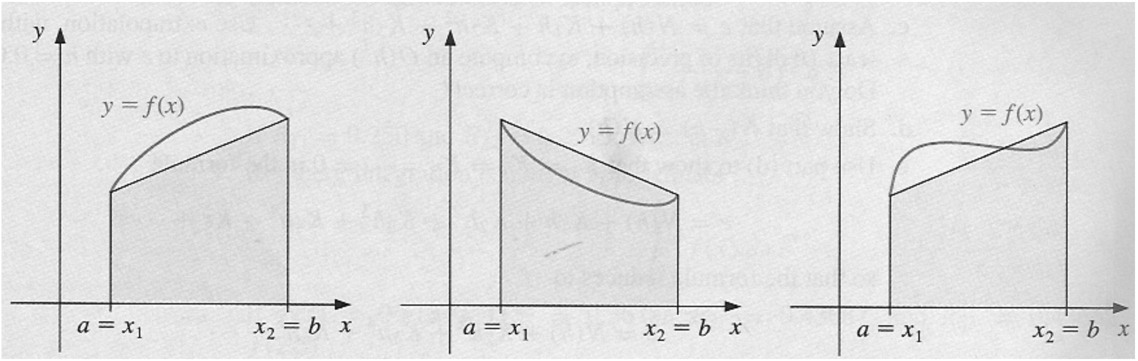
Table 4.5

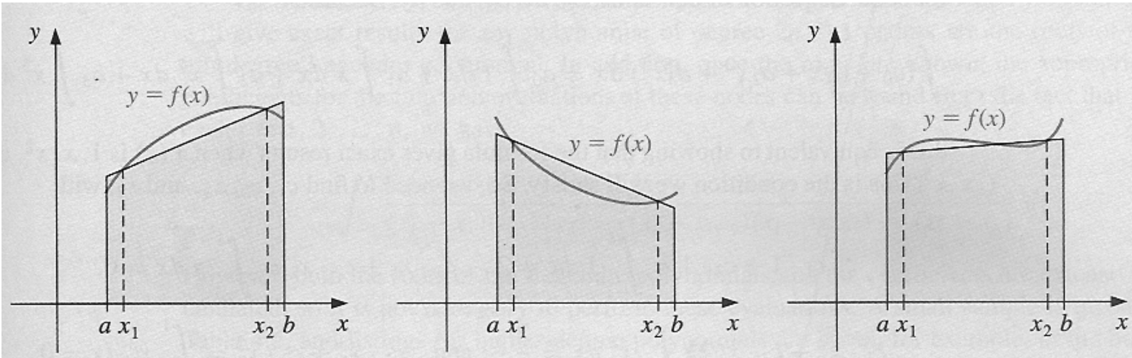
0					
1.57079633	2.09439511				
1.89611890	2.00455976	1.99857073			
1.97423160	2.00026917	1.99998313	2.00000555		
1.99357034	2.00001659	1.99999975	2.00000001	1.99999999	
1.99839336	2.00000103	2.00000000	2.00000000	2.00000000	2.00000000

Problem) x = 0 ~ 0.8 의 구간에서 다음의 식을 Romberg 적분법을 이용하여 적분하라.

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

- Gaussian Quadrature





[a,b] 구간 내의 양 끝점 x=a, x=b 에서의 값을 이용하지 않고 구간 내부에서의 n 개의 data point 를 이용하여 다음과 같이 적분 값을 approximation 하는 방법.

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

위의 approximation 에서 error 가 최소화되도록 계수 c_i 값들과 data 위치 x_i 값들을 결정하는 것이 관건.

Instead of end points, data points inside the interval are used.

How to determine the x values and c values is the issue.

Example) *f*(*x*)가 3 차 이하의 다항식일 때

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

를 만족하도록 c_1, c_2, x_1, x_2 값을 구하라.

Determine c_1, c_2, x_1, x_2 values that satisfy the relation when f(x) is a third order polynomial or lower

$$f(x) = a_o + a_1 x + a_2 x^2 + a_3 x^3$$

$$\int (a_o + a_1 x + a_2 x^2 + a_3 x^3)\ dx = a_0 \int 1\ dx + a_1 \int x\ dx + a_2 \int x^2 dx + a_3 \int x^3 dx$$

이는 *f(x)*가 1, *x*, x^2, x^3 일 때 위 적분식(*)이 성립하는 조건을 구하는 것과 같은 문제임.

$$c_1 \cdot 1 + c_2 \cdot 1 = \int_{-1}^{1} 1\ dx = 2$$

$$c_1 \cdot x_1 + c_2 \cdot x_2 = \int_{-1}^{1} x\ dx = 0$$

$$c_1 \cdot x_1^2 + c_2 \cdot x_2^2 = \int_{-1}^{1} x^2 dx = \frac{2}{3}$$

$$c_1 \cdot x_1^3 + c_2 \cdot x_2^3 = \int_{-1}^{1} x^3 dx = 0$$

$$c_1 = 1, \quad c_2 = 1, \quad x_1 = -\frac{1}{\sqrt{3}}, \quad x_2 = \frac{1}{\sqrt{3}}$$

$$\int_{-1}^{1} f(x)\ dx \approx f(-\frac{1}{\sqrt{3}}) + f(\frac{1}{\sqrt{3}})$$

2 개 이상의 data point 를 사용할 때 (when using more than two data points)

가중인자 c와 Gauss-Legendre 공식에서 사용된 함수의 인자 x.

Points	Weighting Factors	Function Arguments	Truncation Error
2	c_0 = 1.0000000	x_0 = −0.577350269	$\cong f^{(4)}(\xi)$
	c_1 = 1.0000000	x_1 = 0.577350269	
3	c_0 = 0.5555556	x_0 = −0.774596669	$\cong f^{(6)}(\xi)$
	c_1 = 0.8888889	x_1 = 0.0	
	c_2 = 0.5555556	x_2 = 0.774596669	
4	c_0 = 0.3478548	x_0 = −0.861136312	$\cong f^{(8)}(\xi)$
	c_1 = 0.6521452	x_1 = −0.339981044	
	c_2 = 0.6521452	x_2 = 0.339981044	
	c_3 = 0.3478548	x_3 = 0.861136312	
5	c_0 = 0.2369269	x_0 = −0.906179846	$\cong f^{(10)}(\xi)$
	c_1 = 0.4786287	x_1 = −0.538469310	
	c_2 = 0.5688889	x_2 = 0.0	
	c_3 = 0.4786287	x_3 = 0.538469310	
	c_4 = 0.2369269	x_4 = 0.906179846	
6	c_0 = 0.1713245	x_0 = −0.932469514	$\cong f^{(12)}(\xi)$
	c_1 = 0.3607616	x_1 = −0.661209386	
	c_2 = 0.4679139	x_2 = −0.238619186	
	c_3 = 0.4679139	x_3 = 0.238619186	
	c_4 = 0.3607616	x_4 = 0.661209386	
	c_5 = 0.1713245	x_5 = 0.932469514	

Problem) x = 0 ~ 0.8 의 구간에서 다음의 식을 Gaussian 구적법을 이용하여 적분하라.

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

Data point 의 수를 2 개에서부터 증가시켜 가면서 Error 를 check 할 것 (정답: 1.64053334).

적분 구간이 0 ~ 0.8 이 아니라 -1 ~ +1 이 되도록 변수를 변환하고 주어진 식을 변환시켜야 한다는 것에 유의할 것.

2. 수치미분 (Numerical differentiation)

2.1 고차 정확도의 미분 공식들 (Formulas with higher accuracy)

2 개 이상의 data point 를 이용하여 정확도를 높인 공식들

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2}h + O(h^2)$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)$$

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h^2}h + O(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)$$

- 전진 차분 (forward-difference)

※ 1st derivative

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)$$

※ 2nd derivative

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$

$$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2} + O(h^2)$$

- 후진 차분 (backward-difference)

※ 1st derivative

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h)$$

$$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} + O(h^2)$$

※ 2nd derivative

$$f''(x_i) = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2} + O(h)$$

$$f''(x_i) = \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2} + O(h^2)$$

- 중앙 차분 (centered-difference)

※ 1st derivative

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} + O(h^4)$$

※ 2nd derivative

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} + O(h^2)$$

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{h^2} + O(h^4)$$

Example) 다음 함수의 1 차도함수를 x=0.5, h=0.25 에서 O(h^2)로 계산하라. (참값 −0.9125)

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

$f(x_{i-2})$ = 1.2
$f(x_{i-1})$ = 1.103516
$f(x_i)$ = 0.925
$f(x_{i+1})$ = 0.6363281
$f(x_{i+2})$ = 0.2

	Forward O(h)	Backward O(h)	Centered O(h^2)
Estimate Error (%)	−1.155 −26.5	−0.714 21.7	−0.934 −2.4
	Forward O(h^2)	Backward O(h^2)	Centered O(h^4)
Estimate Error (%)	−0.859375 5.82	−0.878125 3.77	−0.9125 0.0

2.2 Richardson extrapolation

$$R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}$$

$$D \cong \frac{4}{3} D(h_2) - \frac{1}{3} D(h_1)$$

Example) 다음 함수 *x*=0.5 에서의 1 차도함수를, *h*=0.5, 0.25 를 사용하여 Richardson extrapolation 법으로 추정하라. (참값 −0.9125)

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

$f(x_{i-2})$ = 1.2
$f(x_{i-1})$ = 1.103516
$f(x_{i+1})$ = 0.6363281
$f(x_{i+2})$ = 0.2

$$D(0.5) = \frac{0.2 - 1.2}{1} = -1.0$$ (−9.6%)

$$D(0.25) = \frac{0.6363281 - 1.103516}{0.5} = -0.934375$$

(−2.4%)

$$D = \frac{4}{3}(-0.934375) - \frac{1}{3}(-1) = 0.9125$$

2.3 부등 간격을 가지는 data 의 도함수 (for non-uniform intervals)

인접한 세 개의 data point 를 2 차 Lagrange 보간 다항식으로 접합

$$f'(x) = f(x_{i-1})\frac{2x - x_i - x_{i+1}}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} + f(x_i)\frac{2x - x_{i-1} - x_{i+1}}{(x_i - x_{i-1})(x_i - x_{i+1})}$$

$$+ f(x_{i+1})\frac{2x - x_{i-1} - x_i}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)}$$

Example) 토양 표면에서의 온도 기울기?

$$f'(x) = 13.5\frac{2(0) - 1.25 - 3.75}{(0 - 1.25)(0 - 3.75)} + 12\frac{2(0) - 0 - 3.75}{(1.25 - 0)(1.25 - 3.75)}$$

$$+ 10\frac{2(0) - 0 - 1.25}{(3.75 - 0)(3.75 - 1.25)}$$

$$= -14.4 + 14.4 - 1.333333 = -1.333333°\text{C/cm}$$