

數值分析

Chapter 4

Numerical Integration and Differentiation

4.2 Basic Quadrature Rules

- Newton interpolatory divided-difference formula

$$\begin{aligned} f(x) &\approx P_{0,1,\dots,n}(x) \\ &= f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + \\ &\quad \cdots + f[x_0, x_1, \dots, x_n](x - x_0)(x - x_1) \cdots (x - x_{n-1}) \\ &\quad + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x - x_0)(x - x_1) \cdots (x - x_n) \end{aligned}$$

- $\int_a^b f(x)dx \approx \int_a^b P_0(x)dx = \int_a^b f[x_0]dx = f[x_0](b - a)$, 若選 $x_0 = \frac{a+b}{2}$, 可使 $f[x_0, x_1](x - x_0)$ 在 $[a, b]$ 之積分爲 0, 亦即使得 truncated error 有效降低.

⇒ midpoint rule:

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

- $\int_a^b f(x)dx \approx \int_a^b P_{0,1}(x)dx = \int_a^b [f[x_0] + f[x_0, x_1](x - x_0)]dx$, 若取 $x_0 = a, x_1 = b$

$$\Rightarrow f[x_0]x + \frac{f(b)-f(a)}{b-a} \frac{(x-a)^2}{2} \Big|_a^b = (b - a) \frac{f(a)+f(b)}{2}$$

, 形成 trapezoidal rule:

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

- $\int_a^b f(x)dx \approx \int_a^b P_{0,1,2}(x)dx$
 $= \int_a^b [f(a) + f[a, \frac{a+b}{2}](x - a) + f[a, \frac{a+b}{2}, b](x - a)(x - \frac{a+b}{2})]dx$
 , with $x_0 = a, x_1 = \frac{a+b}{2}, x_2 = b$

⇒ Simpson's 1/3 rule:

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

, P.113 Example 1.

equally space ⇒

$$\int_a^b f(x)dx = \frac{h}{3}[f(a) + 4f(a + h) + f(a + 2h)] - \frac{f^{(4)}(\xi)}{90}h^5$$

, with $h = \frac{b-a}{2}$

- Simpson's 3/8 Rule

$$\begin{aligned} & \int_a^b f(x) dx \\ &= \frac{3h}{8} [f(a) + 3f(a+h) + 3f(a+2h) + f(b)] - \frac{3}{80} f^{(4)}(\xi) h^5 \\ & \text{, with } h = \frac{b-a}{3} \end{aligned}$$

4.3 Composite Quadrature Rules

- P.116 Example 1, (i) $0 \sim 2$ 用一次 Simpson's 1/3 rule, (ii) $0 \sim 1, 1 \sim 2$ 各用一次 Simpson's 1/3 rule, (iii) $0 \sim 0.5, 0.5 \sim 1, 1 \sim 1.5, 1.5 \sim 2$ 各用一次 Simpson's 1/3 rule.

- 取 n 為偶數, 將 $[a, b]$ 分成 n 個 subinterval, 每兩個 interval 用一個 Simpson's 1/3 rule.

$$\begin{aligned} \int_a^b f(x) dx &= \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x) dx \\ &= \sum_{j=1}^{n/2} \left\{ \frac{h}{3} [f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})] - \frac{f^{(4)}(\xi)}{90} h^5 \right\} \\ &= \frac{h}{3} [f(x_0) + 2 \sum_{j=1}^{n/2-1} f(x_{2j}) + 4 \sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)] - \frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi) \end{aligned}$$

- $\int_a^b f(x) dx$ 的誤差項為 $E(f) = -\frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j)$

$$\text{Since } \min_{x \in [a, b]} f^{(4)}(x_j) \leq f^{(4)}(\xi_j) \leq \max_{x \in [a, b]} f^{(4)}(x_j)$$

$$\text{we have } \min_{x \in [a, b]} f^{(4)}(x_j) \leq \frac{2}{n} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \leq \max_{x \in [a, b]} f^{(4)}(x_j)$$

$$\Rightarrow \exists \mu \in (a, b), f^{(4)}(\mu) = \frac{2}{n} \sum_{j=1}^{n/2} f^{(4)}(\xi_j)$$

Since $h = \frac{b-a}{n} \Rightarrow E(f) = -\frac{(b-a)h^5}{180} f^{(4)}(\mu)$

P.120 Ex 2 Composite Simpson's Rule 的 n 只要 ≥ 18 即可使誤差小於 0.00002, 而 Composite Trapezoidal rule 的 n 卻要 ≥ 360 才會使誤差小於 0.00002.

4.4 Romberg Integration

- Composite Trapezoidal + Richardson Extrapolation
因為爲了加速收斂, 常使用外插法.

- Exact value = M

$$M = N(h) + K_1h + K_2h^2 + K_3h^3 + \dots(*)$$

爲了更精確, $M = N(\frac{h}{2}) + K_1\frac{h}{2} + K_2\frac{h^2}{4} + K_3\frac{h^3}{8} + \dots(**)$

$$2(**) - (*) \Rightarrow$$

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

Define $N_1(h) \equiv N(h)$ and $N_2(h) = N_1(\frac{h}{2}) + [N_1(\frac{h}{2}) - N_1(h)]$

Then we have an $O(h^2)$ approximation formula for M:

$$M = N_2(h) - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \dots \text{ (更接近 M)}$$

We have an $O(h^j)$ approximation of the form

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

- Composite Trapezoidal rule:

切 2^{k-1} 等份得 $R_{k,1}$ approximation

$$= \frac{h_k}{2} [f(a) + f(b) + 2(\sum_{i=1}^{2^{k-1}-1} f(a + ih_k))]$$

- recursive to generate $R_{k,1}$

$$R_{k,1} = \frac{1}{2} [R_{k-1,1} + h_{k-1} \sum_{i=1}^{2^{k-2}} f(a + (2i-1)h_k)]$$

- $\int_a^b f(x)dx - R_{k,1} = \sum_{i=1}^{\infty} k_i h_k^{2i} = k_1 h_k^2 + \sum_{i=2}^{\infty} k_i h_k^{2i} \dots (*)$
 $\int_a^b f(x)dx - R_{k+1,1} = \sum_{i=1}^{\infty} k_i h_{k+1}^{2i} = \sum_{i=1}^{\infty} \frac{k_i h_k^{2i}}{2^{2i}} = \frac{k_1 h_k^2}{4} + \sum_{i=2}^{\infty} \frac{k_i h_k^{2i}}{4^i} \dots (**)$

(只有偶數次之 error 是因為, 原本之 Trapezoidal rule 中, error = $-\frac{f''(\xi)}{12}(b-a)^3 + \dots + (b-a)^5$, 其中只有奇數次方, 但在 composite 後 error = $-\frac{f''(\mu)}{12}(b-a)h^2 + \dots + (b-a)h^4 + \dots$)

- $4(**) - (*)$
 $\Rightarrow 3 \int_a^b f(x)dx - 4R_{k+1,1} + R_{k,1} = 4 \sum_{i=2}^{\infty} \frac{k_i h_k^{2i}}{4^i} - \sum_{i=2}^{\infty} k_i h_k^{2i}$
 $\Rightarrow \int_a^b f(x)dx = \frac{4R_{k+1,1} - R_{k,1}}{3} + \sum_{i=2}^{\infty} \frac{k_i}{3} \left(\frac{h_k^{2i}}{4^{i-1}} - h_k^{2i} \right)$
 $\Rightarrow R_{k,2} = R_{k,1} + \frac{R_{k,1} - R_{k-1,1}}{3}$
 $\Rightarrow R_{k,j} = R_{k,j-1} + \frac{R_{k,j-1} - R_{k-1,j-1}}{4^{j-1} - 1}$

P.131 Table 4.4, Example 2, Table 4.5.

4.5 Gaussian Quadrature

- 在區間中, 找出點, 使求出答案, 不一定要端點.
 Fig 4.10 用 $[x_1, x_2]$ 會比用 $[a, b]$ 好

- 希望找到 (c_i, x_i) , s.t. $\int_a^b f(x)dx \approx \sum_{i=1}^n c_i f(x_i)$

所以總共需要 $2n$ 個參數, 若 $f(x)$ 為 polynomial, 且 $\deg(g) \leq 2n - 1$, 可以算出完全正確的答案.

- P.136 Example 1.

- c_i 與 x_i 之選擇

由 Legendre polynomial (orthogonal in $[-1, 1]$) 之 roots 來求 x_i

$$P_0(x) = 1, P_1(x) = x, P_2(x) = x^2 - \frac{1}{3}, P_3(x) = x^3 - \frac{3}{5}x, P_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}, \dots$$

$$c_i = \int_{-1}^1 \prod_{j=1, j \neq i}^n \frac{x - x_j}{x_i - x_j} dx$$

P.137 Table 4.6

- 由 Table 4.6 可以發現 $\sum_{i=1}^n c_{n,i} \approx 2 \Rightarrow c_{n,i}$ 可想成 $f(r_{n,i})$ 之寬度.

- 若是 $[a, b]$, 而非 $[-1, 1]$, 可用 $t = \frac{2x-a-b}{b-a}$
 $\Rightarrow \int_a^b f(x)dx = \frac{b-a}{2} \sum_{j=1}^n c_{n,j} f\left(\frac{(b-a)r_{n,j}+b+a}{2}\right)$

P.138 Example 2.

- P.138 Ex 2. n 越大, 越精確. 與 Gaussian 比較, Simpson 的誤差很大.

(John Hull-Ch11)

What is Wiener Process (Brownian Motion)?

短暫時間的變化 (影響變化的因素只有一個: 時間)

$$x \sim N(0, \sigma_x^2)$$

$$x + x \sim N(0, 2\sigma_x^2)$$

$$2x \sim N(0, 4\sigma_x^2)$$

- $\Delta Z = \varepsilon\sqrt{\Delta t}$
 因為 $\varepsilon \sim N(0, 1)$
 所以 $\Delta Z \sim N(0, \Delta t)$
 $E[\Delta Z] = 0, \text{Var}(\Delta Z) = \Delta t$
 (描述 ΔZ 的變動不是重點, 而是要知道累積的 ΔZ , 也就是說
 $Z(T) - Z(0) = \sum_{i=1}^N \varepsilon_i \sqrt{\Delta t} = \sum_{i=1}^N \Delta Z_i$)
 $Z(T) - Z(0)$ 是隨時間改變, ΔZ_i 的加總

- 目標:
 要知道平均位移:
 $E[Z(T) - Z(0)] = 0$
 要知道平均 Var:
 $\text{Var}(Z(T) - Z(0)) = N\Delta t = T$
 意思: 隨時間越久, Var 越大

- Generalized W Process
 $dx = a * dt + b * dz \sim N(adt, b^2 dt)$
 where adt is drift and $b^2 dt$ is volatility

- Itô Process (Diffusion Process)
 假設: $dx = a(x, t)dt + b(x, t)dz^{(**)}$ [a, b 是函數]
 對股價做 $\frac{ds}{s} = \mu dt + \sigma dz$ 的成長率假設
 $\sim N(\mu dt, \sigma^2 dt)$
 (股價報酬率是 N 分布) (股價是 lognormal 分布)
 $\Rightarrow ds = \mu s dt + \sigma s dz$ (類似 (**)) 的寫法)
 證明股價是 lognormal 分布 (其實並非正確的) 證明
 $\frac{d \ln s}{ds} = \frac{1}{s} \rightarrow d \ln s = \frac{ds}{s}$
 所以股價報酬率是 N 分布, 股價是 lognormal 分布

- Hull P.247 (12.22式)

$$C = e^{-rT} \widehat{E}(\max(S_T - k, 0))$$

∧: 身處風險中立情況下

[call的價值 = 期望後折現]

爲什麼要有 “∧”

(股票 vs 無風險)

risk averse: 希望出像集中 ⇒ 現實中, 有風險的東西就有風險貼水 ⇒ 報酬率高

risk loving: 希望出像分散 ⇒ 喜歡股票

風險中立 ⇒ 股票跟無風險都一樣好 ⇒ 股票不需要超額報酬

在風險中立下, $\frac{ds}{s} = rdt + \sigma dz$

- How to 處理 $f(S_T)$, S_T 之機率密度函數 (S_T 爲 lognormal distribution)?

P.262

$\ln V \sim N(m, s)$, 求 $E[\max(V - K, 0)]$

引進 $Q = \frac{\ln V - m}{s}$ (變數轉換)

where $Q \sim N(0, 1)$

What's m ? What's s ?

P.235 (12.3式) (一般世界, 所以 μ 要改成 r) Itô Lemma (也就是泰勒展開式)

$$(2 \text{ dimension}) f(x, y) = f(x_0, y_0) + \frac{\partial f}{\partial x}(x - x_0) + \frac{\partial f}{\partial y}(y - y_0) + \frac{1}{2}(\frac{\partial^2 f}{\partial x^2}(x - x_0)^2 + 2\frac{\partial^2 f}{\partial x \partial y}(x - x_0)(y - y_0) + \frac{\partial^2 f}{\partial y^2}(y - y_0)^2) + \dots$$

If $\frac{ds}{s} = \mu dt + \sigma dz \Rightarrow df(s, t) = ?$

[$f(s, t)$ 在極短時間內的波動]

$$df = f(x, y) - f(x_0, y_0) = \frac{\partial f}{\partial s}(ds) + \frac{\partial f}{\partial t}(dt) + \frac{1}{2}(\frac{\partial^2 f}{\partial s^2}(ds)^2 + 2\frac{\partial^2 f}{\partial s \partial t}(ds)(dt) + \frac{\partial^2 f}{\partial t^2}(dt)^2) + \dots$$

⇒

$$df(s, t) = \frac{\partial f}{\partial s}(\mu s dt + \sigma s dz) + \frac{\partial f}{\partial t} dt + \frac{1}{2} \left(\frac{\partial^2 f}{\partial s^2} (\mu s dt + \sigma s dz)^2 + \dots \right)$$

$$\begin{cases} dz = \varepsilon \sqrt{dt} \\ \Rightarrow (dz)^2 = (\varepsilon \sqrt{dt})^2 \approx dt \\ \Rightarrow (\sigma s dz)^2 = \sigma^2 s^2 dt \end{cases}$$

(Rule: dt 很小 $\Rightarrow (dt)^2$ 更小 \Rightarrow ignore)

(次方大於 1.5 都 ignore)

$$\Rightarrow df(s, t) = \left(\frac{\partial f}{\partial s} \mu s + \frac{\partial f}{\partial t} + \frac{1}{2} \frac{\partial^2 f}{\partial s^2} \sigma^2 s^2 \right) dt + \frac{\partial f}{\partial s} \sigma s dz$$

令 $f(s, t) = \ln s$

$$\Rightarrow df(s, t) = \left(\frac{1}{s} \mu s - \frac{1}{2s^2} \sigma^2 s^2 \right) dt + \frac{1}{s} \sigma s dz$$

$$d \ln s = \left(\mu - \frac{1}{2} \sigma^2 \right) dt + \sigma dz$$

$$\Rightarrow \ln S(T) - \ln(S_0) \sim N\left(\left(\mu - \frac{1}{2} \sigma^2\right)T, \sigma^2 T\right)$$

4.6 Adaptive Quadrature

- 萬一函數在某一 interval 較平滑, 某一 interval 變動較大, 則 equally-sized 會不適合, 因變動大的部分, error term 之微分值可能很大或很小, 造成整個的 error bound 上升.

- Fig 4.13

在變動劇烈的地方 \Rightarrow 切割細

在變動不劇烈的地方 \Rightarrow 切割不細

$$\int_a^b f(x) dx = S(a, b) - \frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

(where $\frac{(b-a)^5}{2880}$ 改為 $\frac{h^5}{90}$)

($S(a, b)$ 為 Simpson's 1/3 rule)

$$\approx S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right) - \frac{1}{16} \left(\frac{h}{90}\right)^5 f^{(4)}(\tilde{\xi})$$

($S\left(a, \frac{a+b}{2}\right) + S\left(\frac{a+b}{2}, b\right)$ 為 composite Simpson's rule)

假設 $f^{(4)}(\xi) = f^{(4)}(\tilde{\xi})$, 如果 ξ 與 $\tilde{\xi}$ 很接近, 則之後之推導會很精確.

$$\Rightarrow \frac{h^5}{90} f^{(4)}(\xi) \approx \frac{16}{15} [S(a, b) - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b)]$$

\Rightarrow

$$| \int_a^b f(x) dx - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b) | \approx \frac{1}{15} | S(a, b) - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b) |$$

$$\text{where } | \int_a^b f(x) dx - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b) | \leq \varepsilon$$

$$| S(a, b) - S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b) | \leq 15\varepsilon (\text{iterative error term})$$

- P.143 Example 1

If 需要 error $\leq \varepsilon$

(i) 先看 $S(a, b)$ 與 $S(a, \frac{a+b}{2}) - S(\frac{a+b}{2}, b)$ 之差距, 如果夠小即可.

(ii) 若不夠小, 看 $S(a, \frac{a+b}{2})$ 之 error 是否 $\leq \frac{\varepsilon}{2}$, $S(\frac{a+b}{2}, b)$ 之 error 是否 $\leq \frac{\varepsilon}{2}$

(iii) 若有超過, 則 $S(x, y)$ 放入 (i) 繼續做.

- see Fig 4.13 (越陡峭, 割得越細)

given $\varepsilon = 0.00001$

if $S(1, 3) - S(1, 2) - S(2, 3)$ 還不夠小 \Rightarrow 再切割

$$\Rightarrow S(1, 2) - S(1, 1.5) - S(1.5, 2)$$

看看是否 $< \frac{\varepsilon}{4}$

\Rightarrow 一直做到要求的精確度

**此方法有問題: 不一定每個區間都要都要達目標, 最好是有 + 有 - 正好相消

4.8 Improper Integrals 瑕積分

- $\int_a^b \frac{1}{(x-a)^p} dx$ (as $x \rightarrow a, \frac{1}{(x-a)^p} \rightarrow \infty$)

$$f(x) = \frac{g(x)}{(x-a)^p},$$

$$[g(x) = g(a) + g'(a)(x-a) + \frac{g''(a)}{2}(x-a)^2 + \dots]$$

(where $g(a) + g'(a)(x - a) + \frac{g''(a)}{2}(x - a)^2 + \dots = p(x)$)

$$\Rightarrow \int_a^b f(x)dx = \int_a^b \frac{g(x) - P_4(x)}{(x-a)^p} dx + \int_a^b \frac{P_4(x)}{(x-a)^p} dx$$

$G(x)$ polynomial, 可直接積分

$\int_a^b G(x)dx$ 用 composite Simpson's rule 來算積分, $G(a) = 0$ 當作一邊.

Ex1. 證明出 $\int_0^1 \frac{e^x}{\sqrt{x}} dx$ 的值並非不存在

(當 $x \rightarrow 0$, $\frac{e^x}{\sqrt{x}}$, 所以無法直接用 composite Simpson's rule)

- 如果 Singularity point 在右, 用右邊之 endpoint 作固定點
- 如果 singularity point 在中, 則 $\int_a^b = \int_a^c + \int_c^b$
- 如果 a 或 b 為 ∞ , 則用變數變換將 x 換掉.
- P.161 Example 2

4.9 Numerical Differentiation

- $f'(x_0) = \lim_{h \rightarrow 0} \frac{f(x_0+h) - f(x_0)}{h}$ (微分會有 h 要取多小的問題)

$$f(x_0 + h) = f(x_0) + f'(x_0)(x - x_0) + \dots$$

$$\Rightarrow f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h}$$

- (兩點) $x_0, x_1 = x_0 + h$

$$f(x) = P_{0,1}(x) + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x))$$

$$= f(x_0) \frac{x-x_1}{x_0-x_1} + f(x_1) \frac{x-x_0}{x_1-x_0} + \frac{(x-x_0)(x-x_1)}{2!} f''(\xi(x))$$

(where $\frac{x-x_1}{x_0-x_1} = \frac{x-x_0-h}{-h}$, $\frac{x-x_0}{x_1-x_0} = \frac{x-x_0}{h}$)

微分

$$\begin{aligned} \Rightarrow f'(x) &= -\frac{f(x_0)}{h} + \frac{f(x_0+h)}{h} + \left[\frac{(x-x_0)(x-x_1)}{2!}\right]' f''(\xi(x)) + \left[\frac{(x-x_0)(x-x_1)}{2!}\right] \frac{df''(\xi(x))}{dx} \\ \Rightarrow f'(x_0) &= \frac{f(x_0+h)-f(x_0)}{h} + \left[\frac{(x-x_0)(x-x_0+x_0-x_1)}{2!}\right]' f''(\xi(x)) + 0 \\ &= \frac{f(x_0+h)-f(x_0)}{h} + \left[\frac{(x-x_0)^2-h(x-x_0)}{2!}\right]' f''(\xi(x)) \\ &= \frac{f(x_0+h)-f(x_0)}{h} - \frac{h}{2} f''(\xi(x)) \end{aligned}$$

• 通式

$$f(x) = \sum_{j=0}^n f(x_j) L_j(x) + \left[\frac{(x-x_0)\dots(x-x_n)}{(n+1)!}\right] f^{(n+1)}(\xi(x))$$

where $\sum_{j=0}^n f(x_j) L_j(x)$: 用 polynomial Lagrange 做的,

$$\left[\frac{(x-x_0)\dots(x-x_n)}{(n+1)!}\right] f^{(n+1)}(\xi(x)) \text{ : error}$$

$$x = x_j \text{ 時, } L_j(x) = 1$$

$$f'(x) = \sum_{j=0}^n f(x_j) L_j'(x) + D_x \left[\left[\frac{(x-x_0)\dots(x-x_n)}{(n+1)!}\right] f^{(n+1)}(\xi(x)) \right] + D_x f^{(n+1)}(\xi(x))$$

$$f'(x_k) = \sum_{j=0}^n f(x_j) L_j'(x_k) +$$

$$D_x \left[\frac{(x-x_k+x_k-x_0)(x-x_k+x_k-x_1)\dots(x-x_k+x_k-x_{k-1})\dots(x-x_k+x_k-x_n)}{(n+1)!} \right] f^{(n+1)}(\xi(x))$$

$$\left\| \begin{array}{l} \left[\right] \text{乘開} = a(x-x_k)^n + b(x-x_k)^{n-1} + \dots \\ \left[\right]' = c(x-x_k)^{n-1} + d(x-x_k)^{n-2} + \dots + e(x-x_k) + f, \\ \text{當 } x = x_k \text{ 代入, 只剩下 } f \end{array} \right.$$

$$= \sum_{j=0}^n f(x_j) L_j'(x_k) + \prod_{j=0, j \neq k}^n (x_k - x_j) \frac{f^{(n+1)}(\xi(x))}{(n+1)!}$$

• P.166 Three-Point Endpoint Formula

(可用在 Spline boundary condition 的假設)

$$f'(x_0) = \frac{1}{2h}(-3f(x_0) + 4f(x_0+h) - f(x_0+2h)) + \frac{h^2}{3} f^3(\xi)$$

where ξ lies between x_0 and x_0+2h

**用3點去做 Lagrange (x_0, x_0+h, x_0+2h)

**用點越多越精準 (比較兩點跟三點的 error-三點, error 變小)

- 跟 Three-Point Endpoint Formula 比較
 Three-Point Midpoint Formula 比較好, error 較小
 (where Midpoint: $x_0 - h, x_0, x_0 + h$)
 $f'(x_0) = \frac{1}{2h}(f(x_0 + h) - f(x_0 - h)) - \frac{h^2}{6}f^{(3)}(\xi)$
 where ξ lies between $x_0 - h$ and $x_0 + h$
 **只要帶入兩次 f (endpoint 要代3次), 但 error 比 endpoint 小
 P.168 Ex2. $f(x) = xe^x$, five-point 比 three-point 好, Midpoint 比 endpoint 好

- 在積分時, $h \rightarrow 0$, truncation error 變小, 且雖然用大量之 f 值, 但均為加總, round-off error 之變化約可抵銷.

- 在微分時, $h \rightarrow 0$, truncation error 變小, 但因 f 值之間為相減, 不知 $f(x_0 + h), f(x_0), f(x_0 - h)$ 之間的差距, 是真的差距, 還是 round-off error.

- $f'(x_0) \frac{f(x_0+h)-f(x_0-h)}{2h}, [\frac{\tilde{f}(x_0+h)-\tilde{f}(x_0-h)}{2h}]$ 電腦值
 因為 $f(x_0 + h) = \tilde{f}(x_0 + h) + e(x_0 + h)$
 所以 $|f'(x_0) - [\frac{f(x_0+h)-f(x_0-h)}{2h}]| = |f'(x_0) - [\frac{\tilde{f}(x_0+h)-\tilde{f}(x_0-h)}{2h}]| + |\frac{e(x_0+h)-e(x_0-h)}{2h}|$ (電腦值)
 $\leq |f'(x_0) - \frac{\tilde{f}(x_0+h)-\tilde{f}(x_0-h)}{2h}| \leq \frac{\varepsilon}{h} + \frac{h^2}{6}f^{(3)}(\xi)$
 where $\frac{e(x_0+h)-e(x_0-h)}{2h} = \frac{2\varepsilon}{2h}$, round-off error

$f^{(3)}(\xi)$:truncation error

(h 在分子, 也在分母 \Rightarrow 並不是越小越好)

希望 $\frac{\varepsilon}{h} + \frac{h^2}{6}M$ min \Rightarrow 對 h 微分 s.t. $(\frac{\varepsilon}{h} + \frac{h^2}{6}M)'_h = 0$

$$\Rightarrow h = \sqrt[3]{\frac{3\varepsilon}{M}}$$

- Three-Point Midpoint Formula for Approximating f'' (二階微分)

$$f''(x_0) = \frac{1}{h^2}(f(x_0 - h) - 2f(x_0) + f(x_0 + h)) - \frac{h^2}{12}f^{(4)}(\varepsilon)$$

where ε lies between $x_0 - h$ and $x_0 + h$

**由 $\frac{f(x_0+h)-f(x_0)}{h} - \frac{f(x_0)-f(x_0-h)}{h}$ 而來

	Advantage	Disadvantage
Midpoint rule	Simple	需分割的夠多, 才能很精確
Trapezoidal rule		
Simpson's 1/3 rule (n=2)	Simple and higher accuracy	分割偶數個 intervals
Simpson's 3/8 rule (n=3)	than trapezoidal	分割 intervals 為3之倍數
composite quadrature	比一般 quadrature 來的準	分割偶數個 intervals (composite Simpson's) 可任意分割 equispace (composite trapezoidal) (亦即分割出多個梯形)
Roomberg Integration	可利用一些簡單算術, 將 composite trapezoidal 之 error 降低, 例從 $h^2 \rightarrow h^4$ $(\frac{1}{10})^2 \rightarrow (\frac{1}{10})^4$, 若從分的細著手 從 $\frac{1}{10} \rightarrow (\frac{1}{100})^2$	需分割成 2^k 個 intervals 且 $k = 1, \dots, n$ 都要做 然後才能用 Roomberg Integration
Gauss quadrature	More accuracy than general Simpson's rule	Data points are not equispaced
Adaptive quadrature	處理微分值變動大之函數, 因其變動大 \Rightarrow error term 大 藉由將變動大之 subinterval 之分割, 造成所需之 error bound subintervals 都小於 某個 error bound	有可能永遠達不到 需要之 criteria, 而無限切割, 另外 真正需求是 overall 之 error bound 的限制, 而並不一定要每個 subintervals 都小於 某個 error bound
Newton-Cotes	General rule of simpson's rule	Higher-order formulas are not necessarily more accurate